# CELEBRATION AT A GLANC

Time	Thursday, April 3	Friday, April 4	Saturday, April 5
7:15		Registration Desk Open (Stewart Center, Rm. 310)	
7:30 - 8:00		Continential Breakfast (Stewart Center, Rm. 310)	Continential Breakfast (Purdue Memorial Union, South Ballroom
8:00-8:30		Welcome and Plenary Remarks (Stewart Center, Rm. 310)	School of ME Highlights (Purdue Memorial Union, South Ballroon
8:30 - 10:00		Panel Session 1 (Stewart Center, Rm. 310) Contributions to Heat Transfer Research: Purdue and Beyond	Research Poster Session* (Purdue Memorial Union, South Ballroom) *All attendees are invited to present a research poster at the Poster Session.
10:00		BREAK	9:30 Impact of Purdue Heat Transfer: Alumni Perspectives
10:30 - 12:00		Panel Session 2 (Stewart Center, Rm. 310) <i>Heat Transfer Education</i>	11:30 Meeting Adjounment
12:00 - 1:30		Open Luncheon	<b>1:00</b> - <b>4:00</b> Informal Open House Heat Transfer Laboratories
1:30 - 3:00		Panel Session 3 (Stewart Center, Rm. 310) <i>Emerging Areas</i>	
3:00		Hawkins Lecture Reception (Stewart Center, West Foyer, Loeb Playhouse)	
3:30		Hawkins Lecture (Stewart Center, Fowler Hall) Speaker: John Sununu <i>"The Engineer in the Public Policy Arena"</i>	,
4:30		Hawkins Lecture Q & A (Stewart Center, Fowler Hall)	
5:00		BREAK	
6:00	Registration Desk		
6:30		Cocktail hour (Purdue Memorial Union, West Faculty Lounge)	1
7:15		Dinner (Purdue Memorial Union, West Faculty Lounge)	
7.90			

# TER FROM THE PRESIDENT

It gives me great pleasure to join with many others in welcoming you to this Heat Transfer Celebration at Purdue University.

I began my career as a professor of engineering — aerospace and mechanical engineering — with a strong interest in heat transfer. I am very proud to be associated with the outstanding scholarship and research taking place in heat transfer at Purdue.

I am proud of our entire Schools of Engineering and the level of excellence in our students, faculty and staff. Purdue has drafted Strategic Plans. We have set a goal to become a preeminent university, with world leadership in our strongest programs. Purdue engineering is historically among the highest ranked, most highly regarded in the nation. Now we are working to become even better. We are adding faculty, building new classrooms and laboratories, adding state-of-the-art technology to our teaching. We are expanding our research efforts in interdisciplinary, signature areas that will impact today and tomorrow. We are proud to be a land-grant university. And we are using our missions for learning, discovery and engagement to impact our state, improving the future for people, businesses and industries.

As Purdue moves to the next level of excellence, the Schools of Engineering are a major focus and a major power helping to drive us to our goals. This is the most exciting time I have ever experienced in my years in higher education. We are transforming our university and opening new opportunities for everyone who works and studies here.

Thanks to all of you for joining us and taking part in this important program.

Marhu 1. Swikke

Martin C. Jischke

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# LETTER FROM THE DEAN

Welcome to the Heat Transfer Celebration at Purdue University! Ever since Purdue opened its doors in 1874 as Indiana's land-grant institution, engineering has been a key academic thrust here. That emphasis continues today through twelve engineering disciplines and a number of exciting initiatives.

Among those initiatives is Discovery Park, a new research complex that will house interdisciplinary research at Purdue in nanoscience, bioscience, and e-enterprise. One facility within Discovery Park, the Birck Nanotechnology Center, will bring together engineers and scientists to devise structures and processes that exploit the unique features of the nanoscale. Two new related programs—the NASA Institute for Nanoelectronics and Computing and the NSF Network for Computational Nanotechnology—were funded in 2002. In addition, the Cooling Technologies Research Center was transformed this past year into a designated NSF research center.

Unprecedented growth in the size of our faculty, from 270 to 345 over the next five years, will enable us to significantly increase diversity within our ranks and to strengthen targeted research areas—our "signature areas" of advanced materials and manufacturing; global sustainable industrial systems; information, communications, and perception technologies; intelligent infrastructure systems; nanotechnology and nanophotonics; renewable energy and power systems; tissue and cellular engineering; and "system of systems" studies. All these developments will be supported by our Engineering Master Facilities Plan, which will renovate and expand our facilities by about 60 percent over the next ten years.

I welcome you to experience the vitality of our campus during your stay, and I invite you join us in celebrating the rich tradition of excellence in heat transfer research and education at Purdue. Many of the pioneers in the field have made their home at Purdue, and we will be commemorating their many contributions at this event. You will also find that this wonderful legacy continues in our current faculty and students.

I trust that your time here will be memorable and enjoyable.

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Linda P.B. Katehi John A. Edwardson Dean of Engineering

# R FROM THE HEAD

Welcome to Purdue and the School of Mechanical Engineering! I am really pleased you will be able to join us in honoring a truly outstanding group of faculty and the breadth of their contributions.

The Heat Transfer group at Purdue has long been a world leader in research and education. Beginning in my days as an undergrad here at Purdue in the 1970's taking the renowned undergraduate Heat Transfer ME 315 with Frank Incropera, to the ME 500-level graduate series on Conduction, Convection, and Radiation with Joe Pearson and Bob Schoenhals, and finally to ME 606 Radiation with Ray Viskanta, I have always been profoundly impressed with the stature and sincere focus on education within the group. But in addition, even as an undergraduate student, I was aware of the world-class research reputations of the faculty who made up the group at that time. More recently I have been able to look back and reflect on the other giants of this area (Hawkins, Goss), who also had such a major impact on Engineering and even the whole of Purdue University.

I am also pleased to report that the tradition will continue, as we have been fortunate to attract a cadre of excellent young faculty who are already defining the next generation. They are sustaining the tradition associated with a solid foundation of classical heat transfer, while simultaneously branching out into emerging areas in nanotechnology, microsystems, laser-based micro and nano machining, and bio-heat transfer for medical applications.

I trust that you will enjoy yourself during this weekend of celebration, and thanks again for joining together in honoring our colleagues.

Best regards,

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E. Dan Hirleman, Professor William E. and Florence E. Perry Head

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# WELCOME DINNER & MEALS

# Thursday April 3

## 7:30 р.м.

## Dinner

Join us on Thursday evening at University Inn in West Lafayette for dinner at 7:30 p.m. Not only will you be able to visit with your heat transfer colleagues from around the world, but the registration desk will be open and you can also pick up your Heat Transfer Celebration registration packet and enjoy the meeting Friday morning without delays!

Dinner will be followed by remarks from distinguished faculty alumni.

# 7:30 а.м.

Friday

April 4

Continental Breakfast

All participants are invited to enjoy fresh fruit and pastries before the day begins. This breakfast buffet is provided compliments of the School of Mechanical Engineering.

# 12:00 NOON

# **Exploring Lunch**

You are invited to take advantage of the extended lunch hour to explore Purdue's beautiful West Lafayette campus. Meals are available at several restaurants on the ground floor of the Purdue Memorial Union. Chauncey Village is also within close walking distance and offers many cuisine choices.

6:30 р.м.

## Hawkins Memorial Lecture Dinner

Please join us for cocktails and dinner in the West Faculty Lounge of the Purdue Memorial Union. The dinner is free of charge and will be served at 7:15 p.m. Reservations are requested and your name badge will be required for admission. Door prizes will be awarded throughout the evening, and a performance by the Purduettes is planned.

# Saturday April 5

# 7:30 а.м.

# **Continental Breakfast**

All participants are again invited to start the day with fresh fruit and pastries.

# PANEL SESS

# Friday April 4

**8:00** а.м.

# Welcome

We are pleased that Dr.Vijay Dhir, Dean, School of Engineering and Applied Science, University of California Los Angeles and Technical Editor, *ASME Journal of Heat Transfer*, will deliver the plenary remarks for the Heat Transfer Celebration.

## 8:30 а.м.

#### Contributions to Heat Transfer Research: Purdue and Beyond

### Panel Chair:

M. Pinar Mengüç, University of Kentucky

### Panelists:

Christoph Beckermann, University of Iowa

Vijay Dhir, University of California Los Angeles

Satish Ramadhyani, Data Sciences International

David Zumbrunnen, Clemson University

#### <u>Topics:</u>

**Bio-Heat Transfer** 

Boiling and Two-Phase Flow

Conduction

Convection

Mass Transfer

**Materials Processing** 

Particle Characterization

Polymers

Radiation

# 10:30 а.м.

# **Heat Transfer Education**

### Panel Chair:

Ted Bergman University of Connecticut

## <u>Panelists:</u>

Bashar Abdulnour Ford Motor Company

Louis Burmeister University of Kansas

Gang Chen Massachusetts Institute of Technology

David DeWitt National Institutes of Standards and Technology/Purdue University

Robert Watts Tulane University

### <u>Topics:</u>

**Industrial Perspectives** 

Thermal System Design

Nano- and Microscale Heat Transfer

Integration of Thermal Sciences

Global Scale Environmental Issues

# **Emerging Areas**

Panel Chair:

Richard Chu IBM

# Panelists:

Andrei Fedorov Georgia Tech

Jay Gore Purdue University

Frank Incropera Notre Dame University

Arun Majumdar University of California at Berkeley

Richard Smith National Science Foundation/ Rensselaer Polytechnic Institute

Chao-Yang Wang Pennsylvania State University

# <u>Topics:</u>

Biological Applications Energy

Fuel Cells

- - - -

Funding Trends

Materials Processing

MEMS

Nanoscale Transport





1:30 р.м.

# HAWKINS MEMORIAL LECTURE

# Friday April 4

3:00 р.м.

This annual lecture series was established in 1984 to honor the memory of George A. Hawkins, former Dean of the Schools of Engineering. Renowned for his many contributions as a teacher, researcher, and administrator, he retained a strong commitment to heat transfer and was instrumental in establishing Purdue's eminence in the field. The lecture provides an opportunity for a leader in heat transfer research to present topics of broad interest to the University community. This series is supported by an endowment created with gifts from the Heat Transfer Area faculty at Purdue.

# George A. Hawkins

George A. Hawkins was born in Denver, Colorado in 1907. He attended the Colorado School of Mines and the University of Denver before coming to Purdue where he received three degrees. Dr. Hawkins earned his Ph.D. in 1935 and began an academic career that spanned 41 years. Promoted to Professor of Mechanical Engineering in 1942, he was Dean of the Schools of Engineering from 1953 to 1967 and Vice President of Academic Affairs from 1967 until his retirement in 1971. In addition to his administrative duties, he continued with technical pursuits, writing several textbooks and more than 150 papers and articles dealing with heat transfer, thermodynamics, and other engineering areas.

For his technical, professional, and administrative contributions, he received many honors, including election as member of the National Academy of Engineering, Life Fellow of the American Society of Mechanical Engineers (ASME), Fellow of the American Institute of Chemical Engineers (AIChE), and Honorary Member of the American Society for Engineering Education (ASEE). He received the ASME/Pi Tau Sigma



Gold Medal in 1940. As dean, he was instrumental in effecting major changes in engineering education throughout the U.S., and was awarded the ASEE Medal for Distinguished and Meritorious Service in 1968. He was named National President of ASEE in 1970.

One of his strongest professional commitments was to the subject of heat transfer, and he had an important influence on establishing Purdue as a world leader in this area. In the 1930s and 1940s, he was, with William McAdams on the East Coast, M. Jakob in the Midwest, and L.M.K. Boelter on the West Coast, a major force in promoting the transition of heat transfer from an engineering art to a modern form of engineering strongly based on scientific fundamentals. His early work as a pioneer of heat transfer is well-documented. His program flourished, producing many outstanding graduate students who have enjoyed successful careers in industry, academia, and government.

Following his retirement in 1971, Dr Hawkins continued to be active until his death in 1978.

#### Hawkins Memorial Lecture Series

Ernst R.G. Eckert, University of Minnesota

E.M. Sparrow, University of Minnesota

Arthur E. Bergles, Iowa State University

Chang-Lin Tien, University of California - Berkeley

Wataru Nakayama, Hitachi, Ltd.

Frank Mayinger, Technische Universität München

Raymond Viskanta, Purdue University

R.J. Goldstein, University of Minnesota

Richard C. Chu, International Business Machines Corporation

Robert Siegel, NASA Lewis Research Center

Julian Szekely, Massachusetts Institute of Technology

John R. Howell, University of Texas-Austin

Frank P.Incropera, Purdue University

Boris Rubinsky, University of California-Berkeley

David P.DeWitt, Purdue University

Vijay K. Dhir, University of California-Los Angeles

Robert G. Watts, Tulane University

Martin C. Jischke, Purdue University

Kenneth R. Diller, University of Texas-Austin

John H. Sununu, JHS Associates, Ltd.

# HAWKINS LECT: URE "The Engineer in the Public Policy Arena"

# Friday April 4

# 3:00 р.м.

#### John H. Sununu President, JHS Associates, Ltd.

John H. Sununu of Salem, New Hampshire, is President of JHS Associates, Ltd. and a former partner in Trinity International Partners, a private financial firm.

Governor Sununu attended the Massachusetts Institute of Technology at both the undergraduate and graduate levels, earning his Ph.D. in 1966 in Mechanical Engineering. From 1968 until 1973, he was Associate Dean of the College of Engineering at Tufts University and Associate Professor of Mechanical Engineering. He served on the Advisory Board of the Technology and Policy Program at MIT from 1984 until 1989. He is a member of the National Academy of Engineering.

From 1962 until his election as Governor, he served as President of JHS Engineering Company and Thermal Research, Inc. In addition, he helped establish, and served as chief engineer for, Astro Dynamics, Inc. from 1960 until 1965.

John Sununu became New Hampshire's 75<sup>th</sup> Chief Executive on January 5, 1983, and served three consecutive terms prior to joining the White House staff. He assumed office with a background of nearly 20 years experience as an educator, engineer, small businessman and community leader. The Governor gained both regional and national recognition through his chairmanship of the Coalition of Northeastern Governors, the chairmanship of the Republican Governors' Association, and his election in 1987 to the chairmanship of the National Governors' Association.



Governor Sununu was commissioned Chief of Staff to the President of the United States on January 21, 1989, and served the White House until March, 1992. As Chief of Staff, Sununu oversaw the daily operations of the White House and its staff. He also served as Counsellor to the President. The Governor is a member of the Board of Trustees for the George Bush Presidential Library Foundation.

From 1992 until 1998, he co-hosted CNN's nightly "Crossfire" program, a news/public affairs discussion program.

The Governor is married to the former Nancy Hayes. They have eight children.

# The Engineer in the Public Policy Arena

Good public policy needs engineers to be good public policy makers. There isn't much new and better that happens in the world today that isn't made possible by some innovation in engineering.

But all the changes that make life better also make life a bit more complicated. To deal with those complications, we develop public policies, laws and regulations to provide the framework for the operation of an orderly, beneficial society.

While engineers continue to drive real progress and improvements to the quality of life, they generally have been reluctant to get involved in the process of developing public policy. Unfortunately, they have long considered that arena as being more appropriately the domain for other professions such as lawyers. In fact, however, society needs a more active involvement in policy development by those who understand both the potential and the limitations of technology.

Engineers need to think more seriously about accepting the responsibility of public office. If the problem solvers of the world don't participate in making public policy, then policies will be developed by those who don't know how to solve problems.

# SATURDAY EVENTS

# Saturday April 5

# 8:00 А.М.

#### School of Mechanical Engineering Highlights

Dan Hirleman will discuss the legacy of the School of Mechanical Engineering, ongoing activities, and plans for the future.

# 8:30 а.м.

# **Research Poster Session**

We invite all attendees at the Celebration to contribute a poster at this optional Poster Session. We ask that you choose a topic in your area of expertise or interest for coverage in this poster session. Easels will be provided. Current Purdue heat transfer students will also be participating with posters in this session.

9:30 а.м.

#### Impact of Purdue Heat Transfer: Alumni Perspectives

This event, organized by alumni, will recall memories of their times here, and the impact of their Purdue Heat Transfer experiences.

# 1:00 р.м.

# Heat Transfer Laboratories

Current faculty and graduate students will be available to provide tours of the Purdue Heat Transfer Labs after adjournment of the Celebration.

# **Martin C. Jischke**



President Purdue University

BS 63 Illinois Institute of Technology MS 64 MIT PhD 68 MIT

# Linda P.B. Katehi



John A. Edwardson Dean of Engineering Professor of Electrical and **Computer Engineering** 

BS 77 National Technical University of Athens MS 81 UCLA PhD 84 UCLA

# **E. Daniel Hirleman**



William E.and Florence E. Perry Head Professor of Mechanical Engineering

BS 72 Purdue MS 74 Purdue PhD 77 Purdue





Professor B.Tech. IIT, Kanpur 79

**Heat Transfer Faculty** 

BS Cornell 91

PhD Cornell 98

Timothy S. Fisher

Associate Professor

Suresh V. Garimella

BS IIT Madras 85

MS Ohio State 86

Jay P. Gore

tion Engineering

MS Penn State 82

PhD Penn State 86

PhD California-Berkeley 89

Reilly Professor of Combus-

BE University of Poona 78

Professor

MS Washington State 81 PhD Minnesota 84



Robert J. Schoenhals Professor

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BS Michigan 56 MS Michigan 57 PhD Michigan 61



Raymond Viskanta W.F.M. Goss Distinguished Professor of Engineering

BS Illinois 55 MS Purdue 56 PhD Purdue 60



Lisa X. Xu Associate Professor

BS Shanghai Medical University 86 MS Alabama-Birmingham 88 PhD Illinois 91



Xianfan Xu Associate Professor

BS University of Science and Technology of China 89 MS California-Berkeley 91 PhD California-Berkeley 94

# Alumni Organizing **Committee:**

Christoph Beckermann Ted Bergman Marcus Bianchi **Richard Chu** Andrei Federov Pinar Menguc Brent Webb

Donna Brown, Development Secretary Lori Carte, Heat Transfer Secretary

# The Legends of Purdue Heat Transfer

compiled by

# Brent W. Webb (PhD 1986) Professor of Mechanical Engineering Brigham Young University

In 1935 a young graduate student by the name of George A. Hawkins completed his PhD under the supervision of Professor Harry L. Solberg in the School of Mechanical Engineering at Purdue. Hawkins joined the faculty of Mechanical Engineering that year, and a year later (1936) he was appointed Director of the newly established Heat Transfer Research Laboratory. He was promoted to Full Professor in 1942, and in 1943 was named Westinghouse Research Professor. Hawkins was a visionary academic who nurtured engineering education from art and empiricism to science and analysis. Committed to continual learning, he sought collaboration with the heat transfer "greats" of the day including McAdams, Boelter, Jakob, and Eckert. George Hawkins gathered around him faculty who shared his vision and drive, and together they established Purdue as a pre-eminent university in heat transfer education and research. As the 70<sup>th</sup> anniversary of the establishment of "Purdue Heat Transfer" approaches, we pause to look back on that first generation of faculty who formed the Purdue Heat Transfer Group. While their impact on the discipline will largely be characterized here in "the numbers," let it be said that these early Purdue pioneers of heat transfer have been caring mentors to the students with whom they worked, establishing lasting friendships and providing counsel outside the engineering science for which they became internationally known. Those students who were the beneficiaries of the legacy of Purdue Heat Transfer join in honoring these legendary faculty and celebrating their influence.

The "founding faculty" of the Purdue Heat Transfer Group are shown in Figure 1 with their years of residence at the university. As may be seen, after a developmental start in the first two and a half decades, a significant body of heat transfer engineers joined the group in the late 50's and early 60's. Heat transfer graduate education was in its infancy in those early years, and the pool of qualified faculty in the area was modest. Professor Hawkins and his early colleagues who followed were forced to build a heat transfer corps by training many of the early faculty themselves, building the faculty

expertise with those who studied outside Purdue only as exceptional people surfaced. Among Professor Hawkins' early graduate students, Y.S. Touloukian and R. Grosh joined the Purdue faculty in the Heat Transfer Group. Professor Touloukian was appointed to an academic position in 1944, and he continued to do research in heat transfer and thermodynamics until, recognizing the critical need for characterization of thermophysical properties in the heat transfer science which was emerging, he started the Thermophysical Properties Research Center in 1957. Professor Richard Grosh joined the faculty in 1953 following his doctoral studies. He shared Hawkins' vision for strong heat transfer education and research. Three of Professor Grosh's former PhD students (William Cottingham, Peter McFadden, and Raymond Viskanta) subsequently joined the faculty group. Professor David DeWitt did his doctoral studies under Professor Touloukian, and after two years at the National Bureau of Standards, he returned to join the Purdue group in 1965, affiliated with both the Heat Transfer Group and the Thermophysical Properties Research Center. One of Professor McFadden's PhD students, Calvin Oliver, was appointed to the faculty in 1963, remaining at Purdue for only three years. These Purdue alumni were joined by colleagues in the early 60's who had completed their PhD work elsewhere: R.J. Schoenhals, E.R.F.Winter, FP.Incropera, W. Leidenfrost, and J.T. Pearson. Digital computing began to make inroads in heat transfer research in the late 1970's, and the Group recognized the need for expertise in this area. Professor Satish Ramadhyani joined the faculty in 1983 to provide strength in computer modeling.

As Figure 1 illustrates, the face of the Purdue Heat Transfer Group has evolved since its establishment in 1936. Many of the first generation of Purdue Heat Transfer faculty left the university, accepting positions of influence and leadership in industry and academia elsewhere. After serving as Chair of the Heat Transfer Group, Head of the School of Mechanical Engineering (1962-66), and Associate Dean and Dean of Engineering at Purdue (1966-71), Richard Grosh was named



Figure 1. The founding faculty members of the Heat Transfer Group and their years of residence at Purdue.



W.B. Cottington









G.A. Hawkins





W. Leidenfrost



P.W. McFadden



J.T. Pearson





R.Viskanta



E.R.F. Winter

President of Rensselaer Polytechnic Institute in 1971 at the age of 43. William Cottingham, who led the School of Mechanical Engineering as its Head for four years, became Dean of Academic Affairs at General Motors Institute in 1975, and at age 42, was appointed President of the Institute. Peter McFadden accepted the position as Dean of Engineering at his alma mater, the University of Connecticut. Professor E.R.F.Winter was named Chair of Thermodynamics, Faculty of Mechanical Engineering at the Technical University of Munich in 1973. Professor Frank Incropera served as Chair of the Heat Transfer Group (1976-86), Head of the School of Mechanical Engineering (1989-98), and Assistant Dean of Engineering for Research and Graduate Programs at Purdue before accepting the position of Dean of Engineering at the University of Notre Dame in 1998. A number of others in

that first group also served ably in administrative positions at Purdue. Professor Peter McFadden served as Chair of the Heat Transfer Group from 1962 to 1966, when he took the position as Head of Mechanical Engineering, where he served for five years. David DeWitt was appointed Chair of Heat Transfer in 1986, serving until 2000. He held the position of Deputy Director of the Thermophysical Properties Research Center for a time. The father of Purdue Heat Transfer, George Hawkins' administrative abilities were recognized early at Purdue University. He was the first Chair of the Heat Transfer Group, serving from 1936 to 1953. He was Assistant Dean of the Graduate School where he served as Acting Dean for 15 months (1947-50). Hawkins assumed the position of Dean of Engineering in 1953, serving until 1966, and was also Director of the Engineering Experiment Sta-



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**F.P.** Incropera

tion (1953-61). For the period 1961-63, in addition to his responsibilities as Dean of Engineering, he was Dean of the School of Sciences. In 1967, Professor Hawkins was appointed Vice President for Academic Affairs, a position he held until administrative re-organization when he was designated Vice President Emeritus. He served the engineering education community from 1970-71 as President of the American Society for Engineering Education.

Four of the pioneer faculty in the Heat Transfer Group have been recognized for their influential service in engineering research and education by induction into the National Academy of Engineering. George Hawkins was inducted in 1967, Richard Grosh in 1969 (at the age of 41), Ray Viskanta in 1987, and Frank Incropera in 1996. Arguably the most prestigious recognition accorded engineers, this distinction has been granted to only 174 members of the mechanical engineering community (Source: National Academy of Engineering Web site: www.nae.edu, 2003). They are part of an elite few (only some two dozen) heat transfer engineers in the Academy.

The founding faculty of the Purdue Heat Transfer group have significantly influenced the science of heat transfer. Early work in Professor Hawkins' group was directed at understanding the limits of heat transfer in water at high pressure related to cooling in nuclear reactors. Later, one of Professor Hawkins' hobbies-rifles and pistols-led to his selection to direct another unusual project, U.S. Army Ordnance-supported research on cooling of automatic weapons. His team found ways to improve cooling efficiency and increase firing rate. Stories still circulate on campus about experimental testing of machine guns behind the Mechanical Engineering Building. Over the years, research in the Heat Transfer Group migrated with societal needs to address thermal challenges of timely interest. Looking back, one sees the tremendous contribution to fundamental heat transfer science and application. Their work has been disseminated widely. Figure 2 illustrates the history of publication and presentation for the members of the founding Heat Transfer Group through the year 1995. This year marks loosely the beginning of the "changing" of the guard" in the Heat Transfer faculty-retirements of the founding faculty and the hire of a new generation. Figure 2 shows that the rate of publication has grown

steadily from the mid-1950's as the Group grew, their stature in the technical community matured, and research funding blossomed. Graduate students were attracted to Purdue where it was known that high quality research in thermal sciences was performed. The publication activity of the early Purdue pioneers has been phenomenal, totaling well over 1100 peer-reviewed publications of scientific research<sup>1</sup>. The vast majority of these publications have been with student co-authors—generally with the students as lead author, reporting results of their thesis research. The publications reported in the figure are only a small part of the story of the dissemination of Purdue scholarly activity. Dozens, perhaps hundreds of presentations-invited lectures, short courses, industrial presentations and consulting-also reflect the Group's reach in the discipline both here and abroad.



Figure 2. Publication history of the Heat Transfer Group for the years 1955 to 1995.

The Celebration of Purdue Heat Transfer focuses on the founding members of the Group. The data in Figure 2 therefore includes only publications of the original Purdue Heat Transfer faculty identified here. It should be clearly stated that the current generation of faculty is building on the foundation laid by their predecessors.

<sup>1</sup> It should be stated that an accurate accounting of publication from the Heat Transfer Group is rather difficult. The results reported here represent perhaps the minimum, collected from faculty vitae where available. Further, it is noted that while Professors Touloukian and Winter were part of the original Heat Transfer Group and contributed significantly their works are not included in Fig. 2. As was stated, Professor Touloukian's principal responsibility was the Thermophysical Properties Research Center since 1957, and Professor Winter joined the faculty at the Technical University of Munich in 1973.

<sup>2</sup> The data reported in Figure 3 were taken from the printed version of Science Citations Index (Institute for Scientific Information, Philadelphia, PA) for the years 1961 through 1979. The printed edition lists citations only of lead-author publications. From 1980 through 2000, the online edition (Science Citations Index Expanded. Institute of Scientific Information Web of Science) was used, which reports citations of publications with both lead and secondary authorship. 1980 is the first year for which the online database was available to the author.

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The Heat Transfer Group now includes Professors T.S. Fisher, S.V. Garimella, J.P. Gore, I. Mudawar, J.Y. Murthy, R.J. Schoenhals, L. Xu, and X. Xu, and their work continues to significantly impact the discipline.

One quantifiable measure of the impact of Purdue's founding Heat Transfer Group research is the number of citations of their work by colleagues in the technical community. The history of such citations for the founding members of the Purdue Heat Transfer, in five-year blocks, is illustrated in Figure 3, from 1960 to 2000<sup>2</sup>. The work of Purdue faculty has been cited even from the early days of heat transfer research. The number of citations has risen steadily, and to date (February, 2003), a total over 7000 references of published work of the founding Heat Transfer Group have been identified. In just over two years since January 2001, the Group's work has been referenced nearly 1300 times.



Figure 3. Citations of Purdue Heat Transfer faculty publications by five-year period, 1960-2000.

Some of technical publications of the founding Purdue Heat Transfer faculty might be considered "classical" works, having been referenced many times. Fifty-one publications of eight different faculty members in the Group have been cited thirty or more times since 1979. Twelve faculty publications have been cited sixty or more times; four have been cited more than 100 times (Source: ISI Web of Science, Science Citations Index Expanded, 2003). Professors Incropera and Viskanta were recognized by the Institute for Scientific Information for being among the one hundred mostcited researchers in engineering worldwide (source: ISIHighlyCited.com). The premier heat transfer textbook in the field, Fundamentals of Heat and Mass Transfer, coauthored by two Purdue Heat Transfer faculty, Professors Frank Incropera and David DeWitt, is yet another illustration of the Group's influence on heat transfer education. The text has been adopted at over 200 universities in the United States and has been translated into five languages for use abroad. Since its first publication in 1981, it has appeared in five editions (1981, 85, 90, 96, and 2002), and has been read by more than 300,000 students. In addition to its pre-eminence in undergraduate heat transfer education, the text has become something of a reference for heat transfer research. Its five editions have been cited over 1900 times in technical publications worldwide (Source: ISI Web of Science, Science Citations Index Expanded, 2003).

In addition to the impressive quantity of citations of Purdue Heat Transfer technical publications, several of the early works from the faculty stand even today as foundation additions to the literature. Two of Professor Hawkins' publications on steam properties were cited twice since 2000, nearly seventy years after their publication. Two of Professor Grosh's early published works from the 1950's on heat transfer in welding processes have been cited regularly since their publication, most recently in 2001. Professor McFadden's early research on boiling heat transfer in 1961-62 was cited ten times between 1995 and 2000. These are just three such examples illustrating the enduring impact of quality research from the Heat Transfer Laboratory on the discipline.

The measurable influence of Purdue's legendary Heat Transfer Group has been documented in the foregoing paragraphs. However, it might be argued that the primary product of the faculty has not been the papers, but the people—graduate students, post-doctoral fellows, and visiting scholars with whom they have worked. Figure 4 shows the history of heat transfer student supervision since 1941, mentored by first-generation Purdue Heat Transfer faculty. The numbers are impres-



Figure 4. Student advisement in the Heat Transfer Group by year.

sive, with nearly 600 students—some 250 MS students, 200 PhD students, and 70 post-doctoral and visiting scholars—having completed their studies through 1995. These students have carried the Purdue legacy into positions in academia, industry, business, sharing the heritage of training in careful thought, meticulous research, and concise writing wherever they are. It should not be inferred from Figure 4 that graduate advisement in the Heat Transfer area is "winding down." As the founding faculty in the Group have retired or taken positions elsewhere, they have passed the opportunity and responsibility of student advisement on to the current generation of Heat Transfer faculty. There are currently some fifty students and visiting scholars are pursuing work in the Group.

The worldwide influence of Purdue Heat Transfer alumni is illustrated in Figure 5, where shaded (dark) are the 35 different countries with which alumni have ties (either countries of origin or of current residence). Truly, the influence of Purdue Heat Transfer has been global, spanning North and South America, India, China, Australia, Russia, Western Europe, and Africa. Students have come to Purdue to be educated from Africa, where engineering education is yet immature, to Western Europe, which itself has a rich history of strong engineering training.



Figure 5. Countries (shaded dark) to which Purdue Heat Transfer alumni have ties (i.e., countries of origin or of current residence).

Finally, it should be said that from its inception the faculty in the Purdue Heat Transfer Group have been deeply concerned with their students. Former Dean of the Schools of Engineering John Hancock wrote of George Hawkins:

George Hawkins' leadership in engineering education at both the national and local levels has been well recognized. He has made many outstanding contributions to engineering education during his tenure at Purdue. While George Hawkins is a talented, innovative individual, I feel that much of his success can be directly attributed to the concern and understanding which he has of people. I feel that it is rare indeed to find a man who is just as concerned about a faculty member's health or his family problems as he is about his professional growth and his contributions to Purdue. From my own experience I know that George Hawkins is a humanitarian and Purdue University is richer to day as a result of his leadership in all phases of its life.

The same can be said of Professor Hawkins' colleagues in that group of founding faculty. Discussions with students went beyond technical issues in their work. Their interest was in the development of total, balanced leaders. They did so with the support of their families, who often entertained students in their homes, and who were supportive of long hours in the office and laboratory. On the eve of the 70th anniversary of Purdue Heat Transfer, the alumni honor their faculty mentors, celebrate their achievements, and appreciate their friendship and influence in their lives.

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Purdue Heat Transfer Celebration April 3-5, 2002, West Lafayette, IN

#### **MODELING OF SOLIDIFICATION**

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#### INTRODUCTION

An overview is provided of recent progress in solidification modeling and its application to casting of metal alloys. The overview is structured in the order of increasing length scales: dendrites on a microscopic scale; interactions between dendrites, coarsening, and flow within a unit cell inside the mushy zone; and heat transfer, flow, and species redistribution on a macroscopic scale. It is shown how the transport processes at the different length scales interact to produce certain structures and defects in a casting.

#### DENDRITES

The most common microstructure formed during solidification of metals and alloys is the dendrite. Figure 1 shows an image of a dendrite of a transparent model substance (succinonitrile) grown in the microgravity environment of space [1]. Such images have enabled the study of the scaling behavior of single dendrites growing freely in an undercooled melt [2, 3]. For example, in the sidebranch plane corresponding to Figure 1, the contour length, U, of the solid-liquid interface as a function of distance Z from the tip is given by

$$U/R = 0.38(Z/R)^{1.5}$$
(1)

and the area of the solid, F, by

$$F/R^2 = 0.58(Z/R)^{1.7}$$
(2)

where *R* is the radius of curvature of the dendrite tip. These two scaling relations are valid in the nonlinear sidebranching regime far from the tip, Z/R > 40, up to several hundred tip radii back. They apply not only to the dendrite shown in Figure 1, but to different dendrites grown using a variety of undercoolings. The existence of these relations implies that the dendritic structure remains self-similar far from the tip. It is certainly intriguing that the knowledge of the tip radius alone is sufficient to predict structural features of an entire dendrite.



Figure 1: Enlarged image of a succinonitrile dendrite obtained in the Isothermal Dendritic Growth Experiment of Glicksman and coworkers [1] on the space shuttle.

The simulation of dendritic growth and other solidification microstructures has recently experienced much progress due to the availability of novel numerical techniques and increased computational power. In particular, the phase-field method has been used with great success to model the evolution of complex solidification structures [4]. Figure 2 shows a result from a phase-field simulation of the growth of a single dendrite into an undercooled melt with flow [5]. Such simulations allow the effects of convection in the melt on the growth of the dendrite tips and sidebranches to be quantified and compared to theories and experiments [6-8].



Figure 2: Three-dimensional phase-field simulation of free dendritic growth of a pure substance into an undercooled melt; the melt flows over the dendrite from left to right [5].

#### MUSHY ZONE

One of the challenges in modeling solidification is how to account for processes occurring on a microscopic scale, such as dendritic growth and coarsening, in a model for an entire casting. One approach is to use representative elementary volumes (REV) as building blocks in a macroscopic model. By investigating in detail the solidification and transport phenomena in each REV, an averaged description can be obtained. Here it is important to not restrict attention to a single dendrite, but to take into account the presence of and interactions between multiple dendrites inside the mushy zone of solidifying alloys.

Figure 3 shows two-dimensional phase-field simulations of coarsening and flow for a periodic unit cell inside the mushy zone of an Al-4%Cu alloy [9]. The initial circles (left-most panels) represent cuts through dendrite arms of various diameters. As time proceeds, the structure of the solid coarsens. In the simulations with flow (lower panels in Figure 3), the coarser structures offer less flow resistance, resulting in an increase in the melt velocity with time. This in turn implies an increase in the permeability of the mush element. It is important to realize, however, that while the microstructure of the mush affects the flow, the flow also influences the evolution of the microstructure. In the presence of convection, the interfacial area decreases with the square root of time, as opposed to the classical cube-root-of-time coarsening behavior for purely diffusive conditions [9].

#### CASTINGS

Some of the solidification models developed in the past [10-12] are now being incorporated into commercial software, to enable the casting simulation of complex-shaped, three-dimensional parts.

One important issue in casting simulation is the prediction of macrosegregation (inhomogeneities in the composition on the scale of the casting) [13]. The cause of macrosegregation is the long-range movement of (micro-) segregated liquid and solid in the mushy zone, as shown for a REV in Figure 3. An example of the simulation of macrosegregation formation during solidification of a large steel casting is shown in Figure 4 [14]. It should be noted that due to computer limitations, the prediction of smaller scale macrosegregation features (such as



Figure 3: Phase-field simulations of coarsening in and flow through (lower panels only) a periodic unit cell inside the mushy zone of an Al-4 wt.% Cu alloy; the thick black contour lines show the solid-liquid interface; the gray shades indicate Cu concentrations in the liquid and solid [9].



Figure 4: Simulation of macrosegregation formation in a large (2.65 m height) steel casting; left panel: predicted liquid velocities and solid fraction at an intermediate time during solidification; carbon macrosegregation pattern in the fully solidified casting [14].

freckles or A segregates) in large castings is beyond current capabilities.

Another important area that has recently received increased research interest is the prediction of porosity in castings. Porosity significantly reduces the mechanical performance of castings, and porosity-related defects are a major cause of casting rejection and re-work in the casting industry. Porosity ranges in size from microporosity, such as micron-sized gas bubbles, to macroporosity, such as millimeter- to centimetersized centerline shrinkage porosity, or even larger shrinkage cavities found in inadequately fed cast sections. Porosityrelated defects come about due to the interplay of several phenomena. As the melt cools, the solubility of gases dissolved in the melt decreases. If the solubility limit is reached, gas will precipitate out of the melt. In addition, gases are much less soluble in solid than in liquid, and hence gas is rejected from the solid to the liquid during solidification, which increases gas levels in the remaining liquid. Finally, the pressure gradient associated with metal flowing through the mushy zone to feed solidification shrinkage decreases the pressure in the casting, which further lowers the solubility. Even in the absence of dissolved gases, pores can form solely due to shrinkage.

An example of the simulation of porosity formation in a steel casting is shown in Figure 5 [15]. To validate the predictions, two types of casting trials were conducted: one without applied pressure and one where the solidifying steel was subjected to a higher than atmospheric pressure. Pressurization was accomplished through the top riser. The trials were performed with 3"T x 6"W x 50"L plates, cast with the rigging shown in Figure 5a. The predicted final pore volume percentages for the non-pressurized and pressurized riser cases are shown in Figure 5b. The scale for these results is given at the far right of Figure 5. As expected, pressurizing the riser significantly reduces the amount of porosity that forms in the castings. Figures 5c and 5d provide a comparison between the casting trial radiographs and the simulation results for the non-pressurized and pressurized cases, respectively. Good qualitative agreement is seen. In particular, the simulation nicely reproduces the narrow band of centerline porosity in the plate. However, the visible porosity on the nonpressurized casting radiograph in Figure 5c extends closer to the riser than in the simulation result, and the porosity region in the pressurized casting radiograph in Figure 5d is shorter than seen in the simulation result. The differences in the simulation results and the casting trials are likely due to several factors, including unknown gas levels in the casting trials, uncertainties in the permeability, and the fact that the simulations did not include filling. Still, the simulation results qualitatively capture the phenomena seen in the casting trials. Additional studies are currently underway to validate the porosity model. In addition, the model is being applied to predict microporosity formation in aluminum alloy castings.



Figure 5: Simulation of porosity formation in a steel casting with and without a pressurized riser, and comparison with casting trials: (a) rigging for trial castings; (b) pore volume percentages with and without pressurization; and comparison between radiographs of castings and simulations for (c) an non-pressurized casting, and (d) a pressurized casting [15].

#### CONCLUSIONS

While much progress has been made in solidification modeling during the last two decades, there are several issues that require increased research attention. These include modeling of:

- solidification of multicomponent alloys, taking into account the formation of multiple phases
- grain structure transitions (e.g., columnar to equiaxed)
- deformation of the solid in the mush
- segregation in the presence of moving solid and undercooled liquid
- fragmentation of dendrites
- flow effects on the growth rates and structures of dendrites, eutectics, etc.

Future research on any of the above issues will increasingly rely on first principles, direct numerical simulation of solidification on a microscopic scale using, for example, the phase-field method. However, the use of direct numerical simulation for an entire casting will not be an option until at least the year 2050 [16].

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#### PHASE CHANGE HEAT TRANSFER – A REVIEW OF PURDUE RESEARCH

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#### ABSTRACT

Research carried out a Purdue University in the area of phase change heat transfer (e.g., boiling) has been briefly reviewed in this paper. The hallmark of Purdue research is that basic studies were motivated by industrial applications and the results of basic studies culminated in solutions to practical problems. The reviewed research work is divided into three distinct areas: material processing, electronic cooling, and phenomenological studies of critical heat flux with applications in the power industry.

#### INTRODUCTION

This review is focused on the investigations carried out in the area of boiling heat transfer by Professors F.P. Incropera, I. Mudawar, S. Ramadhyani, and R. Viskanta and their students in the School of Mechanical Engineering at Purdue University. The review is divided into three broad areas: material processing, electronic cooling, and phenomenological studies of critical heat flux with applications in the power industry. These faculty and students deserve to be applauded for their ability to perform basic research while not losing sight of the intended applications. Key results obtained in each of the areas are described in the following.

#### NOMENCLATURE

$C_1C_5$	empirical	l constants
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- *D* tube inside diameter
- G mass velocity
- $h_{f,0}$  saturated liquid enthalpy at outlet
- $h_{fg,0}$  latent heat of vaporization at outlet pressure
- $h_i$  enthalpy of liquid at inlet
- *L* heat length of tube
- $q_{CHF}$  critical heat flux
- $\rho_f$  liquid density

- $\rho_g$  vapor density
- $\sigma$  interfacial tension

#### **Materials Processing**

The product quality from many manufacturing processes depends on thermal response of the material to the cooling methods that are employed during manufacturing. The product quality not only includes physical dimensions, but also the mechanical properties. Some examples of manufacturing processes of interest are hot rolling, casting, extrusions, forging, and annealing.

Zumbrunnen, Viskanta and Incropera [1] investigated the effect of surface motion on forced convection film boiling. This situation arises during cooling by planar jets of a hot plastic steel strip after rolling and during continuous annealing of a cold rolled strip. Figure 1 shows various heat transfer regimes on a steel strip with film boiling being dominant over a larger portion of the plate. It was shown through two-layer integral analysis for laminar flow that with plate motion in the same direction as the subcooled liquid, the vapor film thinned, thereby improving the heat transfer. However, when the plate motion was opposite to the liquid flow direction, the vapor film thickened with a corresponding reduction in heat transfer. Subsequently, similarity solutions were obtained for laminar film boiling and analyses were extended to turbulent film boiling.

Filipovic, Incropera, and Viskanta [2] have investigated, experimentally and theoretically, quenching phenomena associated with a water wall jet as encountered during cooling of a rolled strip or during continuous casting. A quench front (just downstream of the region II in Fig. 1) forms and it travels in the direction of liquid flow. Upstream of the quench front, forced convection and nucleate boiling exist, whereas film boiling prevails downstream. The quench front region, as



Figure 1: Boiling regimes during quenching of steel strip with a planar jet.

shown in Fig. 2, is marked by the existence of transition boiling. It was noted that the length of this region could be as much as 20 mm. The upstream edge of the region marked the critical heat flux condition, whereas the downstream edge, the wetting temperature. At the wetting temperature, liquid-solid contact was established. An apparent quenching temperature was defined at which, as a result of axial conduction in the solid, cooling began to take place at a rate faster than in film boiling. Subsequently, the authors developed an accurate method for quantitatively determining quenching and apparent quenching temperatures from temperature-time plots. It was shown that rewetting temperature and quench front velocity depended on temperature of the solid prior to quenching, liquid subcooling, and flow velocity.



Figure 2: Details of quench front region.

Hall, Incropera, and Viskanta [3] studied the effect of entrainment of gas on quenching characteristics of a planar jet of subcooled water. They found that with gas entrained in the subcooled liquid, heat transfer could be reduced in film boiling, thereby reducing the deformation of a billet during casting. The presence of air also reduced the temperature excursion that occurred after cessation of boiling during quenching by reducing the wall superheat for transition from nucleate boiling to single phase convection. Wolf, Incropera and Viskanta [4] have also experimentally investigated local heat transfer as opposed to average heater transfer during impingement of a planar jet of liquid. They found that jet velocity had influence only on single phase and partial nucleate boiling. The extent of partial nucleate boiling (range of wall superheat) depended on the distance from the stagnation point (decreased with decrease in distance). Single phase heat transfer coefficient was only sensitive to locations near the stagnation point.

Mudawar and co-workers have focused on the use of sprays to quench aluminum products post extrusion, forging, or during continuous casting. A very rapid quenching can lead to plastic deformation which, in turn, can cause warping of the product. On the other hand, slow quenching can lead to undesirable metallurgical properties and degradation of mechanical strength. In their pursuit to develop an ideal quenching rate that avoided the two extremes of warping and low mechanical properties, Mudawar and Valentine [5] and Klinzing, Rizzi, and Mudawar [6] took the first logical step of developing correlations for film boiling heat transfer, minimum film boiling temperature, minimum film boiling heat flux, transition boiling heat transfer, maximum heat flux, heat transfer in nucleate boiling, and temperature for the onset of single phase cooling and single phase heat transfer during spray cooling. A key feature of these correlations as that they were dependent on local spray properties such was Sauter mean droplet diameter, droplet velocity, droplet volumetric flux, and liquid temperature as opposed to properties that are defined at the nozzle exit. Deiters and Mudawar [7] used this information along with a solution of two dimensional transient conduction in the solid, to develop a scheme whereby sprays of desired strengths could be used on different sections of a product. Figure 3 shows their proposed scheme. When heavy density sprays were used on all surfaces a large temperature difference (325°C maximum) could occur at different locations in the solid during quenching. However, when heavier spays were used to quench thicker sections and lighter sprays for thinner sections, the temperature differences were substantially reduced ( $\sim 75^{\circ}$ C maximum). Figures 3a and 3b show the temperature histories at different locations on the solid.

Subsequently, Hall and Mudawar [8] used the quenching rate information to predict the mechanical strength of parts made of aluminum alloys. Through similar studies they developed smart quenching systems that could select spray nozzle configurations and other flow parameters to obtain superior mechanical properties for parts made of aluminum.

#### **Microelectronic Cooling**

With rapid increase in chip switching frequency, and in turn, power densities, we have almost reached the limit where the direct cooling of chips with liquid must be considered. The Purdue Heat Transfer group has been a leader and visionary in this regard, as it started to investigate the liquid cooling of simulated chips almost fifteen years ago. Various cooling techniques that have been considered are pool boiling, forced flow boiling in micro and mini channels, jet impingement cooling, falling liquid films, and spray cooling.

Anderson and Mudawar [9] experimentally studied the effect of artificial cavities and various surface enhancement schemes on hysteresis in the boiling curve and on nucleate and



Figure 3: Variations with time of temperatures in the solid during quenching under unoptimized and optimized conditions.

critical heat fluxes using a simulated chip placed in a pool of dielectric liquid, FC-72. They found that temperature overshoot increased with increase in the waiting period between various experiments. Artificial cavities with a diameter of about 300 µm had little effect on temperature overshoot and on nucleate boiling heat flux. Microfins, microstuds, and microgrooves tended to shift the nucleate boiling curve to the left and increase the maximum heat flux based on a projected area of the chip. The effect of preceding chips placed in an array was to increase the thickness of the void layer on the succeeding chips and thereby increase the wall superheat for a given heat flux. Liquid subcooling tended to reduce the thickness of the bubble boundary layer and increase the maximum heat flux. An optimum (with highest CHF) enhanced surface was developed by placing a single cylindrical stud on the chip and forming microstuds, radial microgrooves, or axial microgrooves on the studs and finally roughening the surface by blasting it with silica, water, and air slurry. On the optimum surface, critical heat fluxes of more than 150 W/cm<sup>2</sup> were obtained, when the liquid had a subcooling of 35°C.

Mudawar and Maddox [10] experimentally investigated critical heat flux on a  $12.7 \times 12.7 \text{ mm}^2$  surface simulating a chip surface placed flush with one of the walls of a vertical rectangular channel having a cross-section of  $12.7 \times 38.1 \text{ mm}^2$ . Using FC-72 as the test liquid, they found that critical heat flux increased with subcooling and velocity. They identified different CHF mechanisms for high and low velocities and developed a correlation applicable for all ranges of velocity. Subsequently, they studied the effect of surface enhancement schemes such as pin fins, microstuds and microgrooves on flow

boiling CHF. They found all the methods enhanced CHF over a plane surface, but pin fins performed the best. Studies of boiling and critical heat when a number of simulated electronic chips were placed in the direction of flow showed that the last chip (#9) was the first to develop nucleate boiling, followed by the upstream chips in order. A slight decrease in CHF in the downstream direction was observed as the vapor boundary layer thickness increased. The CHF data from all of the chips was found to be within  $\pm 12\%$ , which was comparable to experimental uncertainty. Experiments with different channel heights (2, 5 and 10 mm) showed that the temperature overshoot was the highest for the 2 mm high channel. Maximum values of critical heat flux for equal flow velocities were obtained for the 5 mm high channel. It was postulated that it was for this height that bubble removal process from the heater surface was most effective while liquid subcooling persisted throughout the channel.

Heindel, Ramadhyani, and Incropera [11] investigated the cooling of simulated chips placed on the lower wall of a horizontal rectangular channel and protruding into the flow. Ten discrete inline heat sources were used with FC-72 as the test liquid. Temperature overshoot was observed consistent with earlier studies. However, increasing the flow velocity was found to reduce the temperature overshoot. Subcooling of the liquid also reduced the magnitude of the temperature overshoot. A reduction in the height of the channel restricted vapor escape from the heater surfaces, especially those in the downstream direction. As a result, the nucleate boiling heat flux on these heaters, at a given wall superheat, was lower than that in the upstream heaters.

Bowers and Mudawar [12] experimentally investigated the concept of placing mini (D = 2.54 mm) and micro (D = 510µm) channels in the substrate supporting a chip. The effective heated length of the channels was 1 cm and R-113 was used as the test liquid. In both cases a number of parallel channels formed in the copper substrate and connected to common manifolds were operated. No temperature overshoot was reported at onset of flow boiling in the channels. In both mini and micro channels critical heat fluxes higher than 200 W/cm<sup>2</sup> were obtained under a modest pressure drop. Because of spreading of heat across channels, no significant rise in temperature after CHF occurred. As a result, at low flow rates, almost all of the liquid could be evaporated without experiencing large excursion in temperature. Boiling was found to accommodate higher heat fluxes than single phase flow under similar pressure drop conditions. However, a mini channel was preferred because of lower pressure dorp and reduced propensity for blockage. In a subsequent work, Bowers and Mudawar developed design criteria for channel pitch and thickness of the substrate while taking into consideration, the constraints imposed by thermal diffusion. They also developed correlations to two phase pressure drop so that optimum configurations under constraints of pressure drop and flow rate could be determined.

Mudawar and Wadsworth [13] investigated the use of a confined rectangular jet to cool a simulated  $12.7 \times 12.7 \text{ mm}^2$  chip with FC-72. Two regimes for critical heat flux (CHF) were identified. At medium velocities, the critical heat flux increased with flow velocity, whereas at high velocities, the critical heat flux was either insensitive or decreased with velocity. In the medium velocity regime, the critical heat flux increased with liquid subcooling and nozzle width, but was insensitive to channel height. The reduction in CHF at high velocities was postulated to be caused by reduced liquid subcooling in the streamwise direction. Critical heat fluxes as high as 250 W/cm<sup>2</sup> were obtained. A correlation for critical heat flux in terms of fluid properties, jet velocity, nozzle width, and liquid subcooling was developed for the medium velocity regime.

Spray cooling of a simulated electronic chip with full cone sprays of FC-72 and FC-87 has been experimentally investigated by Mudawar and Estes [14]. It was found that the nozzle to surface distance played an important part in determining the magnitude of critical heat flux, which increased with volumetric flux and liquid subcooling. Critical heat fluxes higher than 100 W/cm<sup>2</sup> were obtained. A correlation of critical heat flux in terms of volumetric flow rate, liquid subcooling, and droplet Sauter mean diameter was developed.

Mudawar *et al* [15] investigated cooling of vertically mounted heat sources with a liquid film falling over the surface. Vigorous nucleate boiling was found to disrupt the film and break it into liquid ligaments and droplets. Near critical heat flux condition, liquid was observed to separate from the heater surface and the critical heat flux occurred when thin liquid film left on the surface dried out. Critical heat flux was found to increase with reduction in heater length and increase in film velocity. Onset of the CHF condition was attributed to Helmholtz instability which led to separation of the flow, while leaving a thin liquid film on the surface.

#### Phenomenology and Correlations for Critical Heat Flux in Flow Boiling

Professor Mudawar and his co-workers have conducted a number of fundamental experimental studies to develop a phenomenological understanding of critical heat flux during flow boiling. They have used this understanding to develop mechanistic models/correlations for subcooled critical heat flux. They have also made a significant contribution to the technical literature by collecting and assessing more than 32,000 critical heat flux data points available in the literature.

Galloway and Mudawar [16] carried out photographic observations of the boiling phenomena, pre- and post-CHF, on a  $1.6 \times 12.7 \text{ mm}^2$  heater, mounted flush on the smaller side of a  $1.6 \times 6.4 \text{ mm}^2$  vertical channel. The experiments were conducted with FC-87 as the test liquid. Visual observations showed that, at low heat fluxes, discrete bubbles were formed on the heater surface. At low velocities, nearly hemispherical bubbles lifted off normally to the heater surface. However, at higher velocities, bubbles were elongated and slid along the heater surface before lift off. A liquid film of a thickness of about 60 µm was observed to be trapped between the sliding bubble and the heater surface. With increase in heat flux to about 60% of the value at critical heat fluxes, bubbles merged into large vapor masses which appear to acquire a wavy interface with a well defined wavelength. A thin liquid layer was deposited on the heater when wave troughs touched the heater surface. The regions over which this thin layer of liquid was deposited on the surface shrank with increase in heat flux. Heat was removed from the thin film by evaporation or nucleate boiling in the film. Critical heat flux condition was proposed to occur when the vapor effusion rate from the interface at the wetting front was able to lift the interface, thereby disrupting the liquid supply to the heater. Photographs in Fig. 4 show the wetting front and the interface lift off when the imposed heat flux slightly exceeded the critical heat flux. The lift off fronts progressed in the downstream direction. The dominant wavelength in the vapor liquid interface and its amplitude were found to decrease nonlinearly with flow velocity. In casting the visual observations into a mechanistic model, the two dimensional wavelength was determined from the Kelvin-Helmholtz instability considerations. The maximum heat flux condition was established when the momentum flux of the vapor leaving the interface was able to overcome the pressure difference that existed across the concave interface at the location where liquid-solid contact was established. The mean thickness of the vapor film and superficial velocities of vapor and liquid that were needed to evaluate the pressure difference at the onset of interfacial instability was determined by invoking conservation of mass and momentum across the vapor and liquid streams. Predictions from the model were found to be in very good agreement with critical heat flux data.

Subsequently, Sturgis and Mudawar [17] extended both the visual observations and the modeling of critical heat flux on longer upward facing horizontal surfaces ( $\geq$  102 mm in length). Visual observations similar to those reported by Galloway and Mudawar were made except that wavelength, the amplitude, and liquid contact length were found to increase along the flow direction, but decrease with liquid velocity and subcooling. The ratio of the length of the region wetted by the liquid and that occupied by the vapor was found to remain constant in the flow direction for a given subcooling. Photographs of vapor



Figure 4: Photographs of wetting front and interface lift off.

structure, as given in Fig. 5, revealed existence of both wave like and overhanging configurations. The most prominent configuration was the wavelike. The overhanging structures were seen only at higher subcoolings. A model similar to that developed earlier for the short length vertical surface was developed for the longer surface. This model reflected improvement over the previous study of Galloway and Mudawar in that an analytical expression was developed for the heat flux at the interface lift off. The model was validated with saturated low subcooling data.

To understand, explicitly, the effect of heater length on CHF, Gersey and Mudawar [18] continued their photographic and model studies on horizontal plates of 10, 30, and 110 mm in length, flush mounted along one wall of a rectangular channel. They also investigated the effect of plate angle from horizontal to inclined at  $45^{\circ}$  to vertical. It was found that a mechanism similar to that for shorter plates was present for longer plates, except that the distance between wetting fronts or wave troughs increased in the flow direction. This distance was as much as four times the critical Helmholtz wavelength in the

middle of the longest plate and remained constant further downstream. This, in turn, led to a smaller number of wetting fronts on the plate and reduced critical heat flux. The critical heat flux was triggered with the lifting of the most upstream wetting front which was followed by the downstream fronts. No appreciable effect of surface orientation on the phenomena was found. The earlier model of Galloway and Mudawar, when modified to include the reduction in number of wetting fronts, was found to be compare well with their data.

Mudawar and Bowers [19] experimentally investigated critical heat flux in short, small diameter tubes using highly subcooled water. In the experiments, steel tubes with an inside diameter varying 0.406 - 2.54 mm, and length to diameter ratio of 2.4 to 34.1 were used. The tubes were heated by passing D.C. current through them. Water temperature at the inlet was varied from  $18 - 70^{\circ}$ C with mass velocities varying from 5,000  $- 134,000 \text{ kg/m}^2$ s. The outlet pressures investigated were 2.5 to 172.4 bars. The critical heat flux was found to increase with mass velocity, liquid subcooling, and decrease in tube diameter and decrease in heated length to diameter ratio. The critical



Figure 5: Observed vapor structures prior to CHF under subcooled flow boiling conditions.

heat flux initially decreased with pressure up to 30 bars and, thereafter, remained constant with pressure until it decreased as critical pressure was approached. Because of high pressure drops encountered, it was suggested that a proper account for local pressure be made while developing correlations or models. The highest ever reported critical heat flux of 27.6  $kW/cm^2$  was obtained in a 0.406 mm diameter tube with a length of 5.8 mm at a mass velocity of 120,000 kg/m<sup>2</sup>s and water inlet temperature and pressure of 27°C and 160 bars, respectively. A correlation [20] based on the inlet conditions and employing five adjustable constants was proposed,

$$\frac{q_{CHF}}{G_{h_{fg}}} = \frac{C_1 \left(\frac{G^2 D}{\rho_f \sigma}\right)^{C_2} \left(\frac{\rho_f}{\rho_g}\right)^{C_3} \left[1 - C_4 \left(\frac{\rho_f}{\rho_g}\right)^{C_5} \left(\frac{h_i - h_{f,0}}{h_{fg,0}}\right)\right]}{1 + 4C_1 C_4 \left(\frac{G^2 D}{\rho_f \sigma}\right)^{C_2} \left(\frac{\rho_f}{\rho_g}\right)^{C_3 + C_5}}$$
(1)  
where:  $C_1 = 0.0332$   
 $C_2 = -0.235$   
 $C_3 = -0.681$ 

$$C_4 = 0.684$$
  
 $C_5 = 0.832$ 

The above equation was shown to correlate all of the data within  $\pm 20\%$ .

Hall and Mudawar [21] have made a very important contribution to the literature by collecting and assessing 37,544 critical heat flux data points from the year 1949 onward, and covering more than 100 sources. The data are for water flow in uniformly heated vertical and horizontal tubes. It was reported that some of the data in the literature may be inaccurate because the errors that were introduced when the data were transported from the original sources. They identified a lack of CHF data for tubes smaller than 5 mm in diameter and for flow rates higher than  $10,000 \text{ kg/m}^2\text{s}$ . The authors also developed correlations for subcooled flow boiling CHF based both on inlet as well as outlet conditions. The correlation based on outlet conditions was thought to be most suited for tubes subjected to non uniform heat flux. It was claimed that these correlations were superior to the Look up Tables that have been proposed for use in Thermal Hydraulic Analysis of Nuclear Reactors. The correlation based on inlet conditions was similar to eq. (1) proposed earlier, but the five constants had the values:

 $C_1 = 0.0722$  $C_2 = -0.312$  $C_3 = -0.644$  $C_4 = 0.900$  $C_5 = 0.724$ 

and correlated 4,860 data points with an r.m.s. error of 14.3%. The correlations based on outlet conditions was

$$\frac{q_{CHF}}{G_{hfg}} = C_1 \left(\frac{G^2 D}{\rho_f \sigma}\right)^{C_2} \left(\frac{\rho_f}{\rho_g}\right)^{C_3} \left[1 - C_4 \left(\frac{\rho_f}{\rho_g}\right)^{C_5} x_0\right]$$
(2)

where  $x_0$  is thermodynamic equilibrium quality at exit. Equation (2) with constants having the same values as those for correlations based on inlet conditions, was found to correlate all of the data points with an r.m.s. value of 27.7%.

#### SUMMARY

A review of the studies performed at Purdue University during the last 15 years reveals that many fundamental contributions have been made in advancing the art and science of phase change heat transfer. These studies can be sub-divided into three general areas: material processing, microelectronic cooling, and phenomenological studies of subcooled critical heat flux. The Purdue Heat Transfer Group deserves our congratulations and gratitude for its vision, leadership, and seminal research in these areas.

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### CHARACTERIZATION OF FINE PARTICLES VIA ELLIPTICALLY-POLARIZED LIGHT SCATTERING

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#### PREFACE

This short paper is to give an overview of the particle characterization research we have had during the last decade at the University of Kentucky. This work has been a product of several MS or PhD students, who still continue on advancing the field via their research and development applications. Many different particles have been the focus of our attention, varying from pulverized coal to soot agglomerates, from phytoplankton to cotton fibers, from fat in milk to bubbles in process columns, from foam to metallic nano-colloids. The work has been exciting and rewarding, resulted in several papers, presentations, patents, prototypes. And, all started from that wonderful inspiration I found at the view of reddish/yellowish light scattered by the particles emitted from the Purdue smokestack, long gone from the silhouette of the Purdue campus. Yet, it had a lasting impact!

#### INTRODUCTION

When light, or any electromagnetic wave, is incident on a particle, a surface, or any object, it is absorbed, transmitted, reflected, refracted, and diffracted. These interactions are defined rigorously via Maxwell's equations. If a medium is comprised of several objects, the fate of the incident wave within the medium is determined by considering the cumulative interactions. If a series of assumptions can be made, these relatively complex equations can be replaced with simpler expressions of geometric optics. Using these equations, one can write an expression for the conservation of the radiative energy along a given direction (see Fig. 1). In its simplest form, this equation is the familiar radiative transfer equation, the famous RTE, as can be found in many textbooks or monographs [1-3].

In principle, the RTE represents the change of radiative intensity along a line-of-sight, per unit time, solid angle, and frequency. If we consider a beam of radiation propagating through such a medium in the direction  $\Omega$  (see Fig.1), the intensity at a given location is defined as  $I_{\lambda}(\Omega)$ . As the beam moves along, it will lose some of its energy due to absorption and scattering. Mathematically, the reduction of intensity due to absorption and scattering along a distance *ds* are proportional to the incident intensity, and can be expressed as  $-\kappa_{\lambda}I_{\lambda}(\Omega)ds$ and  $-\sigma_{\lambda}I_{\lambda}(\Omega)ds$ , respectively. Here,  $\kappa_{\lambda}$  is the spectral absorption coefficient and  $\sigma_{\lambda}$  is the spectral scattering coefficient, with units of inverse distance, i.e.,  $[m^{-1}]$ . The total loss of radiation energy, known as extinction, is the sum of absorption and scattering. The spectral extinction coefficient is expressed as  $\beta_{\lambda} = \kappa_{\lambda} + \sigma_{\lambda}$ . The fraction of attenuated (extinct) energy due to scattering is known as the single scattering albedo:  $\omega_{\lambda} = \sigma_{\lambda}/\beta_{\lambda}$ [1-3].

The absorbed energy is promptly converted to thermal energy (heat). The scattered energy is redistributed throughout the medium. This scattered energy carries the information about the medium, and if it is quantified properly, it may help characterization of the objects in the medium.



**Fig.1** Schematic to depict the conservation of radiation intensity along a line of sight.

As shown in Fig. 1, absorption (2) and out-scattering (4) account for the losses, and the emission (1) and in-scattering (3) make up the gain terms. Once these terms are tallied, we arrive at the RTE [1-3].

The term "scattering" refers to the combined effect of reflection, refraction and diffraction, and it is basically because of the presence of particles, or any inhomogeneities. If the frequency or the wavelength of radiation does not change via scattering, it is *elastic scattering*. If the frequency shifts during the absorption/re-emission process, then it is referred to as *inelastic scattering*.

The integro-differential form of the RTE is due to the *inscattering* term. For the solution of the RTE, it is necessary to know how different size and shape particles with different material properties may scatter incident radiation. This information either comes from experiments, or by solving the Maxwell equations, as discussed below, as a function of particle shape, structure, wavelength of the incident radiation, and the dielectric constants of the medium and the particles. The results of these calculations yield absorption and differential cross-section for *single scattering*. In the presence of many particles, the cumulative effect of all need to be considered, which is done by solving the RTE.

If particles are several wavelength away from each other, which is as usually the case for most practical situations, then the single scattering effects can be added linearly (via the inscattering term), and with this approach the multiple scattering can be accounted for in the calculations. It should be understood, however, that there is an implicit approximation made here for multiple scattering calculations. The singlescattering calculations are based on a planar wave being incident on a particle. After scattering, the waves emanated from the particle are spherical, but, as they radiate away they become more planar in shape. If the second particle is several wavelengths away from the scattering center, then the results of single-scattering calculations based on a planar wave are valid, and we can predict the behavior of the scattering by the second particle easily. If the particles closer to each other than two to three wavelengths, or if they are touching each other, then we have to solve more complicated expressions via Maxwell's equations to account for this dependent scattering. In the case of agglomerates of particles, the dependent scattering effects need to be considered as rigorously as possible.

It is obvious that by solving the RTE we will be able to account for the effect of scattering by particles on the scattered intensity distribution outside the boundaries of the medium. This means that if we measure the scattering patterns outside a medium, we should be able to determine the size, shape, and structure of these particles following an inverse radiation analysis. Such an inverse approach requires the availability of an extensive database which documents the scattering patterns of different size and shape of particles with different dielectric constants, or the refractive indices. Therefore, a particle characterization methodology requires first and the foremost, accurate solution algorithms to determine the differential scattering cross-sections of different particles. In the following section, we give an overview of different techniques we have developed and used for this purpose. The next step is the design of an experimental system to obtain the most information for characterization of particles. For this purpose, angular profiles of scattered light can be used. However, if elliptically polarized light is employed, more accurate and detailed characterization will be possible. This requires the detection of Stokes parameters as a function of scattering angle, which can be accomplished by using a predetermined set of polarizers and retarders. This approach will allow us to quantify the change in the ellipticity of the polarization of the scattered light, which yield information about the size, shape and structure of particles. Symmetry is always beautiful to observe and simple to use; however, one can obtain much detailed information from asymmetry. The use of asymmetry in elliptically polarized scattering light is the backbone philosophy of our experimental design.

Below, we will first discuss briefly the theoretical and experimental approaches. After that, we will present a series of results for different physical systems and particles.

#### SINGLE SCATTERING MODELS

The single scattering problem is expressed as: Given a particle of specified size, shape and material properties that is illuminated by an arbitrarily polarized monochromatic wave, determine the electromagnetic (EM) field at all points within the particle and in the medium in which the particle is embedded. The field inside the particle is denoted by  $(E_1, H_1)$ ; the field  $(E_2, H_2)$  in the medium surrounding the particle is the superposition of the incident field  $(E_i, B_i)$  and the scattered field  $(E_s, H_s)$ . (See Figure 2.)



Fig.2 Scattering of EM-waves by an arbitrarily-shaped particle.

The EM field obeys Maxwell's equations at all points. Since an arbitrarily polarized wave can be represented by the superposition of two orthogonally polarized plane waves, we need to solve each scattering problem twice, one for the parallel (s) and one for the perpendicular (p) component, in order to determine the scattering patterns. For the analysis, we assume a planar, harmonic wave incident on the particle, which is expressed as

$$\mathbf{E}_{\mathbf{i}} = (E_{//0}\hat{\mathbf{e}}_{//i} + E_{\perp 0}\hat{\mathbf{e}}_{\perp i})\exp(ikz - i\omega t) = E_{//i}\hat{\mathbf{e}}_{//i} + E_{\perp i}\hat{\mathbf{e}}_{\perp i}$$

where  $k = 2\pi n/\lambda$  is the wave number, n is the refractive index, and  $\lambda$  is the wavelength of the incident light in vacuum. At sufficiently large distances from the origin, (kr >> 1), i.e., in the *far-field region*, the scattered electric field  $\mathbf{E}_s$  is approximately *transverse* ( $\hat{\mathbf{e}}_r \cdot \mathbf{E}_s \approx 0$ ) [4]. The relation between incident and scattered fields is conveniently written in matrix form as

$$\begin{pmatrix} E_{//s} \\ E_{\perp s} \end{pmatrix} = \frac{e^{ik(r-z)}}{-ikr} \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} E_{//i} \\ E_{\perp i} \end{pmatrix}$$

The elements  $S_j$  (j = 1,2,3,4) of the *amplitude scattering matrix* depend, in general, on the zenith angle  $\theta$ , and the azimuthal angle  $\phi$ . The real and imaginary parts of the four amplitude scattering matrix elements can rarely be measured for all values of  $\theta$  and  $\phi$ . It is a very difficult measurement at frequencies corresponding to visible light, which are on the order of  $10^{14}$  Hz. Hence, very few such experiments have been performed. However, the amplitude scattering matrix elements are related to quantities that are much easier to measure than phases.

Once the electromagnetic fields inside and scattered by the particle are obtained, Poynting vector at any point can be determined. The Poynting vector is a measure of the energy flux carried by an electromagnetic wave. It is defined as the cross product of the electric and magnetic field vectors:  $\mathbf{P}=\mathbf{E}\times\mathbf{H}$ . Suppose that a detector is placed at a distance  $\mathbf{r}$  from a scattering particle in the far-field region, with its surface  $\Delta A$  aligned normal to  $\hat{\mathbf{e}}_{\mathbf{r}}$ . The detector records a signal proportional to  $\mathbf{P}_s \cdot \hat{\mathbf{e}}_r \Delta A$ . The detector "sees" only the scattered light provided that it does not "look at" the source of incident light [4].

Now imagine an arbitrarily polarized EM wave. The complete polarization state of the wave is expressed via a column vector of the four Stokes Parameters, where the brackets <> indicate the time average [4,5]:

$$\begin{split} \mathbf{I} &= \left\langle \mathbf{E}_{//} \mathbf{E}_{//}^* + \mathbf{E}_{\perp} \mathbf{E}_{\perp}^* \right\rangle \\ \mathbf{Q} &= \left\langle \mathbf{E}_{//} \mathbf{E}_{//}^* - \mathbf{E}_{\perp} \mathbf{E}_{\perp}^* \right\rangle \\ \mathbf{U} &= \left\langle \mathbf{E}_{//} \mathbf{E}_{\perp}^* + \mathbf{E}_{\perp} \mathbf{E}_{//}^* \right\rangle \\ \mathbf{V} &= \mathbf{i} \left\langle \mathbf{E}_{//} \mathbf{E}_{\perp}^* - \mathbf{E}_{\perp} \mathbf{E}_{//}^* \right\rangle \end{split}$$

These four quantities of the scattered light can be measured by a detector. The Stokes parameters of the incident and scattered beams are related via  $4 \times 4 S$  matrix called the *scattering*, or *Mueller matrix* for a single particle [4,5].

$\left[I_{s}\right]$	$(S_{11})$	$S_{12}$	$S_{13}$	$S_{14}$	$\left(I_{i}\right)$
$Q_s = 1$	S <sub>21</sub>	$S_{22}$	$S_{23}$	$S_{24}$	$Q_i$
$U_{s}\left(\frac{1}{k^{2}r^{2}}\right)$	$S_{31}$	$S_{32}$	$S_{33}$	$S_{34}$	$U_i$
$\left[ V_{s} \right]$	$S_{41}$	$S_{\rm 42}$	$S_{\rm 43}$	$S_{44})$	$\left[V_i\right]$

The Stokes parameters of the light scattered by a collection of randomly separated particles are the sum of those of the individual particles. Therefore, the scattering matrix for such a collection is merely the sum of the individual particle scattering matrices. Only the seven of the sixteen scattering matrix elements are independent if we have large number of particles in the medium. Measurement of S<sub>11</sub>, S<sub>12</sub>, S<sub>33</sub>, and S<sub>34</sub> are usually sufficient for characterization of particles with practical interest [6].

The task now is to solve the Maxwell equations to determine the scattering patterns as a function zenith and azimuthal angles, and then to calculate each of the relevant scattering matrix elements. Finally, using these expressions we determine how much energy would be received by a detector at a given angular location. For an elliptically polarized beam, we will be able to calculate the elliptically polarized scattered intensity incident on a detector. That information, after being corrected for multiple scattering effects, can be used to characterize the size and shape of the particles [6,7].

Below, a series of sample results is outlined in terms of  $S_{ij}$  elements for different shape and structure particles. This information will be needed in the inverse analyses, as it will comprise the database to be used for data reduction after carefully conducted experiments.

#### SIJ PROFILES FOR DIFFERENT PARTICLES

The solution of the Maxwell equations is necessary to obtain the  $S_{ij}$  elements discussed above. The best known approach for such a solution is the Lorenz-Mie (LM) theory, which was originally developed for homogeneous spherical particles (see [4,5] for detailed reviews of the LM as well as all other techniques we discuss here). Even though the symmetry of a sphere is quite convenient for modeling efforts, most of the practical particles are not spherical, and for advanced characterization as well as material process applications, the asymmetrical nature of scattering objects need to be accounted for in the calculations.

In modeling non-spherical particles, we first need to visualize how they look, and then determine how they would scatter elliptically polarized light. It is intuitive to construct particle shapes and structures following a bottom-up philosophy, as this will allow a more realistic representation of irregular shaped-particles. To this end, we consider small monomers, each with 20-50 nm in diameter, and construct any shape we need to model. This concept was discussed in depth by Manickavasagam and Mengüç [6], where fractal-like soot agglomerates were constructed. A series of sample structures



**Fig.3** Different structures modeled using volume integral formulation; each sphere depicts a monomer.

considered for this purpose are depicted in Figure 3.

It is important to realize that each monomer that makes up a structure is either touching at least one other, or within a very close proximity of the others. Therefore, straight forward modeling of scattering phenomena as if they are stand-alone, small spherical particles will not produce acceptable results.



**Fig.4** Angular profiles of  $S_{11}$ ,  $S_{12}$ , and  $S_{34}$  elements, respectively, for different-size soot agglomerates, where number of monomers N changes between 20 and 200; as calculated by AGGLOME. Fractal dimension is 1.8, the value of the fractal prefactor is 8.0, and the wavelength is 500 nm (from [8]).

The dependent scattering effects need to be accounted for in the formulation, as done in discrete-dipole or volume-integral approximations (see references [6,8,9] for the extensive literature reviews).

In Figure 4, we depict a series of results obtained for fractal-like agglomerates using the algorithm developed in [6]. Here, we present three Mueller matrix elements,  $S_{11}$ ,  $S_{12}$ , and  $S_{34}$ , respectively. These elements dictate the scattering pattern of an object, and if they are determined from experimentally measured scattering signals, they help in characterizing particle shapes and structures.

The first panel in Fig. 4 shows the  $S_{11}$  contours as a function of scattering angle and N, the number of monomers that make up soot agglomerate [8]. Practically, the  $S_{11}$  is equivalent to the scattering phase function, and it is obvious that the angular scattered-intensity experiments are not likely to vield much information about the structure of fractals. This is more obvious especially when we realize that performing experiments within the forward 10 to 15 degrees is quite difficult, as forward scattered and transmitted components usually difficult to separate. On the other hand, the second and the third panel show clearly that both  $S_{12}$  and  $S_{34}$  have much more detail, and more sensitive to both the N and the scattering angle. S<sub>12</sub> can be considered as a measure of depolarization and S<sub>34</sub> stems from the change in the polarization of elliptically polarized light. Measurements of these two terms are possible only if we use polarized light and change its ellipticity systematically [6]

Fractal agglomerate concept discussed in Fig. 4 is applicable to many structures, including soot agglomerates. On the other hand, in material characterization one faces many different shapes and structures, and these shapes may change during the actual fabrication process. To explore the possibility of detecting these structural changes, we have constructed several different shapes, again using the bottom-up procedure (see examples in Fig. 3) and determined their scattering signatures using the dedicated computer programs [6]. In Fig. 5, S<sub>11</sub>, S<sub>12</sub>, and S<sub>34</sub> profiles are depicted as a function of scattering angle, for an ellipse, a rectangle, a square, and a triangle shaped particles at a wavelength of  $\lambda$ =632 nm [9]. Again, we note that the phase function information cannot be used alone to identify the particle structures; however, a combined analysis of all three S<sub>ij</sub> profiles will allow us to determine the required shapes. We also note that  $S_{12}$  profiles show that sharp-edged particles depolarize radiation more; i.e., (absolute)  $S_{12}$  values for these particles are larger.

Several other approaches have been considered over the years to determine the  $S_{ij}$  elements for different particle geometries, including coated spheres [10] and multilayer cylinders [11], and recently those of bubbles in a homogeneous media [12,13]. In addition, the discrete-dipole approximation of Draine [14] has been adapted for investigation of agglomerate properties for dependent scattering predictions [15,16] as well as for the interpretation of sooty diffusion flames [17,18]. These models, as well as those available from the literature [5], are likely to provide an extensive database for interpretation of future experimental data.

#### **EXPERIMENTAL RESULTS**

In order to detect the fine structural variations of small particles and agglomerates we discussed above, we have developed several nephelometers over the years and the concept was continually improved [6,8,9,19-24]. In most recent attempts, we used elliptically polarized light, where first we had to determine six unique sets of retarder and polarizer settings to make six different and accurate scattering measurements [6,23]. These unique settings are pre-determined following a series of numerical experiments using the available algorithms. After that, the six  $S_{ij}$  elements,  $S_{11}$ ,  $S_{12}$ ,  $S_{22}$ ,  $S_{33}$ ,  $S_{44}$ ,  $S_{34}$  are recovered from the recorded intensities in a numerical inverse analysis.



**Fig.5** Angular profiles of  $S_{11}$ ,  $S_{12}$ , and  $S_{34}$  elements for different structures: 1: ellipse, 2: rectangle, 3: square, 4: triangle [9].



**Fig.6** Schematic of the experimental nephelometer used for cotton-fiber experiments. L: Lens; P: Polarizer; BE: Beam expander; NDF: Neutral density filter; PMT: Photo-multiplier tube; IR: Iris; RS: Rotary scale. [24].



**Fig. 7** Results of calibration experiments: the Lorenz-Mie predictions are compared against the experimental data obtained for circular cylinders: cylinder diameter: 4.005  $\mu$ m; the quartz index of refraction of *m*=1.457-*i*0,  $\lambda$ =532 nm. [24].

Figure 6 depicts the latest version of the elliptic nephelometer, which is discussed in Aslan et al. [24]. These types of equipment are usually calibrated with particles of known properties. In this case, the system was designed for detection of cotton-fiber properties. For that reason, we tested the system using quartz fibers. The detailed results of these experiments are shown in Fig. 7, where the data for a single quartz fiber are compared against the Lorenz-Mie predictions for cylindrical fibers. The agreement is near perfect for all elements, even though only  $S_{11}$  is shown here.

The system was later used to detect the scattering patterns of convoluted cotton-fibers and the data were compared against a finite element method developed by Jun Yamada (see [24]). Figure 8 shows that the agreement is quite satisfactory. These experiments allowed us to establish a relationship between scattering signals and the cotton fineness and maturity [24].

The same system was later modified and used for detection of various metallic nano-particles. These types of particles are usually difficult to model, as they have large imaginary components of the refractive index, and they tend to agglomerate. Figure 9 depicts the TEM images of three different particles considered in the experiments. And finally, Fig. 8 shows the  $S_{11}$  and  $S_{12}$  profiles recovered from extensive experiments [25]. No theoretical comparisons are provided here, as the models are still in development phase. However, the experimental data clearly shows the difference in the



**Fig. 8** Comparisons of single cotton-fiber experiments with the finite element model predictions. Only the phase function profiles are shown. [24].



Fig. 9 TEM pictures for three different metallic particles: For Silver, the scale is 25  $\mu$ m (left) and 10  $\mu$ m (right); for the others, it is 250  $\mu$ m (left) and 1  $\mu$ m (right). [25].

results. It is obvious that by such shape characterization, a material fabrication process can be better understood and improved to achieve the desired structures and size distributions.

#### SUMMARY

In this paper, an outline of our on-going particle characterization research is presented. Even though we believe that the elliptically-polarized light scattering approach we have developed over the years is a robust and accurate characterization technique for fine particles, by no means we claim that this is the only approach available. Neither have we claimed that this paper is an exclusive review of the literature. However, in each paper we referred, the reader will find more detailed and relevant review of the literature.

This approach can be extended to nano-structures if the novel experimental tools can be developed, which is our current research focus.



Fig. 10  $S_{11}$  and  $S_{12}$  profiles measured for the metallic structures shown in Fig. 7. No appropriate theoretical data available yet for comparisons. [25].

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### DEVELOPING THERMAL THERAPIES FOR DISEASE – THE CONTRIBUTIONS OF THE PURDUE HEAT TRANSFER GROUP

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#### ABSTRACT

This paper describes the development of a mathematical model of transurethral microwave ablation of the prostate. The model, based on the Pennes bio-heat equation, accounts for increases in blood perfusion with increases in tissue temperature. Tissue damage is evaluated by computing the value of the damage integral, and vascular shutdown is simulated by an abrupt reduction in the perfusion when a critical value of the damage integral is reached. The various empirical constants in the model are determined by bench-top experiments as well as by measurements of interstitial temperatures in animal models and human patients. The clinical value of the model is demonstrated by its accuracy in predicting interstitial temperatures.

#### NOMENCLATURE

- At Constant of proportionality in equation 2
- c Specific heat
- k Thermal conductivity of tissue
- P Electrical power input to the catheter
- Q Heat generation rate per unit volume in tissue by microwaves
- q" Microwave power flux from the catheter
- r Radial coordinate
- T Temperature
- Ta Arterial blood temperature
- t Time

Greek Symbols

P

$\rho$	Attenuation constant of microwave radiation in tissue
K	Thermal damage rate constant

 $\kappa_0$  Rate constant at the reference temperature of 47.5° C

#### $\Omega$ Damage integral

#### INTRODUCTION

The development of thermal therapies for various diseases represents a substantial and interesting challenge for the heat transfer engineer. While the equations governing heat transfer in engineering materials are well known, much is yet unknown about heat transfer phenomena in living tissue. Nevertheless, the medical community has been experimenting for at least the past two decades with developing heat-based treatments for the destruction of benign and malignant tissue growths in various parts of the human body. To date, the engineering heat transfer community has largely been uninvolved in this development effort. This paper presents a brief survey of opportunities for research in this arena. The contribution of the Purdue heat transfer group in developing a heat-based treatment for one specific disease state is then described in detail.

It is instructive to review the epidemiological data on the incidence of various disease states to gain perspective on the potential beneficial impact of thermal therapies. In the United States, there are approximately 350,000 new diagnoses and 40,000 deaths each year due to prostate cancer [1]; there are 180,000 new diagnoses and 44,000 deaths each year due to breast cancer [2]; half of all men in the U.S. above the age of 50 suffer from the bothersome symptoms of benign prostatic hyperplasia (BPH) resulting in approximately 300,000 surgeries a year [3]; there are 31,000 new diagnoses for renal cell carcinoma and 12,000 deaths each year [4]. Smaller, but still sizable, numbers of deaths are attributable to liver cancer and pancreatic cancer. In each of the foregoing disease states thermal therapies offer the potential of minimally invasive treatments that yield excellent results with minimal postprocedure morbidity.
Thermal therapies are generally based on either heating or freezing the tissue to sufficiently extreme temperatures to cause tissue necrosis. Tissue heating may be accomplished by a variety of minimally invasive techniques including radio frequency or microwave heating, ultrasonic heating, or circulation of hot water. Tissue freezing is usually accomplished by percutaneous insertion of fine probes that are constructed to utilize the Joule-Thompson effect. In addition to these direct tissue destruction techniques, there is now increasing interest in using milder temperature elevation (hyperthermia) as an adjuvant to drug-based or radiation-based treatments for malignant growths.

The development of the heat transfer theory underlying a minimally invasive thermal therapy for BPH will now be presented. This description also serves to highlight the many technical challenges involved in predicting bio-heat transfer phenomena.

#### **PROBLEM DESCRIPTION**

Trans-urethral ablation of prostatic tissue by microwave radiation is now an accepted modality for the treatment of BPH [5]. The procedure involves elevation of intra-prostatic tissue temperatures by means of a microwave-delivery catheter inserted into the prostate via the urethra. Figure 1 shows a cross-sectional view of the Targis microwave catheter (Urologix, Inc., Minneapolis, MN), one of several commonly used types. The catheter contains a microwave antenna surrounded by coolant channels, the latter serving to reduce the temperature elevation of the urethral surface. Thermal energy generation occurs volumetrically within the prostate, resulting in temperature elevation to between 50 °C and 80 °C within the gland, while urethral surface temperatures typically remain under 42 °C due to the circulating cooling water. Since the urethra is not heated significantly, the procedure may be



Fig. 1: Cross Section of the Targis Microwave Delivery Catheter (Urologix, Inc.)

performed with oral analgesia with little discomfort to the patient. The high intra-prostatic temperatures achieved during therapy result in necrosis of a sizable volume of prostatic tissue. Over a period of weeks, some of this necrosed tissue is removed by phagocytosis, while the remainder resolves into a compact fibrotic mass. The resultant reduction in BPH symptoms is both dramatic and sustained.

A satisfactory response to the therapy hinges on accurate control of the microwave power, the coolant temperature, and the duration of the therapy. The objective is to achieve a sizeable zone of tissue necrosis while maintaining the integrity of the urethra, the prostate capsule, and the adjoining section of the bowel. In the currently approved Targis treatment, all patients are treated for the same time duration. This approach does not allow for patient-to-patient variability and is observed to yield wide variations in patient outcomes. Intrinsic factors affecting the temperature field within the gland include the size of the gland, the magnitude of the blood perfusion and its distribution within the gland, and the composition of the tissue itself. While the size of the gland can be measured with good accuracy by non-invasive ultrasound imaging, the blood perfusion and the tissue composition are not easily determinable. Nevertheless, it is important to be able to predict the spatial and time-wise variations of temperature within the gland in order to control the therapy parameters and achieve the desired volume of tissue necrosis.

#### **Initial Modeling Efforts**

The earliest, and most significant, work on mathematical modeling of transurethral thermal therapy was done by Professor Xu and co-workers. Xu et al. [6] presented a onedimensional, transient, finite-difference model of the prostate and compared its predictions to temperature fields measured in a non-perfused, tissue-equivalent phantom gel as well as temperature distributions measured in several canine prostates. A Urologix Targis catheter was employed for microwave The Pennes bio-heat equation was used in delivery. cylindrical coordinates to predict the radial temperature distributions in the cross sections of the canine prostates. Two different, temporally constant, values of perfusion were used in the calculation region. The peri-urethral region was assumed to be much more highly perfused than the parenchymal region of the gland. While qualitative justification for the use of two different values of perfusion was provided on the basis of the vasculature of the canine prostate (see Yuan et al., [7]), the perfusion values themselves were inferred from fitting the model predictions to one of the data sets. In general, the measured and predicted temperatures in the phantom gel were in very good agreement. The level of agreement of model predictions with the canine prostate data cannot be assessed from the reported results, but the authors observed that better agreement with the data could be obtained by allowing the perfusion to increase in response to increases in local tissue temperature. The physiological thermoregulatory response of vasodilation with increase in tissue temperature is well documented.

A two-dimensional, transient, finite-difference model was developed and presented by Yuan et al. [8]. This model, also formulated in cylindrical coordinates, was capable of predicting the variations of temperature both radially and circumferentially in the cross section of the prostate. The model predictions were compared to experimental data obtained in a non-perfused, tissue-equivalent phantom heated with a Urologix T3 catheter. The model was used to predict temperature fields with various assumed distributions of the perfusion. In a subsequent clinical study, the predictions of this model were compared to interstitial temperatures measured in 22 human subjects. The measured steady-state temperature distributions were in qualitative agreement with model predictions (Larson et al., [9]). However, comparisons of the measured and predicted transient temperature variations during the initial part of the therapy were not provided. Thus, the ability of the model to predict the temperature rise in the prostate during the initial heating period was not tested.

#### **Factors Influencing Model Accuracy**

As noted earlier, spatial and temporal variations of perfusion have an important bearing on the temperature distribution in the prostate. The modeling efforts by Professor Xu and co-workers had hinted at the nature of these variations, but no comparisons had been made between model predictions and measured tissue temperatures during the entire course of a microwave treatment. Therefore, although good agreement had been obtained by adjusting perfusion levels to match the steady state temperatures, there had been no attempt to incorporate the thermo-regulatory perfusion response into a predictive model of the tissue temperatures. Such efforts will have to be guided by direct measurements of the changes in blood perfusion recorded during microwave thermal therapy. A promising start in this direction has been made by Xu et al. [10].

Other important factors in developing an accurate predictive model include accurate thermophysical property data on prostatic tissue, accurate knowledge of the specific absorption rate (SAR) of microwave radiation within the volume of the gland, and an accurate treatment of the thermal effects of blood flow in the tissue volume. Among these factors, the SAR distribution is, perhaps, the most readily quantified on the basis of measured temperature elevations in a volume of phantom gel. Analytical expressions for the SAR distribution produced by the Urologix catheter have been developed in this manner by both Xu et al [6] and by Zhu et al. [11]. The thermophysical properties of human prostatic tissue are not well established, but the properties of canine prostatic tissue have been measured by Yuan et al., [12].

The rate of blood perfusion and its thermal effects are the least well understood of the various factors influencing the model. Most prior modeling efforts have been based on the Pennes bio-heat equation that employs a special term to account for the energy inflow and outflow produced by the flow of blood through a volume of tissue. This term depends on the local "rate of blood perfusion" as well as the difference in temperature between the body core and the local tissue. The perfusion is a nebulous concept, and its measurement is difficult. In humans, blood perfusion in the prostate is known to vary widely from person to person. It is estimated that the range of perfusion values encountered in the elderly male population is between 8 ml/min/100 ml and 50 ml/min/100 ml. Various alternatives to the Pennes model have been developed, but it continues to be used because of its relative simplicity and reasonable accuracy compared to more elaborate formulations (Arkin et al., [13]). In addition to the energy inflow/outflow, a more subtle effect of blood perfusion is an enhancement of the apparent thermal conductivity of the tissue. This enhancement, which is the result of the flow of blood in the microvasculature, has received little attention to date, and little information is available to guide model development.

#### **Recent Advances**

In 1999, the present author joined the staff of Urologix Inc. to further develop the modeling effort initiated by Professor Xu. A brief description of these recent advances will now be provided. The most recent model is closely related to the one-dimensional model in cylindrical coordinates developed by Xu et al. [6]. The computational domain is taken to be a long tissue cylinder of radius R, that encompasses the entire prostate as well as a layer of fatty tissue surrounding the capsule of the gland (see Fig. 2). The temperature field is assumed to be purely one-dimensional, i.e. only radial variations in temperature are considered, while axial and circumferential variations are ignored. The model is based on the Pennes bio-heat equation [14]:

$$\rho_{t}c_{t}\frac{\partial T}{\partial t} = div(k \, gradT) - \omega \rho_{b}c_{b}(T - T_{a}) + Q + Q_{m}$$
(1)

In this equation, T is the tissue temperature, t stands for time, k is the thermal conductivity of tissue, c is the specific heat, Q is the rate of heating produced by the microwave radiation,  $Q_m$  is the rate of heat generation due to metabolism,  $\rho$  is the density,  $\omega$  is the blood perfusion rate and  $T_a$  is the arterial blood temperature. The equation reveals that the time-wise variation of the tissue temperature during microwave treatment is dependent on the properties of the tissue (density, conductivity, specific heat), the rate of heating produced by the microwaves, the metabolic heat generation rate, and the rate of heat absorbed by the circulating blood flow. In microwave treatments for BPH, the metabolic heat generated by the microwaves, and it may be discarded from the equation.

The microwave antenna is assumed to radiate as a uniform line source located at the axis of the catheter. The electromagnetic power flux is, accordingly, taken to have the form

$$q'' = A_t P \exp(-2 \beta r) / r^2$$
, (2)

where  $A_t$  is a constant of proportionality, and P is the electrical power delivered to the catheter. The electromagnetic power flux is maximum at the surface of the catheter and diminishes somewhat faster than the inverse square of the radial distance. The value of  $A_t$  is determined from experiments in tissueequivalent phantom gel. The divergence of the power flux yields the volumetric rate of absorption of microwave radiation per unit volume of tissue, i.e.,

$$Q = (2 \beta + 1/r) q''$$
 (3)



Fig. 2: Computational Model of the Prostate

To predict the temperature distribution within the prostate, Equation 1 is solved subject to the appropriate boundary conditions. At the surface of the catheter (which is the inner boundary of the calculation region) the boundary condition is specified by the temperature of the coolant and the "overall heat transfer coefficient," U, between the tissue and the coolant. The value of U is taken to be 750 W/  $m^2$  K. At the outer boundary of the calculation region, which is taken to be so far from the catheter that the temperature elevation there is small, the conduction heat flow rate is assumed to be zero.

#### **Thermophysical Properties**

Thermophysical properties k,  $\rho$ , and c, obtained from various literature sources, are assigned as follows:

In the prostate and capsular layer:

$$\rho_b = \rho_t = 1000 \text{ kg} / \text{m3}, \ c_b = c_t = 3900 \text{ J} / \text{kg K},$$

In the prostate: k = 0.55 W/m K for T < 49 °C, k = 0.42 W/m K for T > 60 °C,  $k = \{0.55 - 0.13 \text{ * } (T - 49) / 11\} \text{ W/m K for}$ 49 °C < T < 60 °C.

#### **Blood Perfusion Values**

Based on measurements in canine prostates reported by Xu et al [10], the values of the blood perfusion are taken to be different in the peri-urethral zone and the parenchyma of the gland. In addition, the perfusion values are taken to be dependent on the temperature of the local tissue. The following expressions define how perfusion values are assigned:

Peri-urethral zone --

w	$= 1.5 * \boldsymbol{\omega}_{base}$	for T $<$ 40 °C	(4a)
ω	$= 2.25 * \omega_{base}$	for 40 °C < T < 43 °C	(4b)
ω	$= 3.75 * \omega_{\text{base}}$	for 43 °C < T < 48 °C	(4c)

 $\omega = 5.25 * \omega_{\text{base}} \text{ for } T > 48 \,^{\circ}\text{C}$  (4d)

Parenchyma	and capsular layer	
$\omega = \omega_{base}$	for $T < 40 \text{ °C}$	(5a)
$\omega = 1.20 * \omega_{ba}$	se for 40 °C < T < 43 °C	(5b)
$\omega = 1.35 * \omega_{ba}$	se for 43 °C < T < 48 °C	(5c)
$\omega = 1.6 * c$	$\theta_{\text{base}}$ for T > 48 °C	(5d)

The quantity  $\omega_{\text{base}}$  appearing in the foregoing expressions is a baseline value prevailing at the beginning of treatment. This baseline value has to be determined either by measurement just prior to treatment or by inference from measured intraprostatic temperatures during treatment. Equations 4 and 5 attempt to mimic the vaso-dilation observed in canine prostates by Xu et al., [10]. As is evident, the baseline blood perfusion values are incremented by various factors depending on the extent of the local tissue temperature elevation.

The perfusion adjustment rules described by Equations 4 and 5 are invoked as long as the extent of local "thermal damage" of the tissue remains below a threshold level. Once the local thermal damage exceeds a threshold value, the local blood perfusion is taken to diminish abruptly as a consequence of shutdown of circulation in the local micro-vasculature. It was found necessary to incorporate vascular shutdown in the model to replicate certain features of the measured temperature variations in human subjects.

The extent of local thermal damage is computed by evaluating the "damage integral"

$$\Omega = \kappa \, dt \tag{6}$$

as suggested originally by Henriques [15]. The rate constant,  $\kappa$ , is taken to vary with temperature according to the expression  $\kappa = \kappa_0 * 10 (T - T_0)/z$ , where  $\kappa_0$  is the value of  $\kappa$  at the reference temperature  $T_0$  (taken to be 47.5 °C),

and z = 6.5 °C. This computationally convenient expression for  $\kappa$  is derivable from the standard Arrhenius expression for the variation of the chemical rate constant with temperature. The threshold value of the damage integral is taken to be 1.2. Once the local damage integral exceeds this threshold, the local value of blood perfusion is set as follows:

Peri-urethral zone $\omega = 1.70 * \omega$ base	(7a)
Parenchyma $\omega = 0.2 * \omega$ base	(7b)
Capsule – $\omega = 0.0012 \text{ s-}1$	(7c)

The essential details of the model are now complete. Since the complications associated with variations in the thermophysical properties and blood perfusion preclude a closed-form analytical solution, a standard, fully implicit, finite-volume, numerical solution scheme is employed.

## PREDICTION OF INTERSTITIAL TEMPERATURES IN HUMAN SUBJECTS

To facilitate an understanding of the Targis treatment protocol, Figure 3 presents the time-wise variations of the microwave power and the coolant temperature during an actual Targis procedure, along with the measured urethral temperature during the treatment. The coolant is automatically maintained at the recommended set point of 8 °C by the control system through on / off regulation of a thermoelectric refrigerator. The small oscillations in the coolant temperature indicate this regulation. The power is gradually incremented by the physician to drive the urethral temperature to its recommended set point of  $40 \pm 1$  °C. Once the urethral temperature is at its set point, the physician makes small power adjustments to maintain that temperature. In Fig. 3 it is observed that the physician employed larger power increments at the beginning of the power ramp and finer increments as the target urethral temperature was approached. Towards the latter stages of the treatment, it is often necessary to decrement the power as the tissue undergoes progressive necrosis and the vasculature shuts down. Such a reduction in power is seen in Fig. 3.

Figure 4 presents direct comparisons of measured and predicted interstitial temperatures in the human subject whose treatment is depicted in Fig. 3. This particular patient was enrolled in a clinical study involving direct measurements of temperature in the prostate during a Targis treatment. Such temperature measurements are not made in routine treatments because they entail invasive placement of temperature sensors in the gland.

The model was run using the actual coolant and power values used in the treatment. With one exception, none of the model constants was adjusted to improve the level of agreement between the measurements and the predictions. The exception was the value of the baseline blood perfusion,  $\omega_{\text{base}}$ . The value of  $\omega_{\text{base}}$  was adjusted by trial and error to obtain a close fit between the predicted and measured urethral surface temperatures (labeled as P\_ur and M\_ur, respectively, in the figures). Once satisfactory agreement between P\_ur and M\_ur was achieved, the model-predicted interstitial temperatures were compared to the corresponding measured values. The agreement between the predicted and measured temperatures is observed to be excellent.

A comment on the adjustment of the value of  $\omega_{\text{base}}$  may be helpful. The Targis catheter contains a fiber-optic temperature sensor to monitor the temperature of the urethra. Accordingly, it is feasible to adjust the value of the baseline perfusion, during an actual treatment, to obtain a match between the predicted and the measured temperature history of the urethra. The value of the predictive model lies in being able to accurately predict interstitial temperatures once the baseline blood perfusion has been established part way through the treatment.



Fig. 3: Variation of Microwave Power, Coolant Temperature, and Urethral Temperature During a Typical Targis Treatment



Fig. 4: Comparison of Measured and Predicted Interstitial Temperatures in a Human Subject --P1, M1 at 4 mm from Urethra; P2, M2 at 9 mm from Urethra; P3, M3 at 14 mm from Urethra, P\_ur, M\_ur are Predicted and Measured Urethral Temperatures

#### **DISCUSSION AND CONCLUSIONS**

The development of a mathematical model of transurethral microwave ablation of the prostate has been described. This model, which has been developed over a period of about a decade by researchers closely associated with the Purdue heat transfer group, includes the best available representations of the variations of thermal conductivity and blood perfusion as functions of the local tissue temperature and the extent of thermal damage. These functional representations are based on experimental data collected in canines as well as from interstitial temperature mapping studies in human patients.

The ability of the model to accurately predict interstitial temperatures is clinically valuable. The model provides the physician with the ability to adjust the treatment power and duration on a patient-specific basis to achieve optimal therapy temperatures and tissue destruction. With the implementation of this model it is expected that outcomes from the Targis treatment will be better controlled and will display greater uniformity from patient to patient.

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## SMART BLENDING: FUNCTIONAL FINE-SCALE STRUCTURES FORMED BY INTELLIGENT AGITATIONS IN MULTI-COMPONENT MELTS

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#### ABSTRACT

In viscous melts, turbulence often does not arise. Consequently, opportunities exist for controllably organizing melt components into functional structures that can have very small feature sizes. In this paper, concepts and results of smart blending are described. Smart blending entails the controllable development in situ of a variety of fine-scale structures by intelligently agitating melts. Once formed, structures are captured in applicable products by extrusion and solidification. Chaotic advection is an enabling recent sub-field of fluid mechanics for smart blending since it provides a means to stretch and fold melt domains and evolve a multi-layer structure leading to derivative arrangements, or indirectly manipulate solid additives. Applications include the production of plastics with enhanced mechanical properties, electrically conducting plastics and glasses, barrier films, and nano- and molecularscale composites.

#### INTRODUCTION

When engineers develop new processes or materials, they draw from existing knowledge and experience. Plastics are an interesting example. During the last century, it became possible to synthesize a wide variety of polymer molecules with specific characteristics. Some of these polymers were thermally stable and nonreactive. As such, they could be heated to a liquid state and extruded or pressed into desired shapes. Their high molecular weight, however, posed processing challenges. Melt viscosities were typically one-million times greater than the viscosity of water. Consequently, in order to make use of polymers to make plastic products, engineers enlisted equipment originally intended in the 1800s to convey viscous soap and grains [1]. This equipment incorporated a helical shaft (i.e., or screw) inside a cylindrical barrel. By heating the barrel and rotating the screw, polymer pellets were melted and conveyed. It is recognizable today as a screw extruder to many engineers and has become one of the most commonly used manufacturing devices.

In modern times, the majority of plastic products consists of two or more polymer types and may also include additives. Particulate or short fiber additives are used for internal reinforcement or to improve electrical or thermal conductivity, for example. Like any composite material, the physical properties of polymer blends and polymer composites are strongly dependent on the structural arrangement of the components. In this regard, it is interesting that the basic configuration of screw extruders offers little means to controllably develop desired structures, or morphologies, in polymer blends or among solid additives. Nevertheless, the synthesis and processing of polymeric materials is a notable achievement of the past century. Plastics have become common materials and have underpinned advances in diverse fields.

It is time to think anew about polymer blending. New smart blending machines can now be constructed in which blend morphology develops more controllably in response to applied intelligent agitations. Smart blending is enabled by work done in 1984. H. Aref did some independent thinking and articulated in a seminal paper [2] the potential importance of what had been regarded as rather strange fluid motion. When a Lagrangian perspective is taken and in consideration of dynamical systems theory, he noted that the equations of motion for passive markers in a fluid can produce nonintegrable (i.e., chaotic) dynamics. An unsteady flow field is required for flows restricted to two spatial dimensions, whereas chaotic dynamics can occur even in steady, three dimensional flows. This type of fluid motion was appropriately dubbed, *chaotic advection*.

Chaotic advection has been used primarily to elucidate mixing mechanisms and also to enhance mixing of viscous fluids [3]. With this application in mind, the term chaotic mixing has become widely used [4]. Investigators studied almost exclusively patterns formed among passively advected particles or in blobs that were identical to the major component fluid except for color or another passive identifier. To simplify experiments and analyses, flows were often confined to two spatial dimensions or only deformations in small circular blobs were considered. Striations patterns ensued. These had little relevance to polymer blending where melt domains are typically stretched to sheets and interfacial tension and component viscosity differences exist. Moreover, the linear character of striations strongly limits the variety of derivative shapes that can be obtained. For example, a droplet might be extended to a filament, but only droplets can be obtained from its subsequent breakup. As will be shown, the situation is much different if initial minor component bodies are converted to multiple layers.

Although chaotic advection refers specifically to passively advected particles in a fluid, very important characteristics of blending become evident when the aggregate motion of a cluster of particles is considered. A cluster becomes stretched and folded to give patterns denoting horseshoe mappings or baker's transformations. The stretching and folding can occur recursively such that initially large clusters become converted to numerous layers of very small thicknesses. Stretching and folding are very relevant to polymer blending. Due to very high viscosities, refinement due to turbulence effects is not possible. Instead, present day processes attempt to refine polymer components by deforming and reorienting them in response to complex flows in screw extruders. Chaotic advection now allows more controllable refinement in devices of simpler construction [5-8]. It has been used to create a variety of blend morphologies with less restrictions on composition [9]. Because morphology development can be controlled, structureproperty optimizations can be readily done [10,11]. It has also been used to build in situ particle networks to render plastics electrically conducting [12,13]. This line of inquiry has been recently characterized as a new area of chaotic advection research that may hold particular promise [14].

#### METHODOLOGY

A conceptual representation of a smart blending device (SBD) is given in Fig. 1 [8]. The SBD consists simply of a cylindrical barrel and two internal rods. Separate melt flows of polymer A and polymer B enter the device. These can be supplied from metering pumps to ensure a steady polymer flow which are in turn fed from present-day extruders. Chaotic advection can be induced by rotating each rod alternately and periodically. Careful selection of the rotational displacements, rod positions, and other design aspects are necessary for effective performance. Many other physical configurations and rod rotational protocols are possible. These can be estimated from computational simulations of passively advected particles [3,15]. The goal of such studies is to determine component

arrangements and operating procedures such that chaotic advection occurs throughout the smart blending device volume and differences in local stretching rates are minimized. The polymer melt streams of Fig. 1 are initially distributed and flow along the rods. Refinement and reorientation occurs in response to chaotic advection. Thick layers are stretched and folded to give thinner, more numerous layers as the combined melt flows move toward an extrusion point. The amount of refinement depends on the melt residence time and rod rotations.

Instead of small flow clearances associated with screw extruders, comparatively large spaces exist in SBDs in which physically expansive structures with small scale features can evolve. For example, both polymer component melt streams in Fig. 1 are converted to layers that are expansive within their individual planes but can be very thin. The number and thickness of individual layers can be regulated through process control. The layers, while of great practical importance, also are parent structures to other morphologies. Interfacial instabilities arise among the layers leading to morphology transitions and the formation of a variety of derivative morphologies in sequence. Interestingly, by creating physically expansive and numerous multiple layers, a morphology transition that occurs at one location also generally occurs at all other locations having the same degree of layer refinement. Moreover, transitions proceed interactively so that structure uniformity can be promoted. Such progressive morphology development [7] is in stark contrast to existing blending processes where morphology development is localized and transitory. Structure in these processes is broken down instead of evolved. As such, the processing conditions of Fig. 1 offer new opportunities for more controllably creating structures in viscous melts.



Fig. 1 Conceptual representation of a smart blending device.

SBDs receive inputs from computational multicomponent flow models. Modeling morphology development in these devices is challenging due to rapid reductions in length scales and interfacial interactions. As will be shown, layers can develop with thicknesses of only tens of nanometers. Consequently, molecular scale effects such as van der Waals interactions and thermal vibrations in the melt can become important in addition to shear stresses, interfacial tension, and non-Newtonian behavior such as viscoelasticity and shear thinning viscosity. Real-time simulations for process control are currently only possible for early morphology development or for assessing rod motions that give effective chaotic advection conditions.

Multicomponent flow models are implemented currently in parallel with experimentation with SBDs to elucidate progressive morphology development and morphology transitions. For computational approaches, the lattice Boltzmann method (LBM) is computationally efficient for low Reynolds number flows [16] applicable to smart blending. Unlike continuum-based approaches and a Eulerian viewpoint, the LBM is based on the kinetic theory of gases and has also been developed heuristically with cellular automata as a guide [17]. When a sufficiently large number of particles are considered and physically appropriate constraints are placed on their interactions, the LBM correctly represents real fluid motion. It has proved effective in tracking complex morphology changes applicable to smart blending devices [18]. As a new computational fluid dynamics method, restrictions on model parameters such as component viscosity ratio and interfacial tension currently exist. Volume-of-fluid methods [19] for interface tracking and continuum surface force representations [20] for interfacial tension have also been used to study simpler morphology transitions and minor component body interactions in chaotic advection [21-23].

#### **NOVEL POLYMER BLENDS**

In conventional blending processes, polymer components are deformed uncontrollably into disorganized cylinders and sheets often of small spatial extents. The variety of derivative shapes that are obtainable from their breakup is limited. A key concept in smart blending is to instead organize components into alternating layers. As shown in Fig. 1, an alternating layer morphology is a natural consequence in SBDs which make use of chaotic advection. An example is shown in Fig. 2 of very thin and numerous layers in an extruded 500 micron thick film composed of 20% by volume ethylene-propylene-diene terpolymer (EPDM) and polypropylene (PP) [24]. Individual layer thicknesses are about 100 to 200 nm. Several thousand layers were present. Similar layered morphologies have also been formed in extruded 2.5 mm monofilaments where processing conditions were identical except for differences in dies. Details of processing conditions have been described [8].

Instabilities that seek to reduce interfacial area in blends such as the one shown in Fig. 2 can give rise to a variety of derivative morphologies. These can initially retain the very small dimensions of the parent layer thicknesses. By inspecting scanning electron micrographs of blend specimens, insights have been gained of how morphology transitions occur. Continued layer refinement as melt moves toward an extrusion point (Fig. 1) leads eventually to the formation of holes. *Significantly*, if the number of layers is large, changes that occur at one location are also likely to occur at other locations in a multi-layer morphology. Holes thereby form and grow interactively to inherently promote morphology uniformity. The idea of organizing melt components into layers to controllably yield a variety of derivative morphologies constitutes a new approach for making structured materials.

Progressive morphology development due to the growth and interaction of holes has been studied computationally. Results from a LBM simulation are shown in Fig. 3 [18]. Beginning with a periodic array of holes in a periodic arrangement of layers resembling those in Fig. 2, distinct and important derivative morphologies are obtained in sequence. In these simulations, the major component flowed into enlarging holes and caused their source layers to thin. Bulbous regions in



Fig. 2 Polymer melt streams can be controllably converted to numerous thin layers such as these in extruded 500 micron films composed of 20% by volume EPDM and PP.

the minor component enlarged and became closer. The minor component penetrated the thinning major component layer. An interpenetrating blend morphology resulted. Oriented fibers were finally obtained when neck-like regions pinched off by capillary instability. Either morphology can be captured in extrudates where chaotic advection is used to form shapes progressively. Fiber diameters are related to the initial layer thicknesses so that plastics can be produced with an abundance of internal reinforcements. Interpenetrating blends find application in electrically conducting plastics and tough plastic materials due to mechanical interlocking associated with dual phase continuity, among other uses. Results depend chiefly on volume composition and component viscosity ratio C . For 0.3 < < 0.5 and 1 < C < 10, computations indicated that these morphology transitions are applicable. Outside these ranges, other morphologies can arise.



Fig. 3 Interactive hole growth in multiple layers leading to the formation of interpenetrating blends and fiber morphologies.

Interpenetrating blends and fibrous morphologies of LBM simulations such as shown in Fig. 3 have been observed in experiments [5,6,9,11,25]. An example of an interpenetrating blend is given in Fig. 4 where a polystyrene (PS) component has been removed by dissolution in a solvent to expose an interconnected structure in a low density polyethylene (LDPE) component. In Fig. 5, LDPE fibers are shown in PS. Commercially important blend morphologies with single phase continuity, encapsulated structures, thin platelets, and very small droplets have also been documented experimentally. LBM simulations have similarly elucidated how morphology

transitions for these occur. Their characteristic dimensions are directly related to the thicknesses of parent layers. As such, very fine-scale structures are producible where very thin layers can be formed. For example, where interfacial tension is small and viscosity ratio is about unity, instabilities leading to layer breakup occur only after layers become very thin. In such polymer combinations, the production of nanoscale shapes in blends is possible [24].



Fig. 4 Example of an interpenetrating blend resulting from interactive hole growth in multiple layers of polyethylene and polystyrene.



Fig. 5 Low density polyethylene fibers formed in polystyrene from a parent multi-layer morphology.

#### **MOLECULAR- AND NANO-SCALE COMPOSITES**

The multilayer morphology of Fig. 2 incorporates a very large interfacial area on the order of  $10^6 \text{ cm}^2/\text{ml}$ . Opportunities are available to organize additives onto the many internal interfaces to create molecular layers and supramolecular structures among molecules influenced by non-covalent interactions [24]. Although the extent of this potential awaits further study and can make use of specially synthesized molecules, an example is provided that has relation to current practice. In present-day compounding steps, co-polymers are sometimes added to reduce interfacial tension between polymer components and thereby allow smaller structures, most often droplets, to form. Interfaces are stabilized, for example, as an individual block seeks preferentially the polymer component in the melt for which it has greatest miscibility. As such, orientation along the interface occurs. This orientation mechanism can be promoted when melt domains are intermingled by chaotic advection such that numerous and expansive thin layers evolve as in Figs. 1 and 2. In effect and in contrast to common blending, the processing method and molecular characteristics act together to create spatially expansive structures with small internal dimensions. Both molecular scale layers at interfaces and very thin layers of the melt components form so that multiple small scales exist.

This effect is shown in Fig. 6 [11] where blends of LDPE, ethylene vinyl hydroxide (EVOH), and maleic anhydride graftpolyethylene (MA) were organized into layers by smart blending and extruded into 500 micron-thick films. In the left panel of Fig. 6, a film with no MA is shown that consisted of numerous thin EVOH sheets and platelets with thicknesses ranging from about 0.5 to 2 microns. The unique folded morphology was reflective of the chaotic advection used to produce it. In the right panel of Fig. 6, the addition of MA at the EVOH – LDPE interface resulted in a much finer structure with EVOH layer thicknesses below 500 nm. Differential scanning calorimetry tests on EVOH/LDPE film samples indicated that the degree of crystallinity was larger in films containing thinner layers. Molecular orientation, as indicated by higher crystallinity, was promoted upon solidification by confining the melt components to multiple thin layers. Because permeants move more readily through amorphous regions, lower oxygen permeation rates were correlated with smaller layer thicknesses. Higher permeation rates were measured, however, for the EVOH/LDPE/MA films despite the reduced layer thicknesses. Although layer thicknesses were smaller, the intrusion of graft molecule chains into the adjacent thin EVOH layers may have hindered crystallization and increased intrinsic mass diffusivity in the EVOH. Results demonstrate that smart blending is an effective method for producing high barrier (i.e., low permeation) films without the complications inherent in coextrusion now used.



Fig. 6 Formation of thin layers by the placement and orientation of maleic anhydride graft polyethylene at EVOH/LDPE interfaces formed by smart blending.

Because of their very small size, it is impractical to directly manipulate large numbers of nanotubes or other nano-scale additives to produce functional structured distributions for commodity products. Smart blending offers a means to indirectly manipulate additives with nano-scale dimensions to form a variety of structures. An example is shown in Fig. 7(a) of single wall nanotubes (SWNTs) oriented in a PP matrix [24,26]. Internal arrangements among the SWNTs were revealed by fracturing specimens following immersion in liquid nitrogen. Samples were produced with a batch smart blending device [15] in lieu of a continuous smart blending device so that only small quantities of SWNTs were required. The SWNTs were initially concentrated within a cluster occupying a one-quarter sector of a 5 mm high by 5 cm diameter device cavity. Domains were stretched and folded as depicted in Fig. 1 to yield a layered morphology of PP and SWNT-rich PP. Their confinement within layers of decreasing thickness induced the orientation shown. More nanotube rows can be produced by

increasing the SWNT concentration. Although a subject of ongoing work, differences in affinities for polymer components may allow additional opportunities to localize nanotubes within the variety of shapes obtainable in blends.



Fig. 7 Orientation of nano-scale solid additives in polypropylene: (a) exposed ends of single wall nanotubes aligned within a layer for matrix reinforcement; (b) clay platelets arranged into layers for low permeation films.

A relatively new and cost-effective method for producing packaging materials that have high barrier properties involves the addition of inorganic materials to plastics. Such materials can find application in food packaging and beverage containers. Clay is currently being investigated since it consists of very thin (10 nm) platelets having high frontal area. It is currently dispersed in plastics by using screw extruders. Random distributions result that provide diffusion pathways around platelets. Barrier properties in such situations are only marginally improved at preferred small loading levels. In Fig. 7(b), clay platelets were concentrated by smart blending into layers so that distances between individual platelets were reduced and diffusion pathways were significantly impeded [27].

## PERCOLATION AND ELECTRICALLY CONDUCTING PLASTICS

In conventional compounding methods, electrically conducting plastics are often produced via addition of a conducting powder consisting of carbon black or metallic particles. A conducting state is attained at a percolation threshold where the particle concentration is sufficiently high to give abundant contact points by random encounters among particles. In smart blending, percolating structures among particles are instead constructed in situ [12,13]. As such, conducting plastics can be produced with much smaller additive concentrations. This capability is quite important since additives increase costs, reduce processability by raising melt viscosity, and can degrade the desirable characteristics of the host plastics. Moreover, a variety of electrical properties can be deliberately imparted.

An example of the internal structure of a conducting plastic that was produced by smart blending is given in Fig. 8 where carbon black was used [28]. By concentrating the carbon black within one polymer melt stream (i.e., in a 'masterbatch') of Fig. 1, the initial positions of nearby carbon black particles diverged exponentially fast over time as an outcome of chaotic advection. The masterbatch was converted to long striations with the filamentary features in Fig. 9(a). Both the number of striations and their filamentary features in Fig. 9(b), or branches, increased in number and length depending on the specified melt residence time and rod motions in the smart blending device (Fig. 1). Electrical current flow was provided along the striations and also between them via the branches. The formation of branches in striations is an outcome of sensitivity to initial conditions, or in this case, sensitivity to initial locations of particles in the masterbatch. Such behavior is a defining characteristic of the chaotic advection used to implement smart blending. The development of striations and the growth of filamentary features are controllable and repeatable features via selection of process parameters. As such, a variety of electrical properties can be more deliberately imparted to materials produced. Properties and structure characteristics are reproducible since chaotic advection for a particular set of process parameters provides a consistent template for structure formation. However, sensitivity to initial locations necessarily causes the precise particle locations among various extrudates to differ. Such differences have no practical importance since the overall characteristics of the resulting composites are identical.

#### **CLOSING REMARKS**

Chaotic advection and a growing understanding of multicomponent flows provide a basis for reconsidering how blending is performed. It seems probable that smart blending devices will become available to intelligently agitate melts so that desired internal structures among material components can be more deliberately formed. With such devices, an ability to impart desired functionalities to manufactured products will be possible. Blend morphology will be selectable via a computer keyboard in lieu of the often present-day approach of trial-anderror. Smart blending devices may find application to any material that can be processed in a viscous, fluid-like state such that turbulence does not counter structure development. As suggested by examination of Fig. 1, multi-component flow modeling, rheology, instrumentation and control, machine design, polymer science, chemistry, heat transfer and many other topics are pertinent. Opportunities for investigators to make important contributions are manifold.



Fig. 9 Conducting networks formed in carbon black at a concentration of 3% by weight: (a) striations throughout film cross-section, (b) appearance of interconnections by branches between striations.

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### THERMAL SYSTEM DESIGN AT THE UNIVERSITY OF KANSAS

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#### ABSTRACT

The development of a capstone thermal-fluid system design course in the Department of Mechanical Engineering at the University of Kansas is recounted. Next, a rearrangement of courses in the design sequence after that development is described. Finally, the need for flexibility in the definition of "design" in order to accommodate the new biomechanics interest of the department is discussed.

#### INTRODUCTION

It has long been recognized that research, in the words of Wickenden [1, p. 386],

"... transforms the atmosphere of a college from that of a glorified sort of schoolhouse to a place where real things are happening.... An engineer is a man who spends his life in solving problems. He can best learn this art as a disciple, under men actively engaged in solving problems. I mean real ones, and not just exercises in the back of a book."

Design has a similar importance in the minds of many educators and accreditors, although its definition is less sure. As Sabersky [2] wrote in connection with accreditation requirements,

"Now originally, I am sure, design simply meant "machine design" or "mechanical design" and it was typically a required course in a mechanical engineering curriculum. When the need for diversity and flexibility became evident it was realized that a course in "Machine Design," important as such a course may be, was not necessarily the right thing for every mechanical engineering student. The word design, however, carries a lot of tradition and even magic and there was great reluctance to remove it from the curriculum. Rather than dropping the word design entirely, therefore, design was redefined in a broad and rather complex manner. The definition is in fact open to a rather wide range of interpretations."

Because of these views, realistic problems have been a staple of engineering education for decades. Professional consulting, industrial experience and interaction, and research enable engineering professors to identify problems; involving students in contriving solutions is the final step.

The accreditation requirements of the Engineering Council on Professional Development (ECPD) in the 1970s included one-half year of engineering design without further specification. Beginning in the 1980s, the Accreditation Board for Engineering and Technology (ABET) further specified that there must be at least one course that was primarily design, preferably at the senior level, and listed open-ended problems as an important characteristic of the design component of a curriculum. To meet this requirement, design courses, often termed "capstone", of integrative nature to draw on all of the skills learned in prerequisite courses were added to many mechanical engineering curricula.

Opinions about these new requirements were mixed. On one hand, as discussed by Wesner [3], the "capstone" design course was thought of for the senior year because the most integrative experiences come when students have most of the skills and tools that are needed to prosecute the design process. Still, he opined that design experiences should appear throughout the program because one is always taken aback by new situations, and the design situation should not be sprung anew on even a senior. On the other hand, Sabersky [2] believed the design experience is most efficiently and effectively learned on the job in professional employment.

In the following, the creation in the 1980s and instruction of a thermal-fluid capstone design course in the Department of Mechanical Engineering at the University of Kansas will be recounted. Next, a rearrangement of courses in the design sequence after that development is described. Finally, the need for flexibility in the definition of "design" in order to accommodate the new biomechanics interest of the department is discussed.

#### BACKGROUND

At the University of Kansas in the post-WWII period, the Department of Mechanical Engineering had a curriculum that included one senior-level course devoted to design, usually of some sort of machine, always taught by the same professor. A laboratory emphasizing measurement of the performances of compressors, internal combustion engines and so forth was also always taught by the same professor. Shop and foundry experiences were provided in the separate Department of Metallurgy and Materials Engineering, mostly by instructorlevel members of the faculty; the machine tools were available to undergraduate students, many working on projects.

In the 1970s the Department of Mechanical Engineering incorporated the former Department of Metallurgy and Materials and shop instruction was drastically reduced. Equipment remaining from a WWII program to train machinist mates for the United States Navy was used to provide a machine shop capability for the entire School of Engineering and a low-level machine-tool course for undergraduate mechanical engineering students. The laboratory course then emphasized measurements, rather than determination of machine performance. This pattern of adjustment to changed circumstances continued.

In the late 1960s, the School of Engineering started NASAfunded Master of Engineering and Doctor of Engineering programs that emphasized design and project management. The intent was to produce graduate-degree holding engineers who were able to function as members and leaders of design teams. Because only two of the five departments had Ph. D. programs and they were research oriented, these two programs were interdisciplinary so that the faculty and students of the entire School of Engineering could participate.

Through the 1980s and 1990s, the Department of Mechanical Engineering participated in a program funded by the U. S. Department of Energy to establish an Energy Analysis and Diagnostic Center at each of several universities to perform energy audits for regional manufacturing plants. A team of undergraduate and graduate engineering students under the leadership of an engineering professor would gather information at a manufacturing plant in the course of about a day. Their suggestions for reducing the amount of energy used to accomplish the manufacturing task were conveyed in a written report. In many instances, designs for energy management schemes were proposed and evaluated by the students. An energy management course was developed to support this program. To meet the ABET design requirement of the 1980s, two measures were taken. The first was to revise many of the required mechanical engineering courses to include a special design problem of about one-week duration. The second was to require a capstone thermal-fluid design course, ME 656 Thermal Systems Design II, additional to the mechanical design course that had long been required, both to have a semesterlong design project as a major component. The mechanical design course continued to emphasize the design of components, usually mechanical ones. The new ME 656 Thermal Systems Design II course emphasized the design of systems, usually thermal-fluid ones. After instituting these two measures, the Department of Mechanical Engineering received the maximum 6-year accreditation from ABET, compared to the 2-years-and-a-visit outcomes of several prior inspections.

ME 656 Thermal Systems Design II was first taught to a pilot group of 2 graduate students in the fall semester of 1987. This was done to assess the adequacy of preparations for support of the design projects as well as the adequacy of the time allowed for other activities. The textbook and its end-of-chapter problems, computer programs for thermal-fluid system simulation, computational fluid dynamics, and multi-dimensional optimization, reference materials in the School of Engineering library, and several design project topics were tried by and on the graduate students in the pilot group. Enrollments were 10 in the spring semester of 1988, 18 in the fall semester of 1988, and 71 at the peak in the spring semester of 1993.

#### PREPARATION FOR CAPSTONE DESIGN COURSE

Preparation for a capstone thermal-fluid design course began in detail as experience with the pilot group was accumulated. To support the thermal-fluid system design project that was the centerpiece of the course, it was found to be necessary to devote 40% of the course to adding to the information acquired by undergraduates in foregoing courses. The textbook by Stoecker [4], then in the first edition, was used. It was the only one then available, although others [5-8 – the most recent editions are cited for the convenience of the reader] were published later. Although Stoecker offered a good combination of some thermal-fluid design project topics, end-of-chapter problems, basic engineering economy, and basic optimization, it still required extensive supplementation.

It became apparent that the supplemental information would be more effectively imparted if it were incorporated into a textbook for each student to read at his convenience, reducing note taking and easing presentations. Materials that had been gathered, both during the prior 22 years of consulting, researching, and teaching at the University of Kansas and developed with the pilot group, were assembled into a draft for a textbook [9] that was adopted upon its publication. The information was largely taken from other sources in order to present the wisdom of the group, rather than the idiosyncrasies of an individual. Major supplemental topics and the typical number of periods in a semester of 16 weeks plus a 3-hour final exam period were (1) conceptual design and techniques for stimulating it - 3, (2) thermal-fluid equipment - 5, (3) financial figures of merit for competing projects - 4, (4) methods for optimal selection of design parameters - 3, (5) methods for assessing the reliability of a design - 3, (6) product liability and safety - 2. Of course, the details of the supplemental information depended upon the design project for that semester.

The final chapter of the textbook [9] is an illustration of the prosecution and reporting of a typical semester-long, thermal-fluid system design project. The intent of that chapter is more to provide the student with an example of how a design process can unfold, to be read at the student's convenience, than to provide the instructor with a series of presentations.

#### ADMINISTRATION OF CAPSTONE COURSE

Design project topics were developed in consultation with practicing engineers and technologists so that data would be realistic and resulting designs would be practical. Some past topics for ME 656 course system design projects are:

- (a) Use of the Tonganoxie aquifer in a seasonal thermal energy storage scheme to help meet the heating and cooling needs of the University of Kansas campus – consider tree farms, cogeneration, energy from municipal waste, solar energy, and so forth in combination
- (b) Use of the Ogallala aquifer to help meet the heating and cooling needs of a commercial building in Dodge City, KS in a seasonal thermal energy storage scheme – consider evaporative cooling, regenerative energy storage in rock beds, cogeneration, wind and solar energy, and so forth in combination
- (c) Utilization of a blanket of inert gas to enable grain to be dried and stored on the producer's property for a period of at least two years – consider vacuum drying, microwave heating, cogeneration, and so forth
- (d) Recovery or disposal of the solvent vapor from a process in which gold foil is affixed to paper (the vapor is incinerated now) – consider absorption, condensation by compression plus refrigeration, regenerative preheating of combustible air-vapor mixture, and so forth
- (e) Reduction of the costs of cement plant energy and dust removal from its exhaust – consider solar energy (perhaps a laser beam from a geosynchronous earth-orbiting satellite) as an energy source, quenching effluent gases by evaporation of a water spray, storing heat in rock beds by regenerative heat exchange, and so forth
- (f) Use of heat pumps to assist clothes driers optimally select parameters to meet specified loading conditions, utilize continuous rather than batch processes, and so forth
- (g) Improvement of the energy efficiency of an industrial laundry – consider solar energy, regenerative heat recovery, use of heat pumps to recover heat from humid exhaust air, microwave heating for driers, counterflow washers, and so forth.

Design of a component, really just a small system, can also be undertaken, of course. McCoy [10] provided an example of such a topic that can be obtained from the engineering work place:

(h) A pump to purge non-condensable gases and water vapor from the condenser of a distillation assembly – consider a peristaltic pumping mechanism among others, account for heat flow from the environment and the motor, and so forth. While supplementation in elements of each of the six topical areas listed previously was indispensable, a satisfactory base for understanding the information needed to address one of these project topics had been obtained in prerequisite science and engineering science courses, for the most part. However, the use of computer programs for system simulation (TRNSYS [11]), computational fluid dynamics (FLUENT [12]), and optimization (Design Optimization Tools [13]) was new to each student.

Each class was divided into design teams, all working on the same design topic so that the instruction given to one would apply to all. The number, between four and 10, of student members on a team needed to be large enough that working with and coordination of a group was experienced, but small enough that each member had to make a substantial contribution. Each team submitted a description of its design in a written report that included, in addition to the common features of a report, a description of a simulation of the unsteady performance of the system, optimal selection of system parameters, and a computational fluid dynamics evaluation of some aspect of the system.

Each team made five oral presentations. The first presentation described the team organization along with the schedule for project activities. The second and third presentations were of progress and difficulties encountered. The fourth presentation, made during one of the last days of the semester, was of the written final report of the design for the project. Shortcomings of this report were pointed out in a written critique. The fifth and final presentation during the final examination period was of revisions to the design and report to meet adverse criticisms. The instructor's suggestion that teams work on different solutions to the same design problem to ease comparison of alternatives was never adopted.

The semester grade for the course was based on homework (30%), oral presentations (10%), and final report (60%). The homework comprised end-of-chapter problems from the textbook, computer program familiarization exercises, and short problems contrived to illustrate application of information and techniques to the design project.

Limiting the time spent by a student on design projects in a semester required special arrangements. The ME 656 course was scheduled for the fall semester while the mechanical design course was scheduled for the spring semester. And, the ending point of a design team in one semester was often used as the starting point for a design team in the succeeding semester.

#### REARRANGEMENT OF THE DESIGN SEQUENCE

Assessment of the success of an educational scheme should be done with consideration of the thought, said by Hinton [14] to be due to Sir Charles Inglis (professor of engineering at Cambridge University),

"The spirit of education is that habit of mind which remains with the student long after he has forgotten everything that he has been taught."

Boelter [15] thought that such a state occurs about 25 years after graduation. The specific accreditation requirements imposed by ABET for design might have strayed from this 52

thought as excerpts from a paper by Sabersky [2] illustrate. He wrote,

"..., for the education of a present-day-engineer a flexible curriculum would be most suitable. A flexible curriculum which requires a group of fundamental courses and which would teach the student not only certain subjects but also teach her or him how to learn by her or himself and how to absorb new knowledge on her or his own initiative .... Unfortunately as just pointed out, the engineering accreditation process in the last 10 or 15 years has become more rigid rather than more flexible. This trend has been particularly evident in the attitude toward the requirement of "design."... The only thing that is definite in the view of the accreditors is that whatever design means, it is required, and the equivalent of  $\frac{1}{2}$  years of an engineer's education has to be devoted to design. This requirement has been a major cause of trouble for many schools who are attempting to develop forward-looking course programs..., and an even more inflexible policy has been adopted which now requires in addition that each program contain a course -- preferably given in the senior year -- which is largely devoted to "design". This kind of course has been called a "capstone" course by some....It is very hard to understand what brought about this step towards rigidity."

In 2000, the design sequence was rearranged in response to new ABET accreditation criteria that specify only that (1) graduates have an ability to design a system, component, or process to meet desired needs and that (2) in the curriculum graduates must have demonstrated the ability to work professionally in both thermal and mechanical systems areas including the design and realization of such systems. In the rearranged design sequence, all students are instructed in the basics of the design process, emphasizing mechanical design, under the instruction of always the same professor in a required junior-level course. Previously, these basics were nominally covered in each of the two required capstone design courses. Each student is still required to take one capstone-designproject course in either mechanical design, thermal-fluid design, or biomechanical design. These latter three courses are taught by three or four different professors and are concerned only with design projects.

#### **POSSIBLE FUTURE REARRANGEMENTS**

In 2002 the University of Kansas began emphasizing applications to human health in conjunction with the announced desire of the metropolitan Kansas City region to become a center of such activity. The Department of Mechanical Engineering hired its first faculty member in biomechanics in 1996 and by 2001 had five, most of whom have research programs in collaboration with colleagues at the University of Kansas Medical Center, 50 miles away. This shift in educational direction requires the flexibility called for by Sabersky in the definition of "design", perhaps to the extent of giving "design" credit for undergraduate participation in some research projects.

It is expected that there will be another revision of the design sequence in the next several years at the University of Kansas. That design sequence might resemble that of the 1960s with only one required "design" course.

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## **TEACHING MICRO/NANOSCALE HEAT TRANSFER**

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#### ABSTRACT

In this paper, I will share some personal experience and views on teaching micro/nanoscale heat transfer. Due to the diverse science backgrounds underlying the micro/nanoscale heat transfer principles, a big question facing the instructors is what to teach. At the undergraduate level, I believe that micro/nanoscale concepts can be integrated into the current mainstream heat transfer curriculum through some discussion of the length scales of heat carriers and through examples of heat transfer problems in micro- and nanotechnologies. Experimental modules can also be developed for hands-on experience. At the graduate level, a systematic study of micro/nanoscale heat transfer should contain the following four parts: (1) energy states, (2) thermal energy storage, (3) energy transport in the forms of waves and particles, and (4) energy conversion. The principles behind these topics encompass quantum mechanics, condensed matter physics, statistical physics, kinetic theory, electronics and electromagnetic waves. Although integrating these diverse subjects into one course seems to be a daunting task, my experience of teaching such a course at MIT and UCLA convinced me that such an integrated course is feasible.

## THE NEED FOR MICRO/NANO HEAT TRANSFER EDUCATION

Heat transfer as an engineering discipline emerged in the early half of the 20<sup>th</sup> century. Prior to its emergence as an engineering discipline, basic heat transfer principles were laid down mainly by mathematicians and physicists, including such luminaries as Joseph Fourier and Max Planck. The emergence and development of heat transfer as an engineering discipline was mostly need-driven. Examples of the early needs are the power plant, petrochemical plants, and engines. In the 1960s, space and aerospace technologies played a central role in the heat transfer research while in the 1980s, the thermal management of microelectronics became a dominant driver.

What are the application drivers of micro/nanoscale heat transfer education? Micro/nanoscale heat transfer can be

related to a wide range of contemporary technologies including information technology (IT), energy technology, micro/nano fabrication and nanomaterials, and biotechnology [1,2]. Examples of nanoscale heat transfer phenomena related to information technology are the reduced thermal conductivity of various thin films used to build integrated circuits and semiconductor lasers, and the higher temperature rise of nanoscale heat sources due to rarefied phonon heat conduction. These phenomena are part of the thermal management considerations of either individual devices or the whole computer chip. Another type of heat transfer applications in IT is the use of thermal energy for data storage, such as phasechange rewritable disks, the thermal writing of polymers, and the thermal-assisted switching of magnetic bits. In the energy conversion area, some nanoscale heat transfer phenomena can enable particular energy conversion technologies. For example, the reduced thermal conductivity of nanostructured materials can be utilized to improve the thermoelectric figure of merit for solid-state cooling and power generation. The enhanced radiation transfer in small gaps can be exploited to improve the thermophotovoltaic energy conversion efficiency and power density. The fabrication of nanostructures and the synthesis of nanostructured materials often also involve very interesting heat and mass transfer processes, such as the vapor and the liquid phase condensation in the synthesis of nanowires. Nanoscale heat and mass transfer is also seeing increasing applications in biology. Examples are the heating of nanoparticles to separate the DNA strands and mass transfer issues related to the detection of bio-agents.

Another question worth pondering is: what are the technological areas where we can place students educated in heat transfer into the driver's seats. The application examples of micro/nanoscale heat transfer are not necessarily all need-driven. In the last 10-15 years during which micro/nanoscale heat transfer has gone through rapid development, microelectronics was often used as the technological driver for understanding micro/nanoscale phenomena. Although heat transfer in microelectronics remains a crucial issue, it is not a driver for the product development. The intellectual pursuit to

explore the difference between macro and nanoscale heat transfer actually was a much larger driving force for the rapid development of the field of micro/nanoscale heat transfer. The fundamental understanding gained from such intellectual pursuit is now seeing bigger rewards in technological areas other than microelectronics and photonics. Some of the applications put the heat transfer principles into the driver's seats. Examples are energy conversion based on nanostructured thermoelectric materials and based on nanoscale radiation heat transfer phenomena. The heat transfer community should capitalize on these new opportunities by equipping the students with the knowledge to place them into the driver's seats.

## INCORPORATING MICRO/NANO HEAT TRANSFER INTO UNDERGRADUATE CURRICULUM

A typical heat transfer course at the undergraduate level already has very cramped contents and instructors often struggle to cover even the traditional syllabus. How can one include micro and nano topics? While having an advanced course in micro/nanoscale heat transfer is always an option, I believe that we also need to introduce some micro/nanoscale heat transfer concepts in the introductory level course. This can be done in the following three areas without much change to current course contents.

(1) Introduction of fundamental concepts. Some fundamental concepts can be incorporated into an undergraduate heat transfer course. For example, when discussing heat conduction, phonons and electrons as heat carriers can be explained in parallel to molecules for gases and liquids. Two important characteristic lengths of heat carriers should be discussed---the mean free path and the wavelength. Based on the mean free path, the validity of the Fourier law and the non-slip boundary condition can be discussed. The relaxation time can also be introduced together with the mean free path for explaining potential deviations in fast transport processes. The wavelength can be introduced when discussing the Wien displacement law for thermal radiation.

(2) Examples and homework problems from micro and nanotechnology. Many of the heat transfer problems in micro/nanotechnology can be solved based on macroscale constitutive equations. Examples from microelectronics, photonics, and microfluidics can be readily integrated into the teaching of heat conduction and convection. When solving these problems, one may discuss the justification of the classical laws based on the characteristic length and time scales.

(3) **Experiments.** Some experimental modules can be developed with different levels of investments, depending on the institutional resources. Taking thin-film thermal conductivity measurement as an example, different techniques can be employed for measuring the thermal conductivity of thin films. An AC calorimetry method can be used to measure the thermal diffusivity of thin membranes without the need of photolithography tools [3]. Several photothermal methods can also be adapted for thermal diffusivity measurements with little investment [4]. If photolithography tools are available, microfabrication-based experiments will provide students with an even richer experience [5,6]. One can also explore existing

foundry services to obtain microfabricated samples. For fluidic experiments, soft lithography can be a good platform [7].

#### A GRADUATE LEVEL MICRO/NANO HEAT TRANSFER COURSE

At the graduate level, many universities have begun to offer courses related to micro/nanoscale heat transfer with large variations in the course contents, depending greatly on instructors and the targeted student bodies. The courses I developed at UCLA and MIT have targeted students in heat transfer and MEMS, mostly with typical mechanical engineering backgrounds. My philosophy is to start from fundamental physical principles to build microscopic pictures of the heat transfer processes, as shown in Fig. 1. The course contains the following three core parts (1) energy states, (2) thermal energy storage, and (3) thermal energy transport, and if time permitting, two additional topics (4) energy conversion and (5) liquids. I will briefly discuss the essential contents for each part.

The energy states in materials are determined by quantum mechanical principles. Mechanical engineering students normally have had some quantum concepts from their undergraduate physics but have seldom touched these topics in the rest of their engineering curriculum. In contrast, current electrical engineering, materials science, and chemical engineering curricula usually cover such topics in various courses. I believe that understanding the energy states is the starting point for gaining a microscopic picture of heat transfer I cover the Schrödinger equation, the energy states of quantum wells, harmonic oscillators, rigid rotors, hydrogen atoms, and electrons and phonons in crystals. These are usually the contents of quantum mechanics and solid-state physics; each of which is a year-long course in the physics department. The challenge for instructors is to shrink it within 3-4 weeks, preferably 3 weeks. I limit the detailed mathematical treatment using the Schrödinger equation to quantum wells, and for phonons to one-dimensional atomic chains. In addition to the energy states, some key concepts that I emphasize are quantum states, degeneracy, and density of states. Many examples of using the quantum energy states in nanotechnology can be given through these discussions, including semiconductor quantum well, quantum wire, and quantum dots lasers, superlattices, and photonic crystals.

My introduction to heat starts with the thermal energy storage that can be treated based on statistical thermodynamics. Although I favor a rigorous treatment based on ensembles, (microcannonical, canonical, and grand canonical ensembles), a direct introduction of the Boltzmann, the Fermi-Dirac, and the Bose-Einstein distributions are an acceptable alternative. From the distribution functions and the density of states concept, one can derive the Planck law, and the specific heat of ideal gases and of solids. Ideally, the essential statistics should be covered in one week, although my lecture often runs into the secondweek.

The coverage of the energy states and the thermal energy storage is preparatory for a discussion on the thermal energy transport. My treatment of the energy transport is divided into three themes, which will be discussed below.



Figure 1 Contents of a graduate level nanoscale heat transfer course, which are also the major components of a textbook to be published by Oxford Press.

My treatment of transport starts with the heat transfer in the form of waves carried by electrons, phonons and photons. The wave treatment can begin with the quantum mechanics discussion of electron waves. I emphasize a parallel treatment of photons and phonons (throughout the whole course) and thus introduce electromagnetic waves here, with some discussion about acoustic waves. The key concepts emphasized in the wave treatments are the single-interface reflection of waves and related to this, the thermal boundary resistance phenomena, the interference and tunneling phenomena and their impacts on radiation heat transfer. In addition to these important heat transfer phenomena, another advantage of including a wave treatment is that it becomes easy for students to understand the recent development in science and technology. Examples include scanning tunneling microscopes, superlattices, and photonic crystals. The treatment of wave transport will end with a discussion of the criteria for neglecting the phases of the waves so that heat carriers can be treated as particles. Concepts such as wave packets and group velocity will be explained through such a discussion.

My teaching of heat transfer in the form of particles starts with the derivation of the Boltzmann equation, followed by a simplified discussion of scattering mechanisms and the relaxation time approximation. From the Boltzmann equation, classical constitutive laws such as the Fourier law, the Newton shear stress law, the Ohm law will be derived, together with a derivation of thermoelectric effects and a discussion of the Onsager relations. Here, students will see that the laws that they had taken for granted can be derived under various approximations, some of which are not valid in nanostructures. In addition to the constitutive equations, I also briefly discuss the derivation of the Navier-Stokes equation for gas molecules and its counterpart, the electrohydrodynamic equations.

The final topic of transport is classical size effects. This is an area that has had the most development in the micro/nanoscale heat transfer research. My treatment is again based on the Boltzmann equation and treats electrons, phonons, and gas molecules in a parallel fashion. Phenomena discussed are the reduced thermal conductivity of thin films, the velocity slippage in rarefied gas flow and their applications in disk drives, the rarefied phonon gas heat conduction near nanoscale heat sources, and approximate treatments that allow quick estimation of size and interface effects. Some students commented that I should start the course here, although I do not agree.

My past teaching, both on the quarter system UCLA (four lecture-hours per week) or the semester system at MIT (three lecture-hours per week), essentially stops here. There are two additional topics, needing another three weeks, which I would like to cover. These are the microscopic picture of energy conversion and the liquid-based transport.

Regarding energy conversion, the relaxation-time based Boltzmann equation does not include the nonequilibrium between different carriers, such as hot electrons and hot phonons, and the photon-phonon interactions. My treatment of the microscopic energy conversion will deal with the nonequilibrium between different heat carriers, how energy is converted from one-type of carrier to another, and how transport affects such energy conversion processes. Applications include nonequilibrium between electrons and phonons during laser-materials interaction, the hot and cold electron effects in semiconductor devices and thermoelectric devices, and heat generation and heat source distributions. This chapter is also a place to summarize how nanotechnology can be used to improve the efficiency of energy conversion devices.

I have treated all the above-discussed topics in a parallel fashion for electrons, photons, phonons, and gas molecules. Liquids, however, defy such a parallel treatment. Luckily, at least for simple liquid, classical transport equations are still valid except a few atomic layers near the wall region. My treatment of liquid includes surface energy and surface force, and liquid-vapor phase change processes.

The last time I taught the course (Fall 2002), I left the last 10 minutes of each lecture for a student to give a in-class presentation. The topics are chosen from suggested papers for each chapter—ranging,for example, from the original papers of Einstein on photons, to some recent papers on micro/nanoscale heat transfer. Both students and I enjoyed these presentations.

Table 1 shows the weekly coverage of my course at MIT for the Fall of 2002. In retrospect and also in my future agenda, I think at a semester system like MIT, I will further shorten the time I spend on the energy states (currently 4 weeks) and thermal energy storage (currently 2 weeks) to a total of 4 weeks. This will leave time to cover the topics on energy conversion and liquid. Ideally, if a statistical thermodynamics course is offered, it should cover the energy states and the thermal energy storage, which would leave more time to cover the transport and energy conversion.

Clearly, the above-discussed contents include many diverse topics. My experience is that these diverse contents are still manageable and serious students benefit tremendously from such a wide exposure. It was quite gratifying when a student told me that after this course, he suddenly found that he could follow the topics of many papers in current journals (not necessarily just heat transfer journals). For students in my own group, some will continue to take more specialized courses from quantum mechanics and condensed matter physics, to electronics and materials, in addition to mechanical engineering courses and I encourage them to do so.

I would also like to comment that I have attempted to put minimum prerequisites on this course. The expected students background include general physics, introductory thermodynamics and heat transfer. Some junior and senior undergraduate students have taken the course and had excellent performance. There are also students who had not taking heat transfer before and who were still able to survive. One message I do want to deliver to students is that the barriers between different disciplines are actually not high. But it takes students courage and determination to go through the diverse topics and the large amount of new terminologies.

Finally, regarding the textbook. there are currently no published textbooks exist that I can use for the above-discussed contents in my course. I have been working on a textbook [8], which will be published by the Oxford Press as part of the MIT-Papallardo Series in Mechanical Engineering, with anticipated the publication of the book in late 2003 or early 2004. Currently, 10 chapters are planned, nine of which are shown in Fig.1. An additional chapter on numerical simulation techniques, including molecular dynamics and Monte Carlo simulation, will also be included.

#### ACKNOWLEDGMENTS

I would like to thank students who have taken my classes at UCLA and MIT, and students in my group, for their constructive suggestions and comments on the lectures and notes. Also to be thanked are various funding agencies (NSF, ONR, DOE, DARPA, and NASA). Many results of the funded research have been incorporated into the class teaching and used in inspiring new generations of students. Table 1 An example of Course Coverage.

MIT 2.57: Nano-to-Macro Transport Processes Fall, 2002 Schedule

**Week 1.** 9/4 Introduction to nanotechnology and nanoscale transport phenomena. (Ch.1).

Week 2. 9/9 Microscopic picture of heat carriers (Ch.1). 9/11 Mean free path and simple kinetic theory. Basic wave characteristics (Ch.1&2).

**Week 3** 9/16 Material waves and Schrödinger equation, quantum well (Ch.2).

9/18 Quantum wells, 1D and 2D quantum structures (Ch.2).Week 4 9/23 Student holiday, no class.

9/25 Harmonic oscillators, rigid rotors, and hydrogen atoms (Ch.2).

Week 5 9/30 Crystal structures (Ch.3).

10/2 Electronic energy levels in crystals, Kronig-Penney model (Ch.3).

Week 6 10/7 Electronic energy levels in 3D crystals (Chap3).

10/9 Phonons and density of states (Ch.3).

Week 7 10/14 Columbus day, no class

10/16 Density-of-states, Microcanonical ensembles (Ch.3&4).

Week 8 10/21 Midterm No. 1.

10/23 Ensembles, molecular partition functions, specific heat of gases (Ch.4).

Week 9 10/28 Fermi-Dirac and Bose-Einstein distributions, specific heat (Ch.4).

10/30 Specific heat of phonons and electrons (Ch.4), Introduction to heat transfer by waves (Ch. 5).

Week 10 11/4 Energy transfer by waves, plane electron waves and reflection of waves, Introduction to electromagnetic waves (Ch.5).

11/6 Electromagnetic wave reflection at a single interface (Ch.5).

Week 11 11/11 Veteran's day, no class.

11/13 Interference and tunneling, acoustic waves (Ch.5).

Week 12 11/18 Landauer formalism, wave to particle transition (Ch.5).

11/20 Coherence, Energy transfer by particles, Boltzmann equation (Chap 6).

Week 13 11/25 Scattering and relaxation time (Ch. 6)

11/27 Fourier law, Newton's shear stress law, Ohm's law (Ch. 6).

Week 14 12/2 Electron transport, thermoelectric effects (Ch.6). Take home exam out.

12/4 Constitutive equations (Ch. 6), Classical size effects in thin films (Ch. 7), Take home exam due.

Week 15 12/9 Size effects parallel to films Size effects perpendicular to interfaces (Ch. 7).

12/11 Rarefied gas flow (Ch. 7).

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## HEAT TRANSFER EDUCATION: INTEGRATION OF THE THERMAL SCIENCES STEM

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ABSTRACT

Integration of the thermal sciences stem refers to changes in objectives, pedagogy, and content being driven by curriculum reform. We provide a 15-year history of how the discipline has sought to better prepare students for industrial practice. The results of a recent survey identify the drivers for and extent of reform as well as the trends, content and barriers. The reform activities represent a strengthening of the traditional three-course stem, as well as the spawning of combined courses, with opportunities for including materials on new technologies.

#### INTRODUCTION

This paper focuses on the activities over the past 15 years of the ASME Heat Transfer Division as related to heat transfer education in our mechanical engineering programs. Because heat transfer is part of the thermal sciences (TS) stem, we have broadened the discussion to include issues related to thermodynamics and fluid mechanics learning. Our review includes that of several panel sessions and symposia directed toward innovation in teaching. The paper follows a chronological path, which in itself offers interesting insight into how changes in technology – both in engineering practice and in the educational environment – influence our approach, views, and framework for education.

The aims of this paper are to provide a summary of contributions that address the challenges, to assess the impact of change, and to identify opportunities to enhance the educational process. Particular emphasis is given to the curriculum reform effort referred to as the integration of the thermal sciences. Richard S. Figliola Professor Department of Mechanical Engineering Clemson University

#### NATIONAL LOOK IN 1988

As part of the celebration of the 50<sup>th</sup> anniversary of the Heat Transfer Division (HTD) at the 1988 ASME Winter Annual Meeting (WAM), a panel session was devoted to the future of heat transfer education [1]. The four panelists representing industry and academe were in agreement that heat transfer education had been brought to a mature pedagogical approach.

At the undergraduate level, heat transfer was the third in the sequence of courses with thermodynamics and fluid mechanics comprising the TS stem. While the educational process was seen as producing engineers with a strong understanding of the fundamentals, the graduates were thought weak in addressing industrial applications that typically involve complex or multi-disciplinary phenomena. Heat transfer, it was agreed, should be the key course in the TS stem for imparting judgment required to address real-world applications.

The panelists cautioned that the increased accessibility of computers and powerful software using modern computational techniques represented a potential distraction from hands-on analysis requiring judgment. Further, computer accessibility provided opportunities to automate experiments and perform virtual experiments that could seriously diminish students' experiences in experiment design, measurements, and analysis. The industrial panelists raised issues about adequate preparedness in communications, economics and ethics, as the practicing engineer is concerned about matters of reliability, cost, manufacturability, safety and product liability. The challenge was to remedy the foregoing concerns at a time when serious efforts were underway to reduce curriculum total credits, and faculty were faced with increased pressures to maintain productive

research programs. Clearly, meeting the challenge would require significant changes and innovations to the delivery system.

In 1995, the HTD proposed the formation of an Ad Hoc Education committee to strengthen educationresearch-practice interactions and thereby enhance the relevance of education to practice. The main mission of the committee was to organize paper or panel sessions under the general theme of "Innovations in Heat Transfer Education" and student poster sessions entitled "Student Research and Design in Heat Transfer." The committee achieved permanent status (K-21) in 2002 [2]. The outcomes of these sessions are discussed below.

#### INNOVATIONS IN HT EDUCATION

In this brief overview, we describe the general features of advances in heat transfer teaching methods as evidence that serious attention is being given to meet the challenges posed by 1988-WAM panel, as well as to ABET-inspired curriculum requirements.

At the initial session of the new Education Committee in 1997 [3], twelve contributions were presented, half of which dealt with laboratory development. Novel experiments were described for heat exchangers (USNA), two-phase flow (Nevada), microelectro-mechanical systems and integrated circuits (Stanford), and conduction phenomena (Kansas State). At Purdue, the role of the laboratory was expanded to cultivate systems integration and multidisciplinary, complex-problem solving skills by replacing traditional experiments with design-type project assignments developed with an industrial partner. As a means of enhancing classroom theory learning, a simulated fluid flow laboratory at Minnesota allowed students to explore the behavior of Software-related topics included real fluid systems. two learning modules: one illustrating conduction phenomena (Federal University of Santa Catarina, Brasil); and another illustrating classical topics on conduction, forced convection, and radiation view factors (Virginia). An equation-solving package to improve student problem-solving skills and increase their computational productivity was described An elective heat transfer system design (Purdue). course at Virginia Tech provided students with realistic design experience using a commercial industrialstrength software package. Novel ways to teach the classical topics were described including an algebraic, lumped-model approach to solving Heisler-Gröber problems (Idaho State), and an electrical analogy approach to solving two-dimensional conduction problems (Pozan, Poland).

In the 1998 session [4], progress and experiences in the integration of the thermal sciences at Clemson, RPI and Carnegie-Mellon were described. Information was provided on new curricula content, motivations for revising the traditional thermal science three-course sequence, and assessment. Academe-industry relationships at Kettering were presented; one about the process of forming relationships and launching useful collaborations, and another about the experiences derived from using the under-hood compartment of a vehicle as the platform for innovative laboratory experiments and multi-disciplinary projects. An update was given on classroom experiences and impact using the conduction phenomena evaluation educational software (Federal University of Santa Catarina, Brazil) described in the 1997 session.

Khounsary, et al. [5] provided a written summary of the 1996-IMECE panel aimed at identifying issues to keep heat transfer education relevant and exciting. The academe-industry participants thought that steps to ensure the desired outcomes in heat transfer education should include: a better understanding of the interaction between the student, course content, and market needs; an appreciation of the need in multidisciplinary industrial environments for engineers trained with a broad background; and, a revision of introductory heat transfer courses to incorporate insightful industrial examples and case studies that would reinforce problem-solving abilities and emphasize multidisciplinary issues present in modern thermal management applications. These issues have much in common with those identified by the 1988-WAM panel, but there was growing evidence that educators have recognized the importance of forging industry connections and of building students' practical-problem solving skills

In the 1999 session [6], co-sponsored with HTD Energy Systems Committee (K-12), ten contributions were presented. A partnership with the university's engineering services department provided opportunities for students at Michigan State to conduct experiments and perform systems thermal analysis on campus power plant facilities as part of their senior-level heat transfer laboratory course. A laboratory course at Michigan State was organized in two parts, the first with traditional skill-building experiments, and the second a design-project competition. The project work required synthesis of thermal and mechanical systems skills for the design and realization of the device. Serving as synthesizing experiences with interdisciplinary, real-life open-ended problems, senior-level projects were described in separate papers on a hybrid combustion-fuel cell cogeneration plant (Tufts) and a loop heat pipe with transient heat load (Clemson).

Novel ways were described for teaching classical topics including implications of critical radius on conduction heat rates for cylindrical and spherical coordinate systems (Southern Illinois - Carbondale) and a finite-difference method to obtain temperature distribution and heat rates in annular fins in place of an analysis using Bessel functions (Idaho State).

Progress was reported on work at Clemson to implement an introductory thermal-fluids sciences course. The transformation of the introductory heat transfer course from a lecture format into a partial studio model at Virginia was described. Lectures were supplemented with a two-hour session using computerbased teaching modules that allow students to explore with tools for solving classical conduction, convection and radiation problems.

This session saw the first appearance of contributions on learning techniques. From Nevada, an evaluation was given of cooperative learning, a technique where students work in small groups to accomplish specific educational tasks jointly. The peer-group setting has been more commonly used in design-type projects, and less so in problem-solving classes involving engineering science and analysis. From Texas Tech, an evaluation was presented on investigative active learning, a more rational alternative to learning by rote memorization. Implicit in this notion were the concepts of investigation, mentoring, feedback, modeling and interaction that can be implemented with computer-based instruction techniques.

In the 2000 session [7], a description was given on the collaboration between RPI and Tufts to establish a research-curriculum development program in the area of thermal manufacturing and materials processing. A central aspect of the collaboration was the concurrent development of two new graduate courses at their respective institutions, one with a process-physics focus and the other dealing with thermal aspects. Also reported were experiences with a distance-learning version of one of these courses. A description was given of a program at Iowa State in practical thermal system design that encompassed project-oriented teaching for undergraduate, graduate and off-campus professional students. The approach integrated the thermal science disciplines, and involved industryuniversity collaboration and community outreach. Extensive use was made of information technologies for virtual project group meetings, interactive designlaboratory sessions and computational software. Virginia Tech's experiences were described in implementing a new sophomore-level course that provided a sequential introduction of thermodynamics, fluid mechanics and heat transfer; majors were expected to take follow-on courses in each of the disciplines.

The outcomes of these sessions covering a period of five years provided evidence that heat transfer education is undergoing enrichment and notable changes, and that the issues identified by the 1988WAM and 1996-IMECE panels were being seriously addressed.

#### NATIONAL LOOK IN 2001

In summer 2001, the K-21Committee sent a survey to all 250-plus ABET accredited mechanical engineering programs in the United States. The intent of the survey was to identify new trends in TS education and to understand the motivation behind and the experiences gained from such changes. The respondent was either the department chair or, as in a few cases, the program coordinator. While we recognize that their comments reflect individual opinion, we take the collective responses from 101 respondents as being representative of the current state and trends in mechanical engineering education.

The survey results were presented as part of a panel session on integrating the thermal science curriculum at IMECE 2001. Panelists were D.A. Kaminski (RPI), F.A. Kulacki (Minnesota), R.A. Gaggioli (Marquette), and R.S. Figliola (Clemson ) with P. Norris (Virginia) serving as moderator. The panelists from Marquette, RPI and Minnesota related their experiences in how discipline materials were integrated, and provided student and faculty reactions on the new formats. The overall message was that integration efforts are underway, but the packaging of the new content is challenging, and the student outcomes, as well as faculty views, vary between the schools.

The survey queried the following topics: comparison of curriculum content in 1990 to 2000; current required TS stem courses; future plans or considerations for changes in the curriculum; barriers to change in curriculum; assessment information on integrated course offerings, if any; and, any other relevant comments.

The results indicated that while the fractional portion of the curriculum specific to TS education has not changed much over the past few decades, the approaches to how we introduce, present and package the delivery of these subjects are changing. Further, technological and political pressures on the entire mechanical engineering curriculum are likely to force continued changes in TS education. However, there appear to be barriers to changing a system that has been in place for so long and that has successfully served the profession in the past. Clearly, the challenge is for TS education to be represented in the curriculum in a manner that is relevant and reflective of changes in the profession.

#### **Curriculum Content**

Over the past decade, the portion of the mechanical engineering curriculum devoted to TS education has remained at between 12 to 16 semester

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credit hours (or equivalent in quarter credit hours). This is to be expected. as past mechanical engineering accreditation requirements have mandated that there be a visible stem of course study devoted to TS education. Through the late 1990's, the credit hour equivalent of one full semester was still expected. Current ABET Engineering Curriculum 2000 (EC 2000) requirements are more flexible in order to allow programs to be innovative in how a capability in thermal systems is facilitated and in how to package such material to meet individual degree program objectives. But directed study in thermal systems is still required in EC 2000 [8]. As a consequence, and due to other pressures discussed later, we should expect to see TS concepts remaining well represented in our curriculums but the portion directed specifically to TS education reducing in the future.

The most traditional program of study in TS education became well established over the past 50 years. With the exception of a few distinctively different programs, this meant programs offered at least a separate course in each subject of fluid mechanics, thermodynamics, and heat transfer, with extra study in thermodynamics and/or fluid mechanics, and accompanying laboratory study. Electives and design courses completed the study. To this end, textbooks were written and their pedagogy fine-tuned, but most reflected the approach that featured a strong individual subject focus. It should also be noted that subject topics developed 50 years ago still hold a prominent position in our textbooks. For example, we can still see a strong emphasis on large power systems in these texts: power cycles, heat exchangers, and corresponding devices. Over time, new material has been added to keep pace with technology, but without a change in emphasis. Certainly while many applications of TS principles to design are mature concepts (such as large energy exchange systems), there are a host of applications, typically at smaller scales (such as in microdevices and nanomanufacturing), that challenge our knowledge and skills and will be the focus of many of our students during their professional careers. As educators, we now want to address these new challenges, provide experiences that prepare our new engineers for their careers, and enable young engineers for a lifetime of learning.

### **Curriculum Trends**

The major shift occurring in our programs is a growing trend towards requiring some sort of integrated TS course; that is, combining the subject matter of the disciplines of fluid mechanics, thermodynamics, and/or heat transfer within a single course devoted to this material. In fact, about one-half of all programs now include some type of integrated TS introductory course. There are many variations in how such an integrated course is offered. Some programs integrate material through a design experience that incorporates the three disciplines. Others choose to blend the material within a systemsoriented, engineering science format. And others package a sequential treatment of the disciplines within a single course.

A growing number of programs now follow the introductory integrated course with a second offering, effectively replacing the traditional stand-alone discipline courses. One of every six programs reports abandoning the three discipline course approach, substituting a suite of integrated courses, and leaving advanced study in any discipline as a technical elective.

A second shift is placing a stronger focus on TS design and realization. About two out of three programs now offer a course emphasizing integrated thermal design or projects as part of their culminating program experiences. With this approach, a few programs introduce heat transfer fundamentals within a design course format.

Other important recent shifts are attempts to integrate new topics not previously stressed in the undergraduate curriculum into TS courses. Material pertinent to length scales and basic science applications (chemistry and biology) were mentioned most often. These topics relate to a broader discussion on new directions in mechanical engineering and how to accommodate the growing needs of the profession within an undergraduate curriculum [9].

#### **Motivations for Change**

Why are these changes occurring, and where will they lead? Fully one-half of the respondents mentioned that their curriculum is under review for change. There appear to be a number of drivers for change which include: a desire for design integration; a fascination with a multi-disciplinary systems approach to problem solving; the less prescriptive accreditation requirement environment; and state imposed credit limits.

An often-mentioned reason is the desire to add more TS design-oriented courses and projects, and to address vertical integration of design into the programs. This reason is consistent with an accreditation requirement for students to be able "to work professionally in the thermal systems area including the design and realization of such systems [8]." The introduction of TS concepts in an integrated format makes available early in the curriculum a natural palette of systems material for problem-solving and project activity. Proponents of the systems-oriented approach argue that it is more indicative of professional practice and, with its implementation during the early courses, allows a new engineer to develop a systems-level mentality for design as s/he matures within the program. It also fills a need for a broad TS course for non-mechanical engineering majors. Certainly, the softer accreditation requirements that provide more freedom for programs to decide how their graduates will develop the capabilities to practice thermal systems opens the door for trying new approaches.

One strong influence for change is the pressure most programs are under to reduce credit hour requirements. Fully 40% of the respondents noted this. Some state legislatures are mandating credit hour limits for state-assisted, undergraduate degree programs, typically requiring substantial cutbacks in engineering programs. Driving this political pressure are the tuition costs and a desire to increase four-year graduation rates. Likewise, neighboring schools are obligated to match these requirements closely or risk losing a traditional source of quality students. Reducing the number of explicit course offerings in thermal systems and repackaging essential material can accommodate these financial and political pressures. The acute question arises: if fewer credit hours are a goal, and we must scale back material, then what material is critical?

Further pressure comes from the growing needs of the mechanical engineering discipline requiring instruction in other areas and the application of TS material across disciplines, including material sciences, manufacturing and biologically-inspired applications. A recent workshop conducted by the ASME Mechanical Engineering Department Heads Group [9] developed recommendations for the future of mechanical engineering education that will have a broad impact on curricula and TS education: expanding faculty expertise in emerging technologies; revising curricula to include new material on atomic and molecular physics, quantitative biology, organic chemistry, micro fabrication, and modern computing; and, revising ME labs to include biotechnology and micro/nano-scale systems. This message makes clear the need for repackaging and integration, given the real matriculation time and credit hour limits, and given the nature of future needs in the mechanical engineering profession. Cited was the need for drawing mechanical engineering faculty from a broader, multidiscipline pool of expertise, producing agile graduates who can absorb and use new tools from other disciplines to develop new products, and focusing on a systems approach to broaden the "design-space" of mechanical engineering.

#### **Barriers to Change**

Even though significant changes are underway, there are roadblocks, as many survey respondents suggested. Changing the mode of business that has been in place for decades is not a clear or simple process.

First and foremost, the need was brought up for adequate textbooks and teaching materials. Our modern subject-specific textbooks have evolved to provide sound pedagogy and a complete treatment of their subject. Developing new textbooks having a different slant takes time and trial. Development is impeded because the specific materials to be covered in an integrated course of study are not well codified. As a consequence, instructors are spending large amounts of time developing their own materials, both written text and software tools. Transportability to a national scale has not been their focus. But these may be growing pains that will work out with time. The larger questions may be: do these approaches by nature require a substantially higher commitment from the faculty and students; and, if so, are the outcomes advantageous to justify this? We don't have good answers to these questions yet.

The second most cited impediment was a lack of instructors with that special ability to synthesize, integrate and teach combined TS applications. This situation can be expected to compound as universities hire more multidisciplinary professionals into their faculty. For example, should someone specializing in solid-state thermodynamics be expected to be sufficiently proficient in the broad area of thermalsystems design to develop teaching materials?

In project-based courses, students tend to learn subjects as needed to complete the project. Should a student's exposure to material in any of the subjects be well established? How do we ensure understanding with depth on critical material? With project-oriented learning, outcomes may be harder to tie to basic concepts, emphasis changes with tasks, and student proficiency may change with the projects used to integrate the subjects. This is a significant pedagogical issue.

#### CONCLUSIONS

Many of the changes we've identified through the sessions and survey must be viewed as events in an evolutionary process to improve the delivery system. Faculty has been continually seeking novel ways to involve industry as partners, import applications-driven issues into the classroom, cultivate problem-solving skills, address thermal systems analysis / design, and use computer-based learning tools.

However, the process has become complicated because of the urgent need in all schools to include materials on the new technologies, and because of the reduction at many schools in credit hours available to the TS stem. The traditional three-course sequence TS stem remains intact in many programs, while elsewhere it's being reduced into fewer courses that combine the traditional disciplines in novel ways to meet newly defined learning objectives. Dealing in creative ways with the aforementioned barriers for change will strengthen the stem regardless of what path reform will take. New textbooks and learning materials are driven by need, which is evolving as different teaching approaches are tried and assessed. Staffing the stem with faculty having nontraditional specialties will enrich the enterprise through new cultures and content. Capitalizing on the use of project assignments to learn and reinforce fundamental concepts is a worthwhile adjunct to the usual lecturehome problem methodology. In a broader context, the barriers represent opportunities that will be seized by those who have the vision and energy to support change.

Surely there are other creative approaches for dealing with TS stem changes. The reform should also be viewed from the perspective of the total curriculum. Reform isn't just about yielding or sharing turf (credit hours), but about how to prepare engineers under conditions of diminished resources for the marketplace that has higher expectations. We should seek and promote changes in all parts of the curriculum, including general education courses that could strengthen thermal science education.

#### ACKNOWLEDGMENTS

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## HEAT TRANSFER ON PLANETARY SCALES

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#### ABSTRACT

The Earth is a very complex dynamic/thermodynamic system. Predicting things like weather patterns is notoriously difficult, especially on small local scales. In fact the system of equations that predict weather behave chaotically, as has been shown by Lorenz<sup>1</sup>. But what if we are interested in some large-scale average quantities such as globally averaged surface air temperature?

#### INTRODUCTION

In a local and transient sense, the thermal, physical and dynamical properties near the surface of Earth constitute the weather. I will be concerned in this brief paper not with local daily events that make up the weather, but with suitably longterm averages of seasonal or annual averages of properties. These averages are what we refer to as climate. While weather predictions exhibit chaotic oscillations, they are bounded, and when suitably averaged, the predictions are useful.

General Circulation Models are very complex models that incorporate models of the troposphere and the lower stratosphere, the ocean, land ice and snow, and often sea ice. Clouds are currently crudely parameterized, as is sea ice. Most of the important physical phenomena are included, but sometimes crudely. Models of the global temperature increase that is expected following a doubling of atmospheric carbon dioxide (after the system reaches equilibrium) typically agree within a factor of two or three. What is more important than globally averaged temperature are the regional changes of such things as temperature and soil moisture. The models in some cases differ in sign about changes in soil moisture, which is obviously very important to agriculture.

If theories are nets cast to capture the essence of the physical world, our net here is perhaps too fine. Trying to understand climatic change by using huge computer models is a bit like trying to drink from a fire-hose. Because of this a variety of simpler approximate models have been developed. These simpler models serve several purposes. They give us a broad idea of the cause and effect of long-term climate change, and they often give very valuable insight into how to better design and understand experiments with more complex models. I will first present an analysis of a global energy balance model to show what it can tell us about the temperature rise associated with a doubling of atmospheric carbon dioxide. Next, I show how the huge heat capacity of the global ocean can affect climate transients and, indeed can affect the detection of a carbon dioxide/climate signal in the atmosphere.

#### NOMENCLATURE

- A + BT: Infrared flux leaving Earth/atmosphere system
- c: Specific heat in the ocean
- D: Depth of ocean mixed layer
- F: Infrared flux leaving top of atmosphere
- h: Average cloud height
- K<sub>V</sub>: Effective diffusivity of global ocean
- Q: S/4
- N: Cloud fraction
- S: Solar constant = 1360 w/m<sup>2</sup>
- t: Time
- T: Earth surface temperature, or ocean temperature
- T<sub>e</sub>: Effective Earth/atmosphere radiating temperature
- T<sub>P</sub>: Temperature of water sinking at poles
- w: Average upwelling speed in global ocean
- $x_s$ : Area of Earth covered by ice and snow
- y<sub>C</sub>: Atmospheric CO<sub>2</sub> content
- z: Vertical coordinate
- y<sub>W</sub>: Atmospheric water vapor content
- $\alpha$ : Albedo (reflectivity) of the Earth/atmosphere
- ρ: Density of ocean water

#### **A Zero-dimensional Earth**

First consider the simplest possible thermodynamic model of Earth. The value of the solar constant at the distance from the Sun to Earth is approximately 1360 w/m<sup>2</sup>. Because of the rotation and geometry of Earth the average amount at the top of the atmosphere is one-fourth of this. A fraction  $\alpha$  (which climate modelers call the albedo) is reflected away by clouds and the surface. F is the infrared flux leaving the top of the atmosphere. At steady state

$$(1- \alpha)S/4 = F \tag{1}$$

The albedo is a function of several things, the most important of which are the fraction of Earth covered by clouds, N, the height of the clouds, h, and the area covered by ice and snow,  $x_s$ . Thus the change in the albedo due to a change  $dy_c$  in the CO<sub>2</sub> content is

$$d\alpha = \frac{d\alpha}{dy_C} dy_C + \frac{\partial\alpha}{\partial N} \frac{dN}{dT} dT + \frac{\partial\alpha}{\partial h} \frac{dh}{dT} dT + \frac{\partial\alpha}{\partial x_S} \frac{dx_S}{dT} dT$$
(2)

The change in the infrared flux is a function mainly of the  $CO_2$  content, the water vapor content and cloud fraction and height. Thus,

$$dF = \frac{dF}{dy_C} dy_C + \frac{\partial F}{\partial T} dT + \frac{\partial F}{\partial y_W} \frac{dy_W}{dT} dT + \frac{\partial F}{\partial N} \frac{dN}{dT} dT + \frac{\partial F}{\partial h} \frac{dh}{dT} dT$$
(3)

After a perturbation in the infrared flux, dF, and once equilibrium is reached,

$$-(S/4)d\alpha - dF = 0 \tag{4}$$

From these expressions we can see that the change in temperature when the  $CO_2$  content is raised by  $dy_C$  is

The terms in the numerator represent the rate at which the net radiative flux at the top of the troposphere changes with  $CO_2$  content, all other variables remaining constant. Its value has been determined by a number of investigators using radiative-convective atmospheric values to be  $-4.2 \text{ w/m}^2$  and is generally felt to be accurate to within 25% at least.

The first term in the denominator is the rate at which the infrared flux changes with temperature, all other variables remaining constant. Its value may be estimated by supposing that the Earth/atmosphere system radiates as a blackbody at some equivalent temperature  $T_e$ , so that  $F = \sigma T_e^4$ . The appropriate temperature to be used is that seen by a viewer in space, which is approximately 265K. Thus,  $\partial F/\partial T = 3.8 \text{ w/m}^2$  °C. With no feedbacks at all doubling CO<sub>2</sub> would lead to an increase in the average temperature of the atmosphere of 4.2/3.8 = 1.1 °C.

The largest of the feedback terms in the denominator is likely the water vapor term. Atmospheric radiation studies imply that this term is approximately -2 w/m<sup>2</sup> °C with an uncertainty of perhaps 0.5w/m<sup>2</sup> °C.

Cloud feedback is the most controversial and least understood feedback. I has been variously estimated as zero to both positive and negative. I give it here a value of zero with an uncertainty of  $0.3 \text{ w/m}^2 \,^{\circ}\text{C}$ . Ice/snow albedo feedback is  $0.3 \text{ w/m}^2 \,^{\circ}\text{C}$  with an uncertainty of  $0.1 \text{ w/m}^2 \,^{\circ}\text{C}$ . Taken altogether we find that the increase in average Earth surface temperature for a doubling of CO<sub>2</sub> in the atmosphere is between 1.6 and  $4.7 \,^{\circ}\text{C}$ . It is worth noting that the above is taken from a paper published 23 years ago (Watts, ref.2). The current estimate from many GCM studies and reported by the Intergovernmental Panel on Climate Change (IPCC) <sup>3</sup> is 1.5 to 4.5  $\,^{\circ}\text{C}$ .

So we expect an increase in Earth's temperature if and when the  $CO_2$  concentration doubles. But it won't happen immediately because the heat capacity of the system, particularly the ocean, is so large. It has been only fairly recently that coupled ocean-atmosphere GCMs have been able to run in the transient state following gradually increasing atmospheric loading of  $CO_2$ . The results of transients are given in the IPCC reports, but they are not the results of GCM runs. Rather, they are the results of a slightly more complex energy balance model called an upwelling-diffusion model. It involves the same kind of radiation model as before but connected to a one-dimensional (depth only) ocean.

$$dT = \frac{-\left(\frac{\partial F}{\partial y_{c}} + \frac{S}{4}\frac{\partial \alpha}{\partial y_{c}}\right)dy_{c}}{\frac{\partial F}{\partial T} + \frac{\partial F}{\partial y_{w}}\frac{dy_{w}}{dT} + \frac{\partial F}{\partial N}\frac{dN}{dT} + \frac{\partial F}{\partial h}\frac{dh}{dT} + \frac{S}{4}\left(\frac{\partial \alpha}{\partial N}\frac{dN}{dT} + \frac{\partial \alpha}{\partial h}\frac{dh}{dT} + \frac{\partial \alpha}{\partial x_{s}}\frac{dx_{s}}{dT}\right)}$$
(5)

#### A one-dimensional Earth: Transients

There has been much discussion in recent years of the influence of the ocean's thermohaline circulation in delaying the onset of greenhouse induced climate a change. The thermohaline circulation is essentially the vertical overturning of the ocean. More recently, attention has been given to how change in the strength of the thermohaline circulation can itself affect the climate. A one-dimensional ocean model provides a kind of "toy" with which to at least qualitatively understand the situation. The ocean is modeled as a mixed layer sitting atop a deep ocean. As in the real ocean, cold water at high latitudes sinks locally into the deep ocean and upwells more or less in the remainder of the ocean. The governing equation for the ocean interior is

$$\frac{\partial T}{\partial t} + w \frac{\partial T}{\partial z} = K_V \frac{\partial^2 T}{\partial z^2}$$
(6)

At the bottom of the constant depth ocean the vertical advective and diffusive terms must equal:

$$w(T - T_P) = K_V \frac{\partial T}{\partial z}$$
(7)

At z=0 (the bottom of the mixed later, where the temperature is assumed to be uniform, but not constant of course) the rate of change of thermal energy in the mixed layer is equal to the radiant energy received from the Sun minus that radiated away plus the net energy received by diffusion and advection from the deep water.

$$\frac{1}{\rho c} \left[ aQ - (A + BT) \right] - w \left( T_p - T \right) - K_V \frac{\partial T}{\partial z} = D \frac{\partial T}{\partial t} \quad (8)$$

The values of the various constants have been thoroughly discussed in the literature (see Watts, ref. 4 and Watts and Morantine, ref. 5) and are listed in the Nomenclature section.

The equations are not difficult to solve for example when the value of A is decreased to represent an increased greenhouse effect. Similarly, if the value of the upwelling speed w is perturbed, a regular perturbation problem emerges.

The globally averaged surface temperature has been reported by several groups of scientists, and of course we know that the values reported indicate a warming of between 0.4 and 0.6 °C over the past century. A puzzling aspect of these reported temperatures is that they all report a period from roughly 1040 until 1980 when there was a decided dip an the temperatures – an unexplained cooling period. Of course the climate signal is expected to be noisy and to vary on its own on many time scales. But this only begs the question. Why?

Two studies that were published in the oceanography literature may provide a possible answer. Roemmich and Wunsch<sup>6</sup> reported data taken on a transect of the North Atlantic ocean in 1957-59 with another taken in 1981. Levitus<sup>7</sup> used several million disposable bathythermograph measurements to compare the temperature and salinity structure of the North Atlantic ocean for the two pentads 1955-59 and 1970-74. Both found that the ocean at intermediate depths (between about 500m and 2500m) had warmed by an average of 0.1°C. If we assume that most of the mid-latitude North Atlantic ocean (only about 6% of the total ocean area) warmed by this amount, the necessary energy input is 1.7 x 10<sup>22</sup> joules<sup>8</sup>. Taken over a period of 15 years the required rate of transfer of heat is 36 million megawatts. Averaged over the entire surface of the Earth this amounts to  $0.072 \text{ wm}^{-2}$ . During this period the increase in surface heat flux due to greenhouse gases was about

 $0.125 \text{ wm}^{-2}$ . Thus if a similar warming of the intermediate depth ocean occurred in just 10% of the world ocean the expected loss of heat from the ocean surface would be sufficient to completely counter the greenhouse effect.

What does our model tell us? We used the model described above to see what would happen if the thermohaline circulation (the upwelling speed, w) were decreased by 10%. The figure shows the resulting temperature variation of the surface temperature superimposed on the globally averaged temperature reported by researchers at the University of East Anglia (which is essentially the same as that reported by a number of other groups). When the upwelling speed is reduced more heat diffuses into the deep ocean, warming the water at intermediate depths and cooling the surface. In the long run, the surface temperature of the surface returns to the value (in our model) dictated by radiation balance at the top, but this takes several decades. Meanwhile the greenhouse may be hiding in the deep ocean.

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# AFM IMAGING OF BIOLOGICAL MEMBRANES: OPTIMAL OPERATION AND DATA INTERPRETATION THROUGH UNDERSTANDING OF TRANSPORT PHENOMENA

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#### ABSTRACT

Living cells grow and communicate with each other by exchanging ions with their environment fluid through complex physiological processes that occur in sequence and/or parallel and involve multitude of temporal and spatial scales. The events involved can be very fast and highly localized requiring spatial resolution in the order of tens of nanometers. An atomic force microscope (AFM) and AFM-based multifunctional scanning probes belong to a new class of instruments that provide a unique opportunity to study cell communication processes in-situ with sufficient spatial and temporal resolution. However, one of the main challenges in AFM experiments lies in data interpretation. Therefore, development of fundamentally sound, yet computationally efficient theoretical models to resolve the multiple interacting transport phenomena underlying the AFM imaging process is necessary, and such models must be general and flexible enough to simulate the complex interactions, geometry, and operating conditions of the instrument and biological membrane under actual physiological conditions. We report the electrohydrodynamic force at the surface of the AFM tip and elastic deformation of the soft biological membranes induced by the AFM probing action, which are essential for quantitative interpretation the AFM images in the aqueous environment. This study is the first theoretical demonstration, that in addition to the electrical force induced by the non-uniform electric field around the AFM tip, the feedback force at the AFM tip during imaging in an aqueous environment is also due to the strong coupling of electrohydrodynamic interactions in the solution and elastic deformation of the membrane.

### INTRODUCTION

Atomic Force Microscopy (AFM) provides unique opportunities to investigate the structure, morphology, micromechanical properties, and biochemical signaling activity of cells, subcell structures, and even single molecules with high temporal and spatial resolutions [1]. In biological applications, AFM imaging needs to be performed in the natural (aqueous) living environment of the cell in order to observe molecular level interactions and biochemical processes in-situ in the electrolyte solution and to avoid the interference due to the capillary adhesion forces. Despite significant advances made in experimental application of AFM in cell imaging, the data interpretation and associated theoretical models are still in their infancy. This is perhaps owing to the overwhelming complexity of the physical/chemical phenomena taking place during an AFM imaging of flexible, electrochemically active biological samples, which includes intimately coupled fluid flow (inside and outside of the cell), dynamics of the cell membrane deformation, and electrodynamics of ionic interactions in the electrolyte and surface double layers. The critical importance of understanding these interactions should not be overlooked, as pointed out by Kamm in his recent review of cellular fluid mechanics [2], because of the critical role of the flow conditions on the biological functions, normal physiology and disease of living cells. In our previous work [3], the physical processes taking place during AFM imaging of soft biological membranes were investigated in detail. A particular emphasis was placed on the understanding of hydrodynamic effects in the fluid inside and outside of the cell associated with elastic deformation of the membrane in response to the AFM tapping action for the entire probing cycle. In this paper, we extend our prior work by including the electrodynamic effects on the fluid motion and surface forces to obtain an integrated electrohydrodynamic model describing the AFM tip and biomembrane interactions. The model couples the fluid flow (inside and outside of the cell membrane), equilibrium ion distribution, electrical forces, membrane surface charge, and dynamics of membrane deformation.



*Figure 1: Schematic view of an AFM tip approaching a cell membrane and definition of the computational domain.* 

#### THEORETICAL DEVELOPMENTS

#### **Scaling and Model Formulation**

Figure 1 shows the schematic of the physical arrangement used for model development. The electrolyte is considered to be homogeneous with uniform electrical and fluid properties on both sides of the cell membrane, whose surface potential or charge density are uniform and described by a symmetric zeta potential. We also assume that the short-range van-der-Waals, hydration, and other molecular level interactions are negligible compared to the electrodynamic forces when the AFM tip penetrates into the electric double-layer of the membrane. Both the environment fluid and the fluid inside the cell are assumed incompressible Newtonian fluids with the same density and viscosity. The membrane thickness is neglected and mathematically treated as an infinitesimally thin interface. Thermal fluctuations are assumed to be negligible so that the membrane surface is perfectly smooth. We do not consider the ion transport across the cell membrane and the Lorentz electric force is the only body force involved in the probing process. The system dynamics is modeled by the electrically forced nonhomogeneous Stokes equation for fluid flow, the linearized Poisson-Boltzmann equation for the electric potential distribution in the electrolyte environment, the Laplace equation for the electric potential within the dielectric AFM tip, and the Helfrich and Zhon-can's equation is used to describe the equilibrium shape of the bio-membrane. То make the results general, we render the governing equations dimensionless by using the following scales: length scale is given by the AFM tip radius R, velocity **u** is scaled by the tip approach velocity  $V_0$ , time is scaled by  $R/V_0$ , the local surface tension  $\gamma$  is scaled by  $V_0\mu$  with  $\mu$  being dynamic viscosity, the membrane bending rigidity B is scaled by  $V_0 \mu R^2$ , the membrane mean curvature H and spontaneous curvature  $c_0$  are both scaled by 1/R, the Gaussian curvature

K is scaled by  $1/R^2$ , surface force f and pressure p are scaled by  $V_0\mu/R$ , the electric potential  $\phi$  is scaled by  $\zeta(\zeta = kT/e)$  where k is Boltzmann constant, T is an absolute temperature, and e is the single electron charge. Using these scales, the dimensionless governing equations for the electric field potential and electrohydrodynamic stress are: (i) Linearized Poisson-Boltzmann and Laplace equations [4]:

$$\nabla^2 \phi = (\kappa R)^2 \phi, \quad \mathbf{x} \in \Omega_1 + \Omega_2 \tag{1}$$

$$\nabla^2 \phi = 0, \ \mathbf{x} \in \mathcal{Q}_t \tag{2}$$

(ii) Quasi-steady, electrically forced Stokes equation and the continuity equation with combined hydrodynamic and Maxwell electric stresses [5]:

$$\nabla \cdot \left( \boldsymbol{\tau}^{h} + \boldsymbol{\tau}^{e} \right) = -\nabla p + \nabla^{2} \mathbf{u} + \alpha \phi \nabla \phi = 0, \qquad \mathbf{x} \in \Omega_{1} + \Omega_{2} \quad (3)$$
$$\nabla \cdot \mathbf{u} = 0 \quad , \quad \mathbf{x} \in \Omega_{1} + \Omega_{2} \quad (4)$$

where  $\mathbf{x}$  denotes a position vector in the Cartesian coordinate system, and the volumetric charge density has been linearized about the equilibrium ion distribution. The Maxwell stress tensor and the electric field can be written in dimensionless form as

$$\boldsymbol{\tau}^{e} = \boldsymbol{\omega} \left( \frac{\partial \phi}{\partial x_{i}} \frac{\partial \phi}{\partial x_{j}} - \frac{1}{2} \frac{\partial \phi}{\partial x_{k}} \frac{\partial \phi}{\partial x_{k}} \delta_{ij} \right), \quad \mathbf{E} = -\frac{\zeta}{R} \nabla \phi \qquad (5)$$

with the term in front of the Kronecker delta  $\delta_{ij}$  denoting the isotropic stress component.

(iii) Dynamic boundary condition at the membrane interface is given by the Landau's general dynamic interface model [6] combined with Helfrich membrane mechanics and Zhong-can's equilibrium shape equation [7,8], in terms of normal and shear components of the total (hydrodynamic and electric) stress tensor as described in detail in [3],

$$(\boldsymbol{\tau}_{2} \cdot \mathbf{n} - \boldsymbol{\tau}_{1} \cdot \mathbf{n}) \cdot \mathbf{n} = -2\gamma H + B(2H + c_{0})(2H^{2} - 2K - c_{0}H) + 2B\nabla^{2}H$$
(6)

$$(\boldsymbol{\tau}_2 \cdot \mathbf{n} - \boldsymbol{\tau}_1 \cdot \mathbf{n}) \cdot \mathbf{t} = \nabla_s \boldsymbol{\gamma} \tag{7}$$

(iv) Finally, the formulation is completed by introducing the local area constraint condition  $\partial (dA) / \partial t = 0$  [3] in order to find an unknown tension/compression force  $\gamma$  due to the surface force jump given by Eqs. (6) and (7).

Dimensionless parameters in Eqs. (1, 3, 5) are the electric force and electric stress parameters  $\alpha$  and  $\omega$ , respectively, both scaled by the viscous force  $V_0\mu/R$ , and the characteristic diffusion length  $\kappa R$  of the electric double layer based on the Debye length  $\kappa^{-1}$ :

$$\alpha = \frac{\varepsilon \varepsilon_0 \kappa^2 R \zeta^2}{\mu V_0}, \quad \omega = \frac{\varepsilon \varepsilon_0 \zeta^2}{\mu V_0 R}, \quad \kappa = \sqrt{\frac{e^2}{\varepsilon \varepsilon_0 k T} \sum_i \left( z_i^2 n_i^\infty \right)} \quad (8)$$

where  $\varepsilon$  is the relative electric permittivity,  $\varepsilon_0$  is the permittivity of the vacuum, and the summation term inside the

$$\mathbf{u}(\mathbf{x}) = 1 \ \hat{\mathbf{e}}_{x} , \ \mathbf{x} \in \partial \Omega_{t} ; \ \mathbf{u}(\mathbf{x}) = \mathbf{u}_{m}(\mathbf{x}) , \ \mathbf{x} \in \partial \Omega_{m} ; \ \mathbf{u}(\mathbf{x}) = 0 , \ \mathbf{x} \to \infty ;$$
  
$$\phi_{1}(\mathbf{x}) = \phi_{2}(\mathbf{x}) = \phi_{m} , \ \mathbf{x} \in \partial \Omega_{m} \text{ toward } \Omega_{1} \text{ and } \Omega_{2} ;$$
  
$$\phi(\mathbf{x}) = 0 , \ \mathbf{x} \to \infty ; \qquad \phi_{1}(\mathbf{x}) = \phi_{t}(\mathbf{x}) , \ \mathbf{x} \in \partial \Omega_{t} ;$$

$$\varepsilon_r \nabla \phi_t(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = \nabla \phi_1(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}), \ \mathbf{x} \in \partial \Omega_t$$
(9)

where the relative dielectric constant is defined by  $\varepsilon_r = \varepsilon_t / \varepsilon_1$ . Several assumptions are made in the boundary conditions to simplify problem: (i) the AFM tip approach speed remains constant during imaging process, (ii) the membrane electric potential is small,  $|\phi| \ll \zeta$ , so that the Poisson-Boltzmann equation can be linearized, (iii) the polar groups of the lipid molecules keep the electric potential unifom across the membrane, (iv) the AFM tip has zero surface charge density. **Boundary Integral Formulation** 

The model equations are intimately coupled and solved by the boundary integral method. According to Ladyzhenskaya [9], the integral form of the dimensionless, nonhomogeneous Stokes equation combines the contributions from *Stokeslet*, *Stresslet*, and nonhomogeneous source terms and is given by:

$$\lambda u_{j}(\mathbf{x}_{0}) = -\int_{\Omega} S_{i}(\mathbf{x}) G_{ij}(\mathbf{x}, \mathbf{x}_{0}) dV(\mathbf{x})$$
  
$$- \int_{\partial \Omega} \tau_{ik}(\mathbf{x}) n_{k}(\mathbf{x}) G_{ij}(\mathbf{x}, \mathbf{x}_{0}) dA(\mathbf{x})$$
(10)  
$$+ \int_{\partial \Omega} u_{i}(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_{0}) n_{k}(\mathbf{x}) dA(\mathbf{x})$$
  
$$= 0$$

where  $\lambda = 0$  for  $\mathbf{x}_0 \notin \Omega$ ,  $\lambda = 8\pi$  for  $\mathbf{x}_0 \in \Omega - \partial \Omega$ , and  $\lambda = 4\pi$ for  $\mathbf{x}_0 \in \partial \Omega$ . Also, the unit surface normal vector  $n_j$  points into the fluid domain,  $S_i$  represents the vector source term due to Lorentz electric force in Eq. (3),  $u_i$  and  $\tau_{ik}$  represent the velocity and electrohydrodynamic stress fields. Note that when the source point is located at the boundary,  $\mathbf{x}_0 \in \partial \Omega$ , the double layer Stresslet contribution has to be interpreted in the sense of Cauchy principal value because of the stronger singularity in the integral kernel  $T_{ijk}$ . The fundamental solution (*Stokeslet*) and its corresponding stress field (*Stresslet*) are given by [10],

$$G_{ij}(\mathbf{x}, \mathbf{x}_0) = \frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3}, \qquad T_{ijk}(\mathbf{x}, \mathbf{x}_0) = -6 \frac{r_i r_j r_k}{r^5}$$
(11)

respectively, where  $\delta_{ij}$  is the Kronecker delta function,  $\mathbf{r} = \mathbf{x} \cdot \mathbf{x}_0$  is the position vector between the field and source points, and  $r = |\mathbf{x} \cdot \mathbf{x}_0|$  is the distance between them. Further, the domain integral of the source term  $S_i = -\alpha \phi \nabla \phi$  can be transformed into the surface integral by incorporating the divergence free property of the *Stokeslet*,  $\nabla \cdot G_{ii} = 0$ , i.e,

$$\int_{\Omega} \phi \frac{\partial \phi}{\partial x_i} G_{ij} \, dV = \frac{1}{2} \int_{\Omega} \nabla \cdot \left( \phi^2 G_{ij} \right) dV \tag{12}$$

Thus, the boundary integral formulation of Eq. (3) becomes

$$\lambda u_{j} = -\frac{\alpha}{2} \int_{\partial\Omega} \phi^{2} G_{ij} n_{i} dA$$
  
$$-\int_{\partial\Omega} \tau_{ik} n_{k} G_{ij} dA + \int_{\partial\Omega} u_{i} T_{ijk} n_{k} dA$$
 (13)

Eq. (13) is valid for the fluids on both sides of the biomembrane, and the domains can be effectively combined leading to the following unified domain formulation [3]:

$$\begin{aligned} \lambda u_{j} &= -\int_{\partial \Omega_{m}} \Delta f_{i} G_{ij} \, dA \\ &+ \int_{\partial \Omega_{t}} \left( f_{i} + \frac{\alpha}{2} \phi_{t}^{2} n_{i} \right) G_{ij} dA - \int_{\partial \Omega_{t}}^{p.\nu, \mathbf{x}_{0} \in \partial \Omega_{t}} \int_{\partial \Omega_{t}}^{q.\nu, \mathbf{x}_{0} \in \partial \Omega_{t}} \end{aligned} \tag{14}$$

where  $\lambda = 8\pi$  for  $\mathbf{x}_0 \in \Omega_1 + \Omega_2 + \partial \Omega_m$ , and  $\lambda = 4\pi$  for  $\mathbf{x}_0 \in \partial \Omega_t$ . Note that the traction term is replaced by the surface force  $f_i = \tau_{ik} n_k$  for convenience, and the surface force jump condition  $\Delta f_i = f_i^{(2)} - f_i^{(1)}$  in the kernel function can be interpreted as the source density acting on the fluid from the cell membrane surface. Clearly, the solution of linearized Poisson-Boltzmann and Laplace equations, Eqs. (1) and (2), can also be expressed in terms of integral equations:

$$\lambda_{1}\phi_{1} = \int_{\partial\Omega} \left( G_{PB} \frac{\partial \phi_{1}}{\partial n} - \phi_{1} \frac{\partial G_{PB}}{\partial n} \right) dA , \qquad (15)$$

$$\lambda_t \phi_t = \int_{\partial \Omega} \left( G_L \frac{\partial \phi_t}{\partial n} - \phi_t \frac{\partial G_L}{\partial n} \right) dA \tag{16}$$

respectively, where  $\lambda_1 = 0.5$  for  $\mathbf{x}_0 \in \partial \Omega_t + \partial \Omega_m$ ,  $\lambda_1 = 1.0$  for  $\mathbf{x}_0 \in \Omega_1$ ,  $\lambda_t = 0.5$  for  $\mathbf{x}_0 \in \partial \Omega_t$ , and  $\lambda_t = 1.0$  for  $\mathbf{x}_0 \in \Omega_t$ . Note that the coefficient value 0.5 is for the smooth boundary. And the fundamental solutions are given by

$$G_{PB} = e^{-(\kappa R)r} / 4\pi r$$
,  $G_L = 1/4\pi r$  (17)

As shown in Fig. (1), the AFM tip and cell membrane are axisymmetric, so the complexity of the integral formulations can be further reduced by using the cylindrical coordinate system and expressing the fundamental solutions in terms of the Green's functions of the ring source type. Finally, the membrane constraint equation can be expressed in terms of the arc-length with the local surface tangent  $\hat{\mathbf{t}}(\mathbf{x} \in \partial \Omega_m)$  [3]:

$$\sigma \left( \frac{\partial u_x}{\partial s} \hat{\mathbf{t}}_x + \frac{\partial u_\sigma}{\partial s} \hat{\mathbf{t}}_\sigma \right) + u_\sigma = 0 , \qquad \mathbf{x}_0 \in \partial \Omega_m \qquad (18)$$

In the final form, the complex three-dimensional system of integral equations for the coupled electric field/fluid flow/ membrane deformation problem, described by Eqs. (14-16, 18) and boundary conditions Eqs. (6,7,9), is reduced to one-

dimensional form using axisymmetric integral representation and is solved numerically using the boundary element method with discretization along the surface of the AFM tip and the cell membrane [3]. Due to the limited space, the details of all transformations are not shown, but reported elsewhere [3,11].

#### **RESULTS AND DISCUSSION**

#### Hydrodynamic Interactions

We consider three basic interaction processes in respect to direction of the tip movement to characterize the fundamental modes of tip-membrane interactions: first, the AFM tip is approaching an initially horizontal membrane with a constant velocity in positive x direction (forward); second, the tip returns to its initial position moving in negative x direction (reverse); and third, the tip stops at its upper state and the membrane is allowed to freely relax and slowly return to its undeformed horizontal shape (relaxation). It should be noted that the driving mechanisms of the membrane deformation are different than those responsible for the free liquid-liquid interface evolution because of the additional effects arising from the surface bending energy and the local tension or compression force induced by the constant area constraint reflecting the assumption of local membrane incompressibility. The results of presented simulations are based on the geometry of the computational domain defined by the following dimensionless quantities: the AFM tip has total height 10R(where R is the tip radius), the tip opening angle is  $\pi/3$ , and the initial tip-sample separation is 10R. The dimensionless time step is set to 0.1 and is increased to 1.0 in the final stage of the slow membrane relaxation. A test case with the spontaneous membrane curvature  $c_0 = -2.0$  is investigated and the dimensionless bending rigidity B = 0.1, 1.0, 5.0, and 20.0 are used for the simulation of the force-distance curves.



**Fig. 2.** A full cycle evolution of the fluid membrane with bending rigidity B = 1.0 and spontaneous curvature  $c_0 = -2.0$  induced by the AFM tip with an opening angle  $\alpha = 60^{\circ}$ .

Figure 2 shows the membrane evolution during forward, reverse, and relaxation modes of AFM imaging. As a result of viscous flow induced by an AFM motion in fluid outside the cell, the membrane is pushed forward (bends down) by the hydrodynamic piston force, and the fluid within the cell is in turn moved by the membrane with the highest local velocity around the center location. This coupled behavior of two fluids above and below the membrane is consistent with the continuous velocity distribution and the viscous stress jump condition across the infinitesimally thin cell membrane. The curvature-dependent bending energy continuously changes with the membrane bending, thereby providing a local resistance to any deformation away from the planar, equilibrium state of the membrane with the minimum energy. This resistance causes different transient evolution behavior during forward and reverse modes of AFM operation. In the forward (push) motion mode, an increase in the bending energy induces upward motion of the fluid above the membrane (negative local migration velocities of the fluid 1) against the hydrodynamic (forward directed) forces. On the other hand, in the reverse (pull) mode of operation, a decrease in the bending energy assists initially the membrane to withdraw from its highly deformed bend-down state. However, once the membrane returns to and passes its equilibrium position going upward, the bending energy again starts increasing and begins to resist any further deformation of the membrane until the membrane reaches its maximum negative deformation when the AFM tip stops in its upper position. In the final relaxation stage, the migration of the membrane is slow and solely depends on its bending energy and the fluid viscosity. The flow field evolution shows that the viscous hydrodynamic forces affect the membrane state even in the far field along the radial direction, which is a typical dragging behavior of the Stokes flow. If the simulations are continued for sufficiently long time, the membrane eventually returns to its original equilibrium planar shape and the fluid velocity, the hydrodynamics forces, and the membrane surface forces vanish everywhere.



Fig. 3. Isotropic local tension/compression force of deforming membrane with bending rigidity B = 1.0 and spontaneous curvature  $c_0 = -2.0$  probed by the AFM tip with an opening angle  $\alpha = 60^{\circ}$ .

Figure 3 depicts the local isotropic tension ( $\gamma > 0$ ) or compression ( $\gamma < 0$ ) forces in the membrane with respect to the radial position during forward, reverse, and relaxation modes of operation. When the AFM tip is moving forward, the membrane is pushed down by the fluid flow and the tension force is induced to drag the membrane into the center area to satisfy the surface area constraint imposed by the membrane incompressibility. In the reverse motion, compression is observed as the membrane is pulled back and forced to adopt a new shape with smaller area. Even when the membrane recedes over its neutral equilibrium position in the reverse motion (Fig. 2), the surface force is still in the compression mode because the strong hydrodynamic forces overcome the force induced by the slow membrane self-relaxation, thereby maintaining the compression state of the membrane on a shorter time scale.



**Fig. 4.** Effect of the bending rigidity on the hysteresis curve of the membrane deformation vs. tip-sample separation distance for the membrane with spontaneous curvature  $c_0 = -2.0$  and the AFM tip opening angle  $\alpha = 60^{\circ}$ .

Figure 4 shows the instantaneous maximum deformation of the membrane (at the center) as a function of the instantaneous tipmembrane separation distance in a full cycle simulation. Clearly, this plot is analogous to the typical sampling forcedistance curves obtained experimentally during actual AFM imaging of biological cells. The larger bending rigidity translates into stronger membrane resistance to deformation as demonstrated by the smaller variation range for the trace curve along the y-axis. At the same time, when bending rigidity is sufficiently large, the membrane can move faster than an AFM tip initially during the reverse operation mode, which is caused by the strong bending force acting on the membrane. This fact is manifested on Fig. 4 by a decrease of the tip-membrane separation distance below 1.0 at the time moment just past 12.6, for the case of B = 5.0. The lagging response is also observed when the minimum tip-membrane separation distance (equal to 1.0) is maintained at time t = 18.6, 15.9, and 12.6 for the cases with bending rigidity B = 0.1, 1.0, and 5.0, respectively. In the AFM imaging experiments, such an irreversible "hysteresis" behavior in respect to the forward and reverse motion of an

AFM tip is frequently observed for soft samples, and our simulations provide the first theoretical evidence that this behavior is due to coupling of hydrodynamic and elastic membrane effects.

#### **AFM Feedback Force**

The total force acting on the AFM tip is due to: (i) the electrohydrodynamic stress owing to the electrically (Lorentz force) driven fluid motion, and (ii) the Maxwell stress generated by the electric field in the vicinity of the AFM tip induced by the charged biomembrane. The first part is obtained by direct integration of the integral solution  $f_i$  of Eq. (14) along the surface boundary of the AFM tip,

$$\mathbf{F}_{tip}^{eh} = 2\pi \int_{\partial \Omega_t} \sigma f_i \, d\ell \tag{19}$$

and the second part, contributed by Maxwell stress, is obtained by surface integration of the solution  $\phi_1$  of Eq. (15),

$$\mathbf{F}_{tip}^{M} = 2\pi\omega \int_{\partial\Omega_{t}} \sigma \frac{\partial\phi}{\partial x} \frac{\partial\phi}{\partial n} - \frac{\sigma}{2} \left[ \left( \frac{\partial\phi}{\partial x} \right)^{2} + \left( \frac{\partial\phi}{\partial\sigma} \right)^{2} \right] n_{x} d\ell \qquad (20)$$

The Maxwell stress contribution to the force acting at the AFM tip, given by Eq. (20), has been studied before, see for example [12]. Here we only demonstrate the electrohydrodynamic effects by considering three basic interaction processes in respect to direction of the tip movement to characterize the fundamental modes of tip-membrane interactions: first, the AFM tip approaches an initially horizontal membrane with a constant velocity in positive x direction (forward); second, the tip returns to its initial position moving in negative x direction (reverse); and third, the tip stops at its upper state and the membrane is allowed to freely relax and slowly return to its undeformed horizontal state (relaxation). Three typical cases A to C with increasing ionic strength of the electrolyte solution are examined and compared to the purely hydrodynamic case D. The results are shown in terms of the AFM force-distance curve for the tip with 60° opening angle, constant tip approach speed, the membrane bending rigidity B = 1.0, and the relative dielectric constant  $\varepsilon_r = 0.075$ . AFM tip velocity, electrolyte viscosity and electrical permittivity are given by the following set  $(V_0 = 10^{-5} m/s, \mu = 1.5 \times 10^{-3} kg/m/s, \varepsilon_1 = 80)$ . The test conditions are listed in Table 1.

Table 1: Simulation conditions

А	В	С	D
R = 50 nm	15 nm	5 <i>nm</i>	50 nm
$\kappa^{-1} = 96  nm$	30.4 nm	9.6 <i>nm</i>	$\infty$
$n_c^{\infty} = 10^{-5} M$	$10^{-4} M$	$10^{-3} M$	0
$\kappa R = 0.52$	0.493	0.52	0
$\alpha = 160$	479	1601	0
$\omega = 590$	1968	5903	0
$\phi_m = \pm 0.25$	±0.5	±0.5	0

where  $n_c^{\infty}$  is a representative ionic strength with 1:1 electrolyte concentration.


**Fig. 5**: Electrohydrodynamic force (scaled by  $V_0\mu R$ ) vs. tipmembrane separation distance (scaled by R) in a full probing cycle for varying ionic strength of the electrolyte.

Figure 5 compares the force vs. tip-to-membrane separation curves for the purely hydrodynamic system [3] and when Lorentz force contribution is taken into account. The results show that the homogeneous Stokes system (i.e., case D with no Lorentz force) can be a good approximation for the system A owing to its low ionic strength. At higher ionic strength (system B) the Lorentz force contribution increases as the AFM tip approaches the electric double layer of the membrane, and it becomes significant when the AFM tip is penetrating into the double layer (i.e., smaller tip-to-membrane distances). For the system C the strong ionic effect exists for an entire probing cycle (i.e., in the near and far fields) because of the very large ionic strength of the electrolyte solution. In the cases B and C, even in the reverse motion of the AFM tip, the repulsive electric force overcomes an attractive hydrodynamic force and dominates the system dynamics. Also, as the ionic strength increases, the strong screening effect confines the electric double layer into a small region near the membrane and the system can be practically separated into two distinctly different domains. Outside of the double layer, the AFM tip is controlled by the purely hydrodynamic attractive forces well described by the homogeneous Stokes system; whereas when the AFM tip penetrates into the thin double layer, the feedback force is dominated by the strongly repulsive osmotic pressure forces and the viscous fluid forces can be neglected. Analysis of governing equations and numerical tests show that the feedback force acting at the AFM tip is mainly controlled by (i) the two correlated dimensionless parameters,  $\alpha$  and  $\kappa R$ , (ii) the separation distance between an AFM tip and membrane relative to the double layer thickness, and (iii) the membrane surface charge and the material dielectric constants. When Maxwell stress is accounted for, one more dimensionless parameter  $\omega$ needs to be considered to assess contribution of the Maxwell stress relative for Lorentz and hydrodynamic viscous forces.

#### **CONCLUSIONS**

We have investigated fluid mechanics of the AFM imaging of biological membranes in physiological environment to describe the mechanisms of the elastic deformation of the soft sample induced by the AFM tip probing action from the fluid mechanics prospective. In the full probing cycle, a number of interesting and sometimes counterintuitive phenomena was observed such as: (a) dominance of the compression force in the membrane in the reverse (pull-back) mode of operation even after the membrane passes its equilibrium state; (b) a local instantaneous decrease in separation between the AFM tip and the membrane in the beginning of the reverse mode operation when bending rigidity of the membrane is sufficiently large; and (c) the "lagging" behavior (i.e., when the AFM tip-tomembrane separation distance does not change with a decrease in the membrane deformation in the reverse mode of operation) lasts longer in the case of softer membrane with smaller bending rigidity. Relative contributions of the electric Lorentz and hydrodynamic viscous forces to the feedback force acting on the dielectric AFM tip during tapping mode imaging of biomembrane in the electrolyte solution have been quantified. Finally, perhaps the most profound result of this study is that the "hysteresis" observed in the probing experiments using AFM for imaging soft biological samples is due to strong coupling of hydrodynamic effects (fluid motion) and elastic deformation of the membrane. The proposed theoretical methodology provides new insight and quantitative information that cannot be directly measured during the AFM experiment, but essential for interpretation of the imaging data.

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# NANOSCALE MASS TRANSPORT IN LIQUIDS

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#### ABSTRACT

Intermolecular forces in liquids — van der Waals, electrostatic, steric — range over a distance of about 1-100 nm. When liquids are confined to such length scales, their properties and behavior can be significantly altered. In this paper, I have discussed how confined liquids can be used to study biomolecules and biomolecular reactions. Much of the fundamental knowledge is yet to be developed, although this may have direct impact on biotechnology.

## INTRODUCTION

It is fair to say that over the past decade, micro/nanoscale heat transfer has been perhaps the most exciting and active area of research within the heat transfer community, and has also attracted the most amount of research funding. Activity in this area started sometime in the late 1980s. The research was partly driven by the tremendous success of microelectronics and a clear vision that devices were going to become smaller and faster, and that future developments would require an extensive knowledge base for the continuously shrinking time and length scales that would reach tens of nanometers within decades. This also coincided with the invention of a wide variety of experimental tools such as the scanning tunneling and force microscopes and femtosecond lasers, which provided immediate access to phenomena at nanoscales. The ability to make microdevices using MEMS technology became standardized at around the same time. In addition, computing power became readily available such that molecular dynamic and stochastic simulations of micro/nanoscale thermal phenomena became feasible. All these factors put together led to an intense influx and genesis of new theoretical concepts, experimental techniques, and device designs, which led to a remarkable pace of progress. While the research activity continues to grow, one may ask if there is anything left to do or if there are research areas that we should be exploring in the future.

I argue in this paper that while micro/nanoscale heat transfer has received much attention, the fundamentals of nanoscale mass transport, especially in reacting flows, have not been fully explored. Yet they are found in energy conversion devices such as fuel cells. Furthermore, molecular biology provides many examples were mass transport and reactions at nanoscales are not only important for life processes, but a

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Energy Carrier $\Rightarrow$	Molecules in Gas	Molecules in	Electrons in Metal	Phonons in
Characteristics↓	Liquid		and	Dielectric or
			Semiconductors	Semiconductor
Mean Free Path, $\ell$ [nm]	100	0.1-1	1-50	1-500
Wavelength, $\lambda$ [nm]	< 0.1	< 0.1	0.1-50	0.1-5
Relaxation Time, $\tau$ [s]	$(0.1-1)x10^{-9}$	$(0.1-1)x10^{-12}$	(10-100)x10 <sup>-15</sup>	$(1-10)x10^{-12}$
Propagation Speed, v [m/s]	$(0.2-2)x10^3$	$(1-5)x10^3$	≈10 <sup>6</sup>	$(3-10) \times 10^3$
Equilibrium Statistics	Maxwell-	Maxwell-	Fermi-Dirac	Bose-Einstein
	Boltzmann	Boltzmann		

fundamental understanding can lead to new technologies. So what is unique about micro/nanoscale mass transport in reacting flows?

Table 1 provides some characteristic length and time scales for transport phenomena in solids, liquids and gases. For solids and gases, the mean free path is one of the fundamental length scale that demarcates the transition between classical and microscale transport phenomena. For electrons and phonons in solids, the wavelength of energy carriers is also important and lead to the quantum mechanical aspects of transport. Table 1 provides the mean free path of molecules in liquids, which is on the order of 0.1-1 nm. Given this, one would expect no transitions in behavior until one reaches these length scales. It is important to note, however, that the mean free path is not the characteristic length scale that determines transitions in a liquid's behavior. The thermophysical and transport properties of liquids are determined instead by intermolecular and surface forces. So what are these forces and what are the range of length scales that they operate in?

# NOMENCLATURE

- $f_o$  = equilibrium statistical distrubution
- $k_B$  = Boltzmann constant
- $\ell = \text{mean free path}$
- $\ell_{\rm D}$  = Debye length
- T = temperature
- $\varepsilon$  = dielectric constant
- $\varepsilon_o$  = permittivity of vacuum
- $\eta$  = ion concentration
- $\rho$  = electrical resistivity
- $\tau$  = relaxation time

#### INTERMOLECULAR FORCES IN LIQUIDS

When a liquid is in close proximity to a solid surface or a biological molecule, there are four types of forces that are significant - hydration, electrostatic, van der Waals forces, and elastic strain.

# **Hydration Forces**

Solid surfaces such as silica, mica or any other oxides or biological molecules such as DNA or proteins that contain a polar group, are hydrophilic and form hydrogen bonds with water. The H-bond strength between water molecules and the surface can be so strong that the first few layers of water completely wet the surface and are often highly structured. Experimental evidence of such highly ordered 2-dimensional phase of water has been obtained by several investigators [1], which suggest that the strong binding energy decays exponentially away from the surface with a characteristic length scale of 1-2 nm.

#### **Electrostatic Forces**

A solid surface or a biological molecule can be charged in two ways: (i) by ionization or dissociation of a surface group - for example, removal of  $H^+$  ions from a glass surface; (ii) adsorption of ions from solution to a previously uncharged

surface - for example adsorption of  $Ca^{2+}$  ions from solution to replace the K<sup>+</sup> ions in mica. When a surface or molecule is charged, a region of oppositely charged counterions in solution are attracted to the surface. The charge density of counterions decreases exponentially with distance from the surface and approaches the bulk value far away. The combination of surface charge and counterions in solution forms a region near the surface called the *electric double layer*. The length scale that characterizes the exponential decay of electrostatic forces is called the Debye length,  $\ell D$ , which can be expressed as

$$\frac{1}{\ell_D} = \sqrt{\sum_i \frac{\eta_{\infty i} e^2 v_i^2}{\varepsilon \varepsilon_o k_B T}} \tag{4}$$

where  $\mathcal{E}$  is the dielectric constant of the medium,  $\mathcal{E}_o$  is the permittivity of vacuum, e is the charge of an electron, vi is the valence of the ith specie ion and  $\eta_{\infty i}$  is the concentration of the ith ion specie far away from a surface. Typically,  $\ell D$  is on the order of 1-50 nm depending on the ion concentration in the bulk.

#### van der Waals Forces

Although not as strong as hydration or electrostatic forces, van der Waals forces are always present whenever a liquid is adsorbed onto a surface. They arise from interactions of induced dipoles between two or more atoms and are typically effective below 1-50 nm.

#### **Elastic Strain**

The fact that water molecules are highly ordered in a twodimensional ice-like structure close to a hydrophilic surface has been established through experiments and molecular dynamic simulations. Therefore, if the lattice constant of the substrate is not exactly equal to that of ice, the bonds between the water molecules will be strained. The fact that strain influences phenomena at the solid-liquid interface has been known for a while. For example, silver iodide (AgI) has been used to nucleate ice and it is commonly believed that it is the lattice match of the crystal structure of AgI and ice that promotes ice nucleation [2]. Experiments have also shown that strain energy can play a significant role in nucleation processes, in particular for heterogeneous nucleation of ice from water on a solid surface [3,4,5].

#### LIQUID TRANSPORT IN CONFINED REGIONS

It is clear from the above discussion that all the surface forces in liquids operate at different length scales — some are near field and others far field. It is important to note, however, that regardless of their origin, they all operate in the range of 0.1-100 nm. Hence, it is only when a liquid is confined to 100 nm and below by solid walls that one should expect to observe changes in transport phenomena. It must be recognized that the increased surface-to-volume ratio of nanostructured solids is widely used to make compact catalytic reactors. An application of such reactors are in fuel cells, where nanoparticle catalysts improve efficiency. In this paper, I will not discuss transport in catalytic reactors, but focus on nanoscale transport phenomena in molecular biology.



Figure 1 A 120 mV bias across  $\alpha$ HL ion channel produces an ionic current of  $\approx$  120 pA. When a single polynucleotide strand passes through the channel, the current drops to 15-50 pA. The amplitude of the current drop and its duration depend on the type of nucleotide [9].

#### **Biological Nanopores**

Recent work has shown that by monitoring the ion current across a nanopore (1.5-4 nm inner diameter) formed by transmembrane protein ion channels, it is possible to detect single-molecule binding events with the specificity of single base pair mismatches of DNA. The work can be broadly classified into two categories, namely: (i) non-functionalized nanopores; (ii) functionalized nanopores. Almost all of the past work has involved the transmembrane protein ion channel  $\alpha$ -Hemolysin ( $\alpha$ HL) (see Fig. 1) embedded in a suspended membrane separating two chambers filled with ionic solution. The entrance on the top (cis) side is about 2.6 nm in diameter whereas the narrow channel through the membrane that is closer to the bottom end (trans) is 1.4 nm in diameter. When a voltage bias [6] of 120 mV is applied across the ion channel, an ionic current of about 120 pA is produced for ionic concentrations of 1 M KCl (the resistance is approximately 109  $\Omega$ ). When single-stranded polynucleotides are introduced in one of the chambers, they electrophoretically flow through the ion channel. By doing so, they block the ionic current, which reduces to levels of 15-50 pA. This is because the size of the polynucleotides is on the order of the pore size. The time of flight of these polynucleotides seems to vary linearly with their length, and inversely with the applied voltage. It has been hypothesized that different nucleotides would have different blocking signatures (either time of flight or amplitude of current drop), which would allow one to rapidly sequence single-stranded DNA (ssDNA) directly [7]. This has led to many attempts over the last decade, and there has been partial success in discriminating between different bases [8]. For example, polyCs seem to produce shorter but deeper (lower current) decrease in ionic current whereas polyAs produce longer but shallower reductions [9]. However, direct and rapid sequencing of ssDNA has been unsuccessful and remains a



Figure 2 A probe ssDNA is attached through a disulphide linkage to a cysteine residue at the cis opening of a  $\alpha$ HL nanopore protein, as schematically shown above [15]. Shown below are the time traces of the ionic current passing through the nanopore. If the complementary target ssDNA is transported through the nanopore, it binds with the probe strand, which reduces the ionic current for approx. 50 ms. However, if a single base pair mismatch is introduced the binding lifetime is reduced to about 1 ms.

challenge, although hairpin DNA molecules have been detected with single nucleotide resolution [10]. The problem in direct sequencing arises from the fact that the time a single base spends in the nanopore is too short and that the number of ions that it blocks is too few (approx. 100), making it difficult to detect it above the noise. Slowing down the polynucleotides could offer a chance of direct sequencing, but that has also remained a challenge.

While it has so far been very difficult to achieve biomolecule specificity using non-functionalized nanopores, recent work using functionalized  $\alpha$ HL nanopores has been most promising. Howorka et al. [11] functionalized the nanopore with a ssDNA probe attached at the *cis* entrance through a disulphide linkage to a cysteine residue in the  $\alpha$ HL protein (see Fig. 2). Then by transporting target ssDNA sequences, they found that when the target was fully complementary, its residence time in the nanopore, as measured by the duration of the reduced ionic current, was much longer ( $\approx 50$  ms) than if even a single basepair mismatch is introduced ( $\approx 1 \text{ ms}$ ). From this, kinetics of the binding reaction can be quantified [12]. Furthermore, the Bayley group [13,14,15] has also functionlized  $\alpha HL$  protein nanopores with other molecules to study reaction kinetics of various molecular interactions such as small molecules with proteins, ions with proteins, etc.

#### Synthetic Nanopores and Nanotubes

While biology can provide exquisite control on the pore structure and chemistry, they are difficult to integrate them on Si or other inorganic platforms. Hence, synthetic ones made of inorganic materials are desirable. However, fabricating nanopores with 1-2 nm precision is extremely difficult. Recently, Li et al. [16] have demonstrated that artificial nanopores made of inorganic materials (SiNx) can be fabricated using ion beam sculpting, and that they show similar behavior in blocking ionic current when ssDNA passes through them(see Fig. 3). However, direct sequencing of ssDNA has not been



Figure 3 Synthetic nanopore fabricated in  $SiN_x$  by ion sculpting [16]. Passage of a 500bp double-stranded DNA produces a drop in ionic current in response to a 120 mV bias across a nanopore in the presence of a 1M KCl solution.



Figure 4 (Top) Flow chart of the fabrication process for making silica nanotube arrays from vertical silicon nanowire templates. (Bottom) Transmission electron micrographs for the as-prepared silica nanotubes.

reported so far and parallel processing of those artificial nanopores proves to be very difficult with Li's approach.

We have recently developed a process of converting nanowires into nanotubes [17]. Figure 4 shows the fabrication process and some SiO2 nanotubes. It must be noted carbon nanotubes, which have been widely used for nanoscale science and engineering, are hydrophobic in nature and it is very difficult to introduce water inside them. Silica nanotube are, in contrast, hydrophilic such that capillary pressure is sufficient to fill it with liquid. Hence, such nanotubes could be used to study biomolecular transport and reactions. We plan to use these nanotubes to study transport and reactions of biomolecules, perhaps single molecule at a time.

# SURFACE BIOMOLECULAR REACTIONS

One of the technologies that has revolutionized the way genomics research is performed nowadays is DNA microarrays. Figure 5 shows an image of thousands of spots where fluorescently labeled target single-stranded DNA (ssDNA) have hybridized with their complementary strand that is



Fig. 5 Fluorescent image of a DNA microarray showing more thousands of fluorescent spots indicating DNA hybridization.



Fig. 6 Surface reaction of DNA hybridization occurs in DNA microarrays.

attached to a solid substrate (generally glass). Such gene chips allow one to simultaneously study the occurrence or mutations in thousands of genes. In addition, the expression of these genes in the form of messenger RNA (mRNA) can also be quantitatively measured, thus giving insight about the molecular machinery inside a cell. Such DNA microarrays are used not only in basic science but also in applications as well, including forensics, drug discovery, diagnostics etc.

The fundamental process that occurs in such DNA microarrays is a surface chemical reaction, as illustrated in Fig. 6. The speed and efficiency of this reaction depends on a number of factors, namely: concentration of target ssDNA, density of probe ssDNA, length of probe and target ssDNA, and ion concentration. Although DNA microarrays are widely used, to a large extent their performance, although critical, is not well understood. Georgiadis and coworkers [18,19] have performed careful experiments to study the dependence on various factors. Figure 7 shows the effect of surface probe molecular density on the hybridization efficiency. The surface molecular density varies from 2-12 x  $10^{12}$  cm<sup>-2</sup>, which relates intermolecular distance of 3-7 nm. This falls in the regime of hydration, electrostatic and van der Waals forces, such that biomolecular reactions would be significantly altered in such confined regions over that in bulk fluid. The difference in the time taken as well as the efficiency of the reaction suggests that it would be very important to control the mass transport as well as reaction kinetics. Fundamental knowledge of nanoscale fluidic interactions through changes in intermolecular forces is the key to designing such biochips with optimized performance.

While DNA microarrays are commercially produced and widely used, protein microarrays that utilize antibodies as probe molecules are starting to be developed. Here again the speed



Fig. 7 Target hybridization kinetics as a function of probe density. The probe density, determined by surface plasmon resonance, varies from  $2 \times 10^{12}$  to  $12 \times 10^{12}$  molecules/cm<sup>2</sup>. Heating of the probe film prior to hybridization increases the hybridization efficiency. All runs are 1  $\mu$ M target in 1 M NaCl with buffer.

and efficiency of surface reactions would depend on the density of probe molecules, intermolecular forces between them and mass transport of target protein molecules to the surface. This would be an important and exciting area of research.

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#### CONCLUSIONS

Most of the intermolecular forces in liquids that determine the behavior such liquids generally occur with a length scale regime of 1-100 nm. Hence when synthetic or naturally occurring structure fall in this regime, fluid behavior in such confined regions can be drastically different. In this paper, I have suggested how biomolecular transport at nanoscales can be studied and utilized to make contributions both in basic science as well as in biotechnology. I believe this is an exciting area of research where the heat transfer community, and in general researchers in thermofluid science and engineering, can make contributions.

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# FUNDING TRENDS FOR BASIC RESEARCH IN HEAT TRANSFER: A NATIONAL SCIENCE FOUNDATION PERSPECTIVE

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#### INTRODUCTION

It is particularly appropriate and with great pleasure that I am able to represent the National Science Foundation "Heat Transfer" program at this celebration of heat transfer research accomplishments—past, present, and future—at Purdue. It will be my goal in this short article to provide a description of current and future directions for heat transfer research, at least from my perspective at NSF. It should be emphasized that any opinions expressed here represent those of the author and not necessarily those of the Foundation. Furthermore, my perceptions are based primarily on my activities at NSF, and they may be somewhat different from those of program managers at the mission-oriented funding agencies such as DOE, NIH, ARO, ONR, AFOSR, DARPA, and so forth.

The presentation below will begin with a brief description of the mission and strategic goals of NSF, as the basis for the Congressional appropriations that provide the necessary funds. Some current Foundation Priority Areas will be presented, as will their representation within the Engineering Directorate. I will then describe the Thermal Transport and Thermal Processing Program along with some of the current projects that characterize important new areas. Especially prominent among these are important activities funded here at Purdue. I will conclude with some final observations for the present state of heat transfer research in the United States and how the thermal science community may best take advantage of this somewhat mature area in light of a number of emerging technologies.

#### NSF AND THE ENGINEERING DIRECTORATE

As part of the executive branch, NSF works for the President. We are asked for guidance on intellectual and financial priorities. However, we ultimately receive directions from the Office of Science and Technology Policy (OSTP) on intellectual priorities and the Office of Management and Budget (OMB) concerning financial priorities, in line with the President's Management Agenda and the resources provided by Congress. Major federal departments have Secretaries; independent agencies do not, and NSF is an independent agency.

The NSF Mission is "Enabling the Nation's future through discovery, learning, and innovation". The Strategic Goals associated with fulfilling this mission are embodied in three words, and the order is important:

- People A diverse, internationally competitive and globally-engaged workforce
- Ideas Discovery across frontiers and connections in service to society
- Tools *Accessible, state-of-the-art information bases and shared tools*

When NSF prepares a budget request to the White House and then presents this request as part of the White House budget to the Congress, all initiatives and priorities that are the basis for funding increases (and in fact funding maintenance) are characterized in terms of these missions and strategic goals. It is important that each research program, including Thermal Transport and Thermal Processing, and the constituent communities bear this in mind when trying to leverage future funding and to develop new areas for research. For the FY03 Budget Request, the major Foundation priorities were

- Nanoscale Science and Engineering
- Information Technology Research
- Mathematical Sciences
- Social, Behavioral and Economic Sciences
- Biocomplexity in the Environment
- Learning for the 21<sup>st</sup> Century Workforce

The Engineering Directorate at NSF comprises one of seven that fund the bulk of the basic research. It is one of the youngest directorates, having been elevated from a division of the Mathematical and Physicals Sciences Directorate approximately 25 years ago. The organization and FY03 budget request is shown in the following chart:



It should be noted that the Congressional appropriation passed just in advance of this writing will probably increase these amounts slightly.

Engineering Directorate investment priorities for most recent and current fiscal year are summarized in the following chart:

FY02 Investments	New in FY03				
Nanoscale Science and	Workforce for the 21 <sup>st</sup>				
Engineering	Century				
NSE in FY02 \$199M (ENG share \$86.3M)	ENG and EHR Partnership				
Information Technology Re- search ENG invested \$11.2M	Human and Social Dynamics ENG and SBE Partnership				
Biocomplexity in the En- vironment ENG share \$3M	Mathematical Sciences ENG and Math Partnership				

The principal technological themes for future Engineering research were characterized during a recent retreat that consisted of the Division Directors and selected senior Program Managers. At the heart of all the divisions are the common threads of *Materials*, *Design*, and *Processing*. Important supporting topics include overlapping areas of Energy, Environment, Hazard Reduction, Health, Infrastructure, Manufacturing, and Security (no significance in the order). As a result, the Acting Assistant Director has formed six Working Groups to identify gaps and opportunities related to these themes. Three of these have been charged and three more are being formulated for initiation within the next year:

- **Sensors** (Charged; new program solicitation developed for FY03 funding)
- Transformation of Performance Driven Materials (Charged)
- Energy (Charged)
- Environment (To be charged)
- **Infrastructure** (To be charged)
- Health (To be charged)

Significant cross cutting investment opportunities may be expected from some or all of these Working Groups in the next 2-3 years.

# CURRENT EMPHASIS AND FUTURE OPPORTUNITIES IN HEAT TRANSFER RESEARCH

The Thermal Transport and Thermal Processing  $(T^{3}P)$ Program is one of eight programs in the Chemical and Transport Systems Division, whose focus is the science and technology of operations that involve transformations-physical, chemical, or biological-and transport of matter and energy. The investigator community comes primarily from chemical engineering and mechanical engineering, but also includes aeronautical engineers, physicists, chemists, mathematicians, civil engineers, and materials scientists. The primary emphasis of the T<sup>3</sup>P program is to provide support for research leading to an improved understanding of the basic heat transfer modes and their application to manufacturing, materials processing, energy conversion, and temperature control. Traditionally, it has been a major sponsor of research in heat transfer and thermal processing, and it is affectionately known as the "Heat Transfer Program." The current Program Director and author of this paper humbly follows in a long line of distinguished researchers who have devoted a portion of their careers to the nurturing of the area. These individuals include Stefan Thynell, Ashley Emery, Tim Tong, Debbie Kaminsky, Jack Howell, Mike Chen, Bud Peterson, Joan Gosink, Eph Sparrow, Richard Buckius, Bill Grosshandler and Win Aung to name only a few. It should be emphasized that a Program Director has little opportunity to influence the direction of a program over the short time period when he or she is in residence. Rather, the research community must respond to important new initiatives and recognize the thermal science research needs within the context of emerging areas and Foundation priorities. In addition, reviewers must respond by promoting new advances through the peer review process that is at the heart of the NSF funding process.

The T<sup>3</sup>P program continues to enjoy high visibility and popularity among researchers. The vast majority of American industry, and in fact our everyday lives, involve processes that are either enabled or controlled by thermal energy transfer. Almost every energy conversion process includes a transfer of heat, either as a primary energy source or as a secondary process. In addition, thermal transport plays a dominant role in manufacturing and materials processing, and as such has received significant attention in many different application areas including, among others, crystal growth, optical fiber processing, fast-pulse laser interactions with surfaces for processing, cleaning or tempering, as well as electronic assemblies and chips. Continued advancement in electronic devices, from computers to telecommunications, requires careful control of temperature to permit long-life operation, and the reduction in scale of the basic dissipative mechanisms to only a few nanometers has opened entirely new physical domains for heat transfer research.

The following are some of the major topical themes that have emerged during the past few years. The subtopics represent actual projects currently being funded through the  $T^{3}P$  Program.

- Phase change enabled or driven by thermal transport high speed annular flow unsteady condensation multicomponent solidification, including microporosity and inclusions
- High heat flux applications, especially at small length scales microchannel flow in rough channels microchannel condensation thermal ink jet flows
- Complex flow processes (in terms of driving forces, geometry, etc.)

magnetic and electric fields turbulent combustion with radiation turbulence with real surface roughness turbulence with pin fin structures turbulence in building flow environments fuel cell transport processes

- Manufacturing and materials processing ultrafast, precision laser processing optical fiber drawing and coatings MEMS processing control of industrial crystal growth processes
- Nanoscale transport phenomena novel energy conversion devices

semiconductor devices multiscale conduction modeling sub-nano second thermal transport fuorescence microscopy

#### Properties

non-isotropic conductivity under shearing conditions radiative properties of ultra-thin films functionally graded shape memory alloys high temperature combustion gases

Design, control and optimization

inverse design Second Law optimizaion of transport processes active control of non-linear convection

Exemplary among current directions for heat transfer research are recently funded projects at Purdue, with brief summaries provided here.

Tim Fisher, as part of his continuing CAREER award, is investigating thermal-electrical energy conversion phenomena in vacuum electron field emission microstructures with synthetic diamond and diamond-like cathodes. Guided by new theoretical and computational analyses, new experiments will be conducted to characterize thermodynamic performance for low-temperature refrigeration and high-temperature electrical power generation. The results could have significant impact on emerging needs in portable cooling technology and mobile electrical power generation. Further, the efficiency and simplicity promised by this concept could improve large-scale energy systems, such as renewable solar energy converters.

An Industry/University Cooperative Research Center (I/UCRC) for Compact High Performance Cooling Technologies, under the direction of Suresh Garimella, will address research and development needs of industries in the area of high-performance heat removal from compact spaces. The Center brings together faculty from the Schools of Mechanical Engineering, Electrical and Computer Engineering and Aeronautics and Astronautics at Purdue University, and contribute complimentary competencies in heart transfer, microfluidics, microfabrication, refrigeration, computational techniques, mechatronics, controls, acoustics, sensing and actuation and diagnostics and measurements.

A new Information Technology Research grant was recently awarded to Jayathi Murthy and Xianfan Xu for development of a comprehensive set of numerical models and techniques for the simulation of ultra-fast laser machining and to employ these techniques to obtain a detailed understanding of the fundamental physics of ultra-fast laser processing. Largescale simulation offers the possibility of resolving a number of fundamental questions concerning mechanisms of the ablation process in ultra-fast laser machining. The large-scale parallel computing aspects of the research will broaden the capabilities of thermal science researchers in this important information technology area.

Purdue is playing a significant role in a new Nanoscale Interdisciplinary Research Team (NIRT) category. In a project funded at Vanderbilt under the leadership of Tim Fisher, a multi-university team of researchers will examine direct thermal-to-electrical power generation using electron emission from arrays of carbon-based nanostructured emitters, such as carbon nanofibers and diamond nanotips. With characteristic dimensions of one to ten nanometers, these materials enable highly efficient electron emission and the possibility of quantum confinement effects that enhance the energy conversion process.

Suresh Garimella and Tim Fisher have teamed together to study ion driven air flow at the microscale, integrated within micro-featured heat generating surfaces. The work could advance air cooling technology in a variety of electronic products for which air cooling is the only practical means of thermal management. It is the aim of this work to fill a technological gap in microscale convective cooling by developing a pump that is itself truly at the microscale. Preliminary calculations have suggested that cooling rates that compare favorably to those in many liquid-cooled applications are achievable, providing an air-cooling alternative to meet the needs of future semiconductor devices.

As difficult as it may be to believe, there are a number of high quality research activities underway at competing institutions that represent significant advancement of the thermal sciences. A few of those will be highlighted here to indicate by example some of the directions that the field is taking. Stefan Thynell (Penn St.) is investigating the coupling between anisotropic thermal transport and water management in PEM fuel cell membrane systems. The results will have impact on fundamental understanding of anisotropic thermal transport, will address the critical water management issues for PEM fuel cells, and will serve to expose mechanical engineering students to a technology area often considered to be outside the discipline.

The use of arrays of sensors and actuators to control thermally induced convective flows is being studied experimentally and theoretically by Haim Bau (Penn) and his students. Because such flows are nonlinear with many degrees of freedom, effective control is quite difficult. This is a fundamental study that has the potential of enabling control strategies for modifying transport phenomena in significant industrial processes. The research should also facilitate the integration of active control strategies with thermal transport into new educational materials.

Studies of thermal and mass transport processes that lead to dross formation during the oxidation of molten aluminum are being carried out by Ishwar Puri and co-workers at Illinois-Chicago. Reduction of dross formation has potential for significant increases in energy efficiency and reduction of waste in the secondary aluminum processing industry, which produces 1/3 of the aluminum produced in the United States. The project has enabled the PI and his students to interact with their industrial partners at the Gas Technology Institute. Some secondary investigations have lead to a burner redesign for reverberatory furnaces, which may lead to savings for the aluminum industry of as much as \$24M per year.

Adrian Bejan (Duke) is striving to develop a strategy (method) for optimizing the tree-shaped flow architectures in diverse flow systems such as the collection and distribution of water, the distribution of electric power, vascularized tissues, the cooling of electronics, etc. For vascularized tissues under the skin, Prof. Bejan and his students have explained why blood vessels are assembled into perfectly matched arterial and venous blood trees. The reason is that the objective of the vascularized structure is to be the best thermal insulation possible, to minimize the heat leakage from the body core to the ambient. They also derived analytically the proportionality between body heat loss and body mass raised to the power \_, in warm-blooded animals of all sizes.

A common objective in the design of radiant enclosures is to identify an enclosure geometry that produces a desired heat flux distribution over the design surface. Jack Howell and Ofodike Ezekoye (Texas) have been applying non-linear programming to automatically identify the optimum enclosure geometry.

In the figure below the red shaded surface is heated following a specified temperature history while it is kept spatially isothermal as it moves through the heating chamber. The temperature distribution and the power input for the heaters on top are the unknowns, and the predicted values of the power input at various positions on the top surface are shown on the graph. These are predicted by inverse analysis using a conjugate gradient method limited to a few terms.



The University of Puerto Rico-Mayagüez and Hewlett-Packard of Puerto Rico are collaborating to investigate fundamental thermo fluids problems associated with thermal ink jets. Directed by Jorge Gonzalez-Cruz, the project includes modeling and experimentation of the fluid flow process in flexible porous media, development of non-contact thermal sensors using Laser Induced Fluorescence Thermometry (LIFT), and studies of the microboiling process that occurs in the atomization chamber.

Mike Olsen (Iowa State), as part of his CAREER award, will investigate the effects of controlling the surface microstructure on the single phase flow and heat transfer in microchannels, using whole field temperature measurement techniques. If successful, the research could lead to improved performance of MEMS devices and a variety of small scale, high heat flux devices, such as heat sinks for microprocessors, wearable air conditioners for harsh environments, and portable cooling units.

In another recent CAREER award, Li Shi (Texas) will study the thermal transport of nanotransistors that are influenced by ballistic charge transport, and to characterize thermoelectric properties of nanowires and superlattices with potentially superior thermoelectric figure of merit.

H.S. Udaykumar (Iowa) is using his CAREER award to study the interaction of microscale solidification fronts with embedded particles. The work impact on two important areas: the manufacture of metal matrix composites and the cryogenic preservation of biological tissues.

In a continuation of work that has been active for a number of years, Yogesh Jaluria and Costas Polymeropoulos at Rutgers are conducting research focused on high speed coating of optical fibers, a step in the draw process that is critical to the quality and low cost fabrication of optical fibers for telecommunications and other applications. The work includes comprehensive modeling and simulation of the transport processes within coating applicator/die systems, (b) experimentation with a laboratory off-line system developed previously, allowing measurements with different operating conditions, (c) experimentation on a full-scale draw tower, and (d) measurement of specific properties (thickness, concentricity, integrity, presence of bubbles, etc) of coatings produced under controlled conditions. This approach will therefore provide a quantitative, systematic, and validated means to predict and control fiber-coating characteristics.

The projects highlighted above represent only a brief cross section of the diversity of technological areas and potential industrial impact of the fundamental research activities in the T<sup>3</sup>P program. A complete listing of active and even past grants can be obtained from the NSF web page (<u>www.nsf.gov</u>) by "clicking" on "Grants and Awards" and then on "Award Data."

#### FUTURE FUNDING DIRECTIONS

Over the last decade, the T<sup>3</sup>P program has significantly increased its support of materials processing and micro/nanoscale heat transfer. From a strategic point of view, support for materials processing manufacturing research in the microelectronics area is clearly linked to Information Technology Research, and the micro/nanoscale heat transfer to the Nanoscale Science and Engineering Initiative.

The fundamental mechanisms of macroscale thermal transport and their underlying theories are in large part well understood. However, thermal transport and processing usually involves all of the traditional mechanisms to differing degrees, introducing complexity and challenge to both computational and experimental investigations. For most applications of interest to T<sup>3</sup>P, the major difficulties with applying the fundamental concepts are: a) specification of properties, b) definition of the appropriate constitutive laws, c) development of accurate and efficient methods to solve the combined equations of multi-modal transport, and d) application of theory and algorithms to practical manufacturing or processing situations. For example, radiative properties of most infraredactive molecules at elevated temperatures are not accurately quantified, and modeling both macro- and microscopic behavior during the solidification of metals continues to be a computational challenge. Therefore, future research support is likely to address these difficulties and challenges.

It is expected that funding for research in emerging technologies will continue to increase. The area of particular interest is largely related to micro- and nano-scale heat transfer. Applications of practical interest can be found in electronics, flow and heat transfer in microchannels, laser-induced phase changes for microelectronic manufacturing, coating of optical fibers, optimization of thermal systems and improved gas turbine performance.

Besides investigations at small *spatial* length scales, it is clear that T<sup>3</sup>P will continue to address both fundamental and phenomenological investigations in which the *temporal* length scales are in the subnano- or femto-second range. The impetus for these investigations is the availability of inexpensive, highfluence lasers which have been considered for use in removing contaminants from surfaces in materials processing, altering the crystal structure of material near the surface in displays, or removing coatings from painted surfaces.

An area of some uncertainty with regard to  $T^{3}P$  is the area of biological and bioengineering thermal transport. There has been limited activity in this area in recent years at NSF, despite the overall growth in research devoted to biological advances and health, as evidenced by the extraordinary increases in funding levels to the National Institutes of Health, and the new National Institute for Bio-imaging and Bioengineering. Funding levels in the Division of Bioengineering and Environmental Engineering at NSF are among the lowest in the Engineering Directorate, with a great many research groups striving to compete for those funds. The programs in the CTS Division, in particular T<sup>3</sup>P, have a limited capacity to absorb significant increases in proposals in these areas, despite the importance of thermal transport issues in bioengineering. There is hope that a marshaling of interest in "bioheat" may in the next few years help to mobilize an expansion of investment that may involve a productive partnership between NSF and other federal agencies.

#### ADDITIONAL FUNDING TRENDS

The heart of the core research programs at NSF, such  $T^{3}P$ , will continue to lie in the funding of unsolicited, or investigator initiated, proposals. Over half the total research budget of the Foundation is devoted to such activity. In this way a good, novel idea by an investigator that seeks to break new ground of scientific inquiry can prepare a proposal, obtain a fair peer review, and potentially receive financial support for the activity. However, it is clear that most funding *increases* in the next several years will be tied to multi-disciplinary and crosscutting initiatives, such as Information Technology, Nanoscale Science and Engineering, Sensors, etc. In addition, there will be increasing opportunities and pressures for programs to participate in (that is, devote a portion of their core budgets to) special initiatives and interagency cooperative activities. Examples are the NSF/EPA Partnership for Environmental Research, the NSF/Sandia Program in Engineering Sciencs for Modeling, Simulation, Decision Making and Emerging Technologies, the NSF/HUD Partnership for Advanced Technology in Housing, and the NSF/DARPA High Capacity Optical Communications and Networking Solicitation. The T<sup>3</sup>P Program will "participate" in each of these during FY03.

Another funding trend that merits discussion for both advantages and disadvantages is a perceived emphasis on multi-disciplinary proposals. On the one hand, issues in the thermal sciences area can seldom be understood in isolation. Related problems in computational science, electrical behavior, materials behavior, and mechanical behavior are integrally coupled to the advances of many new technology areas. This naturally calls for multiple investigators partnering to produce a more synergistic research activity. Therein lies dilemma, in that research proposals that are multidisciplinary tend to require greater financial resources to be successful. In addition, they may have to satisfy separate peer reviewer constituencies to receive ratings that are high enough to merit a favorable funding decision. The most difficult aspect of initiating such activity successfully is to develop the true synergistic interaction among different research groups working together. In other words, "one plus one" should come out to be equal to "three."

# **Transport Issues in Polymer Electrolyte Fuel Cells**

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#### Abstract

This paper describes recent attempts to define and understand important transport issues that control performance and durability of polymer electrolyte fuel cells. The transport phenomena occurring in fuel cells are characterized by a large range of length and time scales. As examples, we will discuss oxygen/proton transport and water distribution in the microscopically complex catalyst layer at the pore level (microscale, ~µm), water management in the membraneelectrode assembly (MEA) (mesoscale, ~mm), lateral diffusive transport of species and electron transport in the gas diffusion layer over the land between two neighboring gas channels (mesoscale), and multi-dimensional flow, thermal transport, and multi-component species transport on the macroscale (~cm). In addition, a comprehensive physico-chemical modeling framework of combining electrochemistry with multi-scale transport is presented for an industrial-scale fuel cell. Areas for future research into transport issues in fuel cells are pointed out wherever appropriate.

#### 1. Introduction

Proton exchange membrane (PEM) fuel cells can potentially replace the internal combustion engine because they are clean, energy-efficient, quiet, and have rapid start up transient due to low-temperature operation. A PEM fuel cell consists of an anode, a membrane, and a cathode. The membrane, typically about a few tens  $\mu$ m thick, is also the electrolyte and made of proton-conducting polymers. The anode and cathode are prepared by applying a small amount of catalyst, typically platinum black or carbon-supported platinum, to both surfaces of a thin polymer electrolyte. The catalyst-coated membrane is then sandwiched between anode and cathode gas diffusion layers (GDL), and the three components are bonded together to produce an integral membrane/electrode assembly (MEA). The anode and cathode GDLs are contacted on the backside by flow plates with channels that permit oxidizer and fuel flow. The anode flow channel supplies either gaseous fuel (e.g. hydrogen) or liquid fuel (e.g. methanol), whereas air or oxygen is fed into the cathode flow plate. The fuel flowing through the anode channel dissociates at the catalyst layer into protons and free electrons. The protons migrate through the PEM to the cathode where they combine with oxygen from the oxidizer and electrons flowing from the anode through the external circuit, to form water.

Fuel cell science and technology cuts across multiple disciplines, including materials science, interfacial science. transport phenomena, electrochemistry and catalysis. Through a decade-long R&D and tremendous progress, it appears that currently available fuel cell materials will be adequate for near-term markets with highest cost entry points. As a result, the fuel cell and automotive industries are currently placing their focus on fuel cell design and engineering for improved performance and durability. This new focus has led to an urgent need for identification, understanding, prediction and optimization of various transport processes of chemicals, product water, protons and electrons that occur on disparate length scales in PEM fuel cells. This note presents select transport issues that are currently being pursued by an interdisciplinary group of researchers along with their industrial collaborators at Penn State Electrochemical Engine Center (ECEC).

#### 2. Transport Issues

# 2.1 Pore-Level Transport of Oxygen, Water and Protons in Catalyst Layer

The catalyst layer of a thickness around 10  $\mu$ m is a critical component of PEM fuel cells. Gottesfeld [1] provided a good overview of the catalyst layer structure and functions. Oxygen reduction reaction (ORR) occurs in the cathode

catalyst layer, and the hydrogen oxidation reaction (HOR) takes place in the anode catalyst layer. Both reactions require active catalyst sites to break the molecular bond in the diatomic gaseous reactant molecules because of the low temperature environment of PEM fuel cells. HOR has orders of magnitude higher kinetic rate constant than ORR, which leads to ORR being one of the largest voltage losses in the PEM fuel cell. Due to the acid nature of the membrane electrolyte and low temperature operation, Pt or Pt-alloys are the best known catalysts. In order to enable ORR in the cathode catalyst layer, the layer must provide access for oxygen molecules, protons, and electrons. Therefore, the catalyst layer usually consists of: (1) the polymer electrolyte (its amount is also called Nafion content,  $\varepsilon_{e}$ ) to provide a passage for protons to be transported in or out, (2) metal catalysts dispersed on carbon (the electronic phase volume fraction,  $\mathcal{E}_s$ ) to provide a means for electron conduction, and (3) sufficient porosity ( $\mathcal{E}_{g}$ ) for the O<sub>2</sub> gas to be transferred to the catalyzed sites. The sum of all volume fractions is equal to unity; i.e.  $\varepsilon_e + \varepsilon_s + \varepsilon_e = 1$ , and individual volume fractions must be optimized to provide the best overall performance of a catalyst layer.

ECEC has developed a direct numerical simulation (DNS) model to describe the transport of protons, electrons, oxygen and product water at the pore level (of the order of 100 nm) within a microscopically complex catalyst layer [2]. This model is based on a numerical mesh created by either a digitized catalyst layer micrograph or a computer-generated random pore structure controlled by a specified porosity and an average pore size, and subsequently performs direct simulation of reactant and product transport with reaction at the pore level. Such a DNS model is being used by the industry as an alternative to experimental trial-and-error for the optimization of compositions and microstructure of a highperformance catalyst layer. Figure 1 shows the cathode voltage loss as a result of kinetic polarization, ohmic polarization, and mass transport polarization, for a commonly used catalyst layer composition (circles), an optimized design (squares), and a less optimal design (triangles). The threedimensional contour of the O2 concentration on the right illustrates that the less optimized design exhibits restrictive oxygen transport into the catalyst layer due to a too small porosity.

#### 2.2 Co-Transport of Protons and Water in MEA

Water management is a key to high performance and longevity of PEM fuel cells. This is because currently available membranes such as Nafion require water in order to exhibit good proton conductivity. Figure 2 depicts a complete picture of water transport and generation in the MEA as well as the water uptake by reactant gas flowing through anode and cathode gas channels, respectively. Water is typically supplied in the gas feed streams at both anode and cathode through external humidification; however, the most recent industrial practice has been to keep the gas inlet relative humidity to a minimum extent possible, without drying out the polymer membrane. This allows for the reduction in the cost and volume of external humidifiers. Within MEA, two modes of water transport are operative, electro-osmosis that drags a certain number (between 1 and 2.5) of water molecules along with each proton, and molecular diffusion driven by the water concentration gradient set up between the anode and cathode sides of the MEA. In addition, water is produced on the cathode side of MEA due to oxygen reduction reaction.



**Figure 1.** (a) Cathode voltage loss as predicted by direct numerical simulation of proton, oxygen and water transport in a catalyst layer at the pore level, and (b) a three-dimensional oxygen concentration distribution in a random microstructure of the catalyst layer.

The complex interplay of water transport and generation within MEA leads to two characteristics of water concentration profiles inside anode and cathode channels along the flow direction. These are shown in Figure 2(b) as the dimensionless quantity normalized by the saturated water vapor concentration (a function of temperature and pressure only). It can be seen that the anode water profile undergoes a decrease initially, meaning losing water to the cathode side due to the electro-osmotic drag. Thus an electro-osmotic drag control regime can be defined based on this behavior. After the minimum point, the anode water concentration will increase as a result of enhanced back diffusion due to the cathode water concentration continually increasing from the oxygen reduction reaction. On the cathode side, the water profile can typically take two routes, depending primarily upon the membrane thickness. For thin membranes (i.e. less than 25  $\mu$ m), the back diffusion is so strong that it makes the anode and cathode water profiles reach equilibration. At this point, water distributes uniformly within the entire fuel cell, making a continuous stirred fuel cell reactor model applicable for simple analysis of PEM fuel cell dynamics [3]. On the other hand, thick membranes greater than 25  $\mu$ m tend to make the water concentrations on both sides of MEA more diverging from each other, as is illustrated in Fig.2.

Using an on-line gas chromatograph (GC) and an instrumented fuel cell, ECEC researchers have measured the water distribution along both anode and cathode channels, for the first time [4]. Figures 3a and 3b show the experimental data in the anode and cathode channels, respectively. These data combined with a fundamental water transport model provide a valuable tool to understand and design water management strategies for PEM fuel cells [3].

Figure 2 also nicely describes two possible scenarios of electrode flooding. Defining the onset of electrode flooding by the dimensionless water concentration reaching unity (i.e. gas becomes saturated), Fig.2 shows that both anode and cathode will be flooded by liquid water condensed from the gas phase for thin membranes, but for thick membranes only the cathode is susceptible to flooding by liquid water.



**Figure 2.** (a) A two-dimensional sketch of water management in a PEM fuel cell whereby the membrane-electrode assembly separates the anode feed channel from the cathode, and (b) a diagram of water uptake profiles in anode and cathode channels as well as definition of various regimes of water transport.



(a)



**Figure 3.** Water mole fraction distributions in anode and cathode gas channels of an operating fuel cell measured by a micro-GC: (a) anode gas channel, and (b) cathode gas channel. The cell temperature is 80°C, and anode/cathode pressure of 1 atm, and stoichiometry of 1.5 and 2.0 @ 1A/cm<sup>2</sup>.

#### 2.3 Lateral Species/Electron Transport in Gas Diffusion Layer

The gas diffusion layer (GDL) provides dual functions: to supply reactants to the catalyst layer uniformly and to conduct electrons in and out. The lateral transport of species and electrons is referred to as the transport processes occurring in the in-plane direction of MEA between the channel area and the region covered by the land separating two neighboring channels. Here, we are primarily concerned with a mesoscopic scale of approximately one millimeter. On this mesoscale, non-uniform current distribution may result primarily from the low diffusion rate of oxygen in the restricted area covered by the land and GDL resistance to lateral electron flow. Figure 4 displays the current density distributions in a single-channel fuel cell predicted by a most recent model of Meng and Wang [5]. As can be seen, without accounting for the lateral electron transport in GDL, the current density is highest in the middle of the channel because the reaction zone there has the easiest access to oxygen. However, once considering the electronic resistivity of GDL in the in-plane direction, the highest current density region is shifted towards the edges of the channel because these locations have the best combination of easy access to oxygen and short path for electron transport onto the currentcollecting land. This new study clearly establishes the necessity to include the lateral electron transport on a mesoscale in a comprehensive fuel cell model for high-fidelity computer simulations.



**Figure 4.** *Current distribution in a straight-channel fuel cell with the 1mm wide channel bounded by two half-width lands (0.5 mm wide) on the edges at the cell voltage of 0.6 V: (a) without GDL electronic resistance, and (b) with GDL electronic resistance.* 

#### 2.4 Thermal Transport

A PEM fuel cell produces roughly a similar amount of waste heat to its electrical power (such that the energyconversion efficiency is close to 50%). This is a fairly large amount of heat generation. Heat generation in PEM fuel cells stems from the irreversibility of the electrochemical reactions, ohmic resistance, and mass-transport overpotentials [6]. Furthermore, the polymer membrane has low tolerance for temperature deviation from its operating point. Hydration of polymer membrane also strongly depends upon the temperature as the water vapor saturation pressure is an exponent function of temperature. Thus thermal management of a fuel cell is inherently coupled with water management, and the two factors combine to ensure high performance and longevity of a PEM fuel cell.

ECEC researchers have developed a unique technique to embed micro-thermocouples in a multi-layered membrane of an operating PEM fuel cell so that the membrane temperature can be measured *in-situ* [7]. An array of up to 10 thermocouples can also be instrumented into a single membrane for temperature distribution measurements. These new data in conjunction with a parallel modeling effort have helped in probing the thermal environment of PEM fuel cells for the first time [3].

#### 2.4 Multi-scale Simulation of Industrial-size Fuel Cells

Once sufficient understanding of transport issues occurring at various length scales is obtained, this knowledge can be incorporated with electrochemistry to establish a comprehensive simulation tool for industrial-scale fuel cells featuring tens of flow channels. Such a large-scale simulation is now being made possible by parallel computing on PC clusters using millions of computational cells [8]. Figure 5 shows a current distribution for a 36-channel fuel cell predicted by such a comprehensive fuel cell model using 2,560,000 grid-points. Both large-scale and mesoscale variations in the current distribution are visible.



**Figure 5.** Current density profile in the mid-channel crosssection of a 36-channel fuel cell.

#### 3. Summary

Transport in low-temperature PEM fuel cells is an important and physically rich subject. Despite that experimental and modeling capabilities are emerging, presently this is still a largely unexplored area. Much remains to be done before one can utilize the knowledge of multi-scale transport phenomena occurring in PEM fuel cells directly in the cell design and product development.

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# PORTRAITS THROUGH TIME

In preparation for the Purdue Heat Transfer Celebration event, organizers communicated with alumni, inviting them to share briefly their recollections of graduate student life. Contributions came from alumni whose graduation dates span over fifty years. We thank those that took time to paint a more personal picture of Purdue Heat Transfer. The submissions are arranged chronologically below:

# Cecil F. Warner, PhD, 1945, G.A. Hawkins

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I was fortunate to have been one of the early members of the Heat Transfer Group of the School of Mechanical Engineering under the direction of Prof. George Hawkins. I took ME 100, Heat Transfer under Prof. Hawkins as an undergraduate in 1938 and later returned to Purdue to study under George in 1942. John Agnew, Wilmer Sibbit, and I shared offices in a hallway, near Prof. Hawkins' office in the small Heat Transfer Building. Our group was much enlarged when Prof. Hawkins received a contract to investigate heat transfer and cooling of machine guns from 1942-1946. From 1948 through 1975, I was involved in studying heat transfer in rocket engines at the Jet Propulsion Center of Purdue. (Renamed The Zucrow Laboratories).

# Max W. Carbon, BSME 1943, PhD 1949, G.A. Hawkins

I am pleased to write on my recollections of the Purdue Heat Transfer environment. People stand out - in particular, George Hawkins. I still feel deeply indebted to him. Other standouts include Max Jacob for his brilliance in heat transfer, Dr. Brock for his help on electronics, Mr. Stone - impressive because he was a healthy 80 year old, Jim Mundy [who worked on my experiment with me], and fellow students including Chuck

St. Clair, Jack Silvers, Wayne Jens and Wilmer Sibbitt. My work as an undergrad on .50 caliber machine gun research is still fresh in my mind - I wonder if one could fire such guns in the center of West Lafayette today. And the mercury which was scattered in many cracks on the floor in my dark room is still vivid in my memory - I wonder what the EPA or someone would say about that today. Needless to add, my work in the Laboratory has had a huge, beneficial effect on my technical career, my family, and me.

# Wayne H. Jens, PhD 1949, G.A. Hawkins

Recovering from wounds in WWII, having just been married, we arrived at Purdue in a 10foot trailer that we parked in a residential yard near the Union and we began the three best years of our life. Later barracks housing became available as we expanded our family.

The GI bill, a research grant, and a lot of caring Purdue faculty and fellow graduate heat transfer candidates were a blend that made 1946 to 1949 three great years. My research on heat transfer to recoilless cannons provided an opportunity to experience and understand the research process. It is also noteworthy that in the absence of formal nuclear engineering education at our universities, that Purdue provided the basic engineering and more specifically heat transfer knowledge and discipline which enabled me to perform competitively and make contributions in nuclear engineering at Argonne National Laboratory and in the Electric Utility industry. I am totally indebted to Purdue for being a part of the greatest American generation.

# Bu-Xuan Wang (Former Pu-Hsuan Wang) MSME 1949

I received solid foundation on Thermodynamics and Heat Transfer from Professors George A. Hawkins, Y.S. Touloukian and Visiting Professor Hoyt C. Hottel for his special lectures on radiant heat transmission in Purdue University. I returned back Beijing in September 1949 to join Peking University, and then, to head the Teaching and Research Group of Thermodynamics and Heat Transfer in Tsinghua University since 1952. I established firstly a new specialty "Engineering Thermophysics" (Thermal Science and Engineering) in 1957, and was appointed full professor in Jan. 1961. I was elected a Member (Academician) of Chinese Academy of Sciences. I served as Editor of Int. J. Heat & Mass Transfer since 1982. As China opens to the world, I participated in international activities in the broad field of thermal science and technology. I am 81 years old now, but still act as the Director of (Research) Institute for Thermal Science & Eng. in Tsinghua University and as the Lifetime Honorary President for Chinese Society of Engineering Thermophysics. I am honored as a Purdue Heat Transfer Alumni to celebrate the rich future of research and education in heat transfer.

# Edgar L Galson, MSME 1950, Y.S. Touloukian

I was very surprised by Purdue. The size of the Heat transfer faculty seemed as large as the entire mechanical engineering faculty at Cornell University from which I graduated in 1949.



Locomotive testing at the School of Mechanical Engineering in 1897.



Water jet cooling of railway car wheel.



I was a veteran and eager to work at a real engineering job. Thus I finished my master's requirements including a laboratory thesis in two terms. Although my technical training was superior and timely, I was shocked at the differences between Cornell and Purdue. For instance, Cornell was a ferment of all sorts of cultural and political activity while at Purdue student clubs representing the major political parties were prohibited by law. Great concerts and lectures by the outstanding people who were brought to the campus by the university with free admittance did not generate enthusiastic student response. There was an inordinately large amount of interest in sports. Whereas I was and still am a very active sportsman, the spectator sports emphasis was overwhelming Thus my general feeling was that I was in a fine technical school but Purdue did not meet my personal standards of a great University.

Technically I had fine teachers and the laboratory facilities were outstanding. The training I received proved its worth in my work. I did not have intimate relationships with my teachers but I was not seeking such relationships. When I needed help, I received it. Everyone was friendly and helpful. The staff was dedicated. I am grateful for the experience.

# Paul Lottes, PhD 1950, G.A. Hawkins

I have many fond memories of the old Purdue Heat Transfer Laboratory. There was a very friendly, jovial yet serious atmosphere about the place. We all worked together, sharing problems and suggesting solutions. In particular, I recall the fellows that were there at the same time - Max Carbon, Jack Silvers, Lloyd Wilson, Paul Zmola, and Professors St. Clair, Sibbit and Hamilton (that we nicknamed the "Three Wise Men"- due to their collective wisdom). Those were great times!

# Merl Baker, PhD 1952, G.A. Hawkins and Y.S. Touloukian

I completed my MS degree in 1948 on panel heating and cooling under the direction of F.W. Hutchinson. During this work, I had valuable interactions with the heat transfer team. These supportive experiences prompted me to consider a closer relation with the group in pursuing the doctorate. I worked under the direction of Y.S.Touloukian and George Hawkins, and selected a dissertation project concerning the coefficients for two-phase heat transfer of refrigerants flowing inside tubes. As I soon learned, the analysis had to consider many variables and turbulence relationships. Dr. Hawkins was most understanding when I had the opportunity for a tenure-track assistant professorship at the University of Kentucky and approved of my completing the experimentation for the dissertation while at the University of Ky.I returned to Purdue frequently for consultations with him and others. The 230 mile travel between West Lafayette and Lexington is an easy automobile trip today but with the two-lane roads of the 1940 and 50s, it was a challenging commute. Dr. Hawkins' directions and support were invaluable. The Purdue heat transfer program was exciting and inspiring. I continued my research and teaching and became Director of the U of KY Research Foundation in 1953. In 1963, I became Chancellor of the University of Missouri Rolla. The team spirit of the Purdue heat transfer team inspired me to seek challenging professional opportunities, and the directions given me by Dr. Hawkins and others- plus the team-spirit of the heat transfer program-served as spring boards launching and strengthening my professional career.

# Robert Cess, MSME 1956, R.J. Grosh

My stay as a graduate student at Purdue was actually rather short. I arrived at Purdue in September 1955 and departed in May 1956 after receiving the MSME degree. I recall that Ray Viskanta and I took Dick Grosh's heat transfer course together, and Dick was also my thesis advisor. I also recall that Dick's course was the only ME course I took at Purdue (the others were in mathematics and physics), which raised some eyebrows when it came time to graduate. For me, those nine months at Purdue were extremely rewarding, due largely to the incredible mentorship provided by Dick Grosh, with the result that my MS thesis produced my first two journal publications. And I have been able to give something back to Purdue. The current chair of Purdue's Earth and Atmospheric Sciences Department is one of my former PhD students.

#### Alvon C. Elrod, PhD 1959, R.J. Grosh

Since 44 years have passed, a lot of the details of the work that was being done while I was a student at Purdue have been forgotten. However, memories remain of interactions with the outstanding faculty, including Richard Grosh, Thomas Jefferson, M.J. Zucrow, Bruce Reese, and Peter Liley. Fellow students who have gone on to distinguished careers include Morris Ojalvo, William B. Cottingham and William Gaubatz. Interactions with these people had considerable influence on my work of teaching and research as a faculty member at Clemson University from 1959 until I retired in 1988.

#### Peter W. McFadden, PhD 1959, R.J. Grosh

Wonderful memories of excellent teachers, exciting classes, leading edge research, and outstanding students. Professor Grosh taught us the organized approach to problem solving, the advantage of industriousness and the importance of careful work. While my academic/ research career was relatively brief, all the values learned in the Purdue Heat Transfer Labo-

Mechanical Engineering drafting class (1922).



Prof. J.D. Hoffman's shop work class (1927).

ratory proved invaluable in my administrative career. While I am now retired, those same values are serving me well still.

# Bill Cottingham, PhD 1960, R.J. Grosh

My favorite memories of Purdue are of my colleagues and mentors, Dr. Grosh, Dr. Viskanta, Dr. Garrett, Dr. Incropera, Dr. McFadden and many others. I also want to take every one back to the early days of pre-digital when we were studying heat transfer in gun barrels on the old analog machine in the old heat transfer building where Dr Grosh's office was. I am humbled by the research accomplishments of my colleagues. My career tended more toward education and I attribute my small successes to my association with the Purdue Heat Transfer Group.

# Vernon E. Holt, PhD 1961, R.J. Grosh

Always a gentleman and a scholar who inspired me to pursue higher goals.

Incorporating graduate study courses in Math, Physics, Engineering Science and Aero in a Heat Transfer Major, with graduate research programs emphasizing analytical and experimental design and development; Purdue was "ahead of the curve" even in 1961.

# Charles A. Fritsch, PhD 1962, R.J. Grosh

In the late '50's and early '60's, Heat Transfer was transitioning from an art to a science. As Dick Grosh's students, we were immersed in that transition. Dr. Grosh taught a careful, analytical, and scientific approach to the solution of problems that consisted of a clear description of the system and the assumptions made about it and then an application of the basic equations of conservation of mass, momentum and energy, all seasoned with intuition born from laboratory experience. Being well grounded in such a fundamental approach served me well in my career at Bell Laboratories whether it was solving problems in heat transfer, developing computer aids for hardware and software design, or demonstrating the limitations of grand proposals such as Peter Glaser's space sited power plants or the ABM system of the '60's. In short, we were taught "there is no necessity for recourse to artifice".

# Morris S. Ojalvo, PhD 1962, R.J. Grosh

Dean George A. Hawkins was the first person to interview me in 1956 for a position as Instructor and Research Assistant in Mechanical Engineering. This was my introduction to the warm camaraderie that I felt in my graduate studies in heat transfer at Purdue. In addition to my major professor, Dick Grosh, I was fortunate to have Bob Schoenhals, Val Bergdolt, Y.S. Touloukian, J.B. Jones, and Ernst R.G. Eckert (visiting from Minnesota) as mentors and advisors. The graduate students I met at Purdue (including Ray Viskanta, our Russian language expert) added to the real spirit of friendly familiarity and good will that I experienced as my most vivid recollection of Purdue.

Receiving a Ph.D. led to an engineering professorship at the George Washington University (Washington, D.C.) and later, to a staff position at the National Science Foundation (NSF). While at NSF I was granted a two-year leave of absence to accept an appointment as Mechanical Engineering Expert (Thermal Power) with UNESCO to initiate, with sixteen other experts from many countries, a graduate program at the National Polytechnic Institute (Mexico City) teaching Fluid Mechanics and Heat Transfer, prescribing detailed curricula, setting up laboratories and a library. I also wrote a textbook (in Spanish) in Fluid Mechanics which was published by the Editorial Section of the Institute. At NSF I held successive positions as Program Director of Engineering Energetics, Heat Transfer, Engineering Technology, Particulate and Multiphase Processes, Industry/University Cooperative Research Centers and Interfacial, Transport and Thermodynamics, and was able to support Dan Hirleman, present Head of the School of Mechanical Engineering.

# Rollin Dix, PhD 1963, R.J. Grosh and R.J. Schoenhals

My years working with Professors Grosh and then Schoenhals (1957-1963) became the foundation of my career. Learning the science of heat transfer from the best lecture series I ever attended (ME505 and 506) was great. Among many enjoyable and interesting experiences, one stands out. On a Saturday morning I stopped by the Heat Transfer office (in the old Railroad Building) to pick up a book and was amazed to find everyone else there working. I was careful to not repeat the experience (until trying to finish my PhD thesis). Research opportunities, good colleagues, and the Lafayette living convinced me to send my daughter to Purdue. I've been back many times and look forward to the Celebration happily.

# Tom J. Love, PhD 1963, R.J. Grosh

It was an era of time when the digital computer was just beginning to gain a major role in engineering, but the historic large analog network analyzer still occupied space in the heat transfer laboratories. The main experimental work in the lab was the study of thermody-namic properties of fluids in the region of the critical point. The excitement of learning and discovery permeated the group of graduate students crowded into the limited space of the small building.



Laboratory on Otto gas engine.



Ordinance inspectors used in metrology class (1944).

I was impressed with the exceptional quality of instruction in the graduate courses at Purdue. In particular, Dick Grosh and J.B. Jones were outstanding teachers.

My studies at Purdue served as an excellent foundation for my career in teaching, research, and administration at the University of Oklahoma. I give credit to that foundation for the honors that I received in the 1984 AIAA Thermophysics Award and the 1989 ASME Memorial Heat Transfer Award.

As a note of possible interest, while I served as Director of the School of Aerospace and Mechanical Engineering at Oklahoma, I was fortunate to recruit Martin Jischke (the current President of Purdue), who had just completed his doctoral studies at MIT, to our faculty. He proved to be an exceptional faculty member as he advanced through the ranks to full professor. His leadership abilities were recognized in his election as Chair of the Faculty Senate, and his appointments as Director of the School of Aerospace and Mechanical Engineering, Dean of the College of Engineering, and Interim President of the University. I am confident that Purdue will make dramatic progress during his tenure as President.

#### J. Alan Adams, PhD 1965, P.W. McFadden

I was able to begin my graduate studies at Purdue in the fall of 1961 by the skin of my teeth. The Berlin Wall crisis was just beginning and President Kennedy froze all military personnel at about the same time that I was being released from active duty as a communications officer in the USAF.My wife, Ginger and I were a few days late checking into our apartment at 126 Marshall Drive near the airport. Ginger obtained a position as food supervisor at Cary Hall, along with a valuable "blue staff parking permit". When Professor Peter McFadden found out that I was entering graduate school without any financial aid, his first statement to me was "I didn't know that anybody like you was still around". It just so happened that there was still money available to support graduate study, from both NSF and Proctor & Gamble that led to support as both a TA and RA during the next four years. This allowed a move after two years in married student quarters to a more comfortable home on Harrison Street, two blocks south of the Purdue Union.

My masters degree thesis was the design and construction of a supersonic blow-down wind tunnel for the undergraduate lab, to study combined heat and mass transfer in supersonic flow. The Mach number was controlled by changing the shape of replaceable wooden 2-D nozzles and the test section contained cones and wedges coated with naphthalene. Unfortunately, the noise problem was never really solved and the tunnel along with its air tanks did not survive the first renovation of the M. E. labs, when the balconies along with their graduate student offices were removed. Sharing an office with Warren Stevenson, who was later to become the father of optics research within the department, gave me access to a locally made Mach-Zehnder interferometer and its mercury arc light source. This was patterned after a design by Dr. E.R.G. Eckert when he was at Wright Patterson AFB in Ohio, and helped make accurate Ph.D. experimental investigations of combined heat and mass transfer with opposing body forces a possibility.

My relationship with the faculty was for me the most memorable part of Purdue. Teaching fluid mechanics with J.B. Jones, and heat transfer with Peter McFadden set the standard for my entire teaching career at the U.S. Naval Academy. The social contact with J.B. at Purdue football games (and later at Virginia Tech) and with Peter at his ping-pong table (and later during sailing events in Connecticut and Maryland) led to lifetime friendships. Shooting hoops with Bob Schoenhals at Purdue was icing on the cake. The most frustrating time as a graduate student at Purdue was trying to use the first departmental computer along with its machine language, and running back and forth across the alley with punched IBM cards trying to obtain a converged solution to boundary value problems on the larger computer. On the other hand, the evolution of computing capability had the most significant effect on my career. During the past few years as Professor Emeritus, I have placed much of my undergraduate, pedagogical MathCad software into the public domain, available at www.ew.usna.edu/~adams.

#### Russell M. Holdredge, PhD 1965, P.W. McFadden

After receiving the Ph D I returned to Utah State University where I was on leave from the Department of Mechanical Engineering. I retired from USU in 1997. While at USU I served as department head, associate dean and acting dean. Several items stand out when I think about my Purdue experience. First is the thesis direction from Pete McFadden. He provided the ideal amount of direction and still gave me the freedom to develop my capabilities. Another was the interest the faculty took in me and in my research. Bob Schoenhals. Ray Viskanta frequently came by to look over the experimental data I was obtaining even though they were neither my major professor nor on my committee. The classes in heat transfer from Ray V were demanding and pushed me to my limit. Help in these classes was available when needed and they gave me an exceptional background in heat transfer. The third was the quality of the Ph D students. They were good, competitive in class and would go out of their way to help fellow students. Was heat transfer study at Purdue a positive experience—absolutely.



Research on boiling heat transfer in 1953.



Heat loss from transmission lines are measured using wind velocities up to 60 miles per hour and currents up to 100 amperes (1950).

# Louis C. Burmeister, PhD 1966, R.J. Schoenhals

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A few days after my August 1962 arrival, Richard Grosh (Head of the School of Mechanical Engineering) stopped me as I was walking across campus and gave me a ride to a friend's house, setting the tone for my Purdue experience. He was a good heat transfer man, I already knew from Charles Hebert Treat, my colleague at Sandia Corporation in Albuquerque, NM, who had done a Masters thesis with him. Treat recommended Purdue for a Ph.D. program, not only because the faculty was good in heat transfer, but also because the program was good for students, not placing artificial difficulties in their paths. There were no final examinations in courses—a comprehensive exam after the Ph.D. course work had been completed consisted of a battery of tests in the evening, one per course with about six specified by the major professor. There was no qualifying exam—I was admitted to the Ph.D. program on the basis of existing materials that attested to my record. The faculty treated the graduate students as much like colleagues as possible-graduate students were included in the school annual pre-Christmas social, and I ate my first kumquat there. Work with Peter McFadden's group of graduate students to develop experiments for a new laboratory for the undergraduate heat transfer course was formative. Professor Aspel (Associate Head) told me that the students are a high class of people with whom to work, and I found that to be true. Robert Schoenhals (his wife Betty joined him in being hospitable to my Rosalyn and me) suggested a very good dissertation problem, the effect of pressure fluctuations on film boiling. And, it was on the basis of his course in convection heat transfer that I later was able to write a book on that subject. E. R. F. Winter and Robert Schoenhals let me work with them in preparing a research proposal, adding to my education in an important way. The digital computer was in Chicago-card decks were motored there in the afternoon and returned the next morning with printout, so debugging was time consuming. Later the digital computer was on campus, but it still took up to six hours for turn-around. One day Kenneth McCoy. my former undergraduate classmate at another institution who was also in the heat transfer program, remarked, "there is so much more here!" The blend of experimental and analytical projects made it possible to learn a great deal just by looking over the shoulders of fellow degree candidates.

# Terry L. Libby, MSME 1968, R.J. Schoenhals

My experience in the graduate ME school majoring in Heat Transfer centers on the small attached lab in which we aspiring grads conducted our 'hands on' experiments. Prof. Edgar Winters scrutinized my daily data collection while Dr. Bob guided my sometimes wayward efforts toward thesis completion. My study involved a project for NASA. Specifically, I was observing the stratifying effect on a volume of water resulting from a gradient of heat transferred through the walls of the container while monitoring the changing temperatures of the controlled water volume. My equipment consisted of a Plexiglas rectangular container with a myriad of thermocouples wired to an analog recorder spitting out a cash register type tape of the recorded temperatures. From this crude setup, by today's standards, we were able to establish several empirical relationships that gave support to the advanced study that followed, the study of the stratification of cryogenic fluids and the design of equipment.

# David A. Nealy, PhD 1968, P.W. McFadden

I transferred to Purdue in 1963 to initiate a doctoral program in gas turbine related heat transfer. R.J.Grosh, who was Mechanical Engineering Dept. Head at the time, helped me to decide to come to Purdue, a decision I have never regretted. Owing to a somewhat unusual arrangement which allowed me to do much of my thesis research in absentia, I was only on campus about a year and a half, sharing the barracks-like heat transfer laboratory building with several contemporaries, including Bob Watts, who subsequently joined the ME staff at Tulane. I always thought that building was aptly named thanks to what seemed to be enhanced rates of heat transfer—in during summer, out during winter! My major advisor was Pete McFadden whose constructive advice and patience with my sometimes glacially paced off-campus research progress will always be greatly appreciated. Pete became head of the School of Mechanical Engineering while I was still his student, and I believe I may have been his last Purdue graduate student before he moved to the Dean of Engineering position at the Univ of Connecticut. I continue to feel honored to have been associated with Purdue Heat Transfer and its proud history.

# Kenneth E. Wilkes, MSME 1968, Y.S. Touloukian

I came to Purdue in the fall of 1966, after having graduated from Duke University. There to greet me was Prof. David DeWitt, who also was a Duke alumnus (he and I have a connection through the Duke swimming team: he was a champion swimmer there in the 50s, and I was a champion team manager there in the 60s). Even though Prof. Touloukian was my official advisor, Prof. DeWitt interacted more directly with me, advising me on courses and research work. I managed to take only two heat transfer courses, ME 505 from Prof. Leidenfrost and ME 606 from Prof. Viskanta; the rest of my schedule was loaded up with physics and mathematics courses. My other advisor was Dr. Reginald W. Powell, a senior researcher at the Thermophysical Properties Research Center (TPRC). He was the world's expert on thermal conductivity of materials, and had recently retired from the National Physical Laboratory in the United Kingdom. Other extremely helpful persons at TPRC were Dr. Ray Taylor and Hans Groot. I did some serious damage to Ray's ribs while playing basketball at the old



Thermosyphon loop used to determine boiling heat transfer coefficients in two-phase flow (1954).



A late 1970's project investigates heat transfer to and from latent energy storage materials. The figure shows optical interference fringes in the liquid during melting of n-heptadecane around a heated horizontal cylinder.

YMCA in Lafayette. Ray still has not forgotten about that. My thesis was on measurements of the thermal conductivity of pure metals, and I produced the first experimental thesis from TPRC. The rest of my life has been mostly spent chasing the thermal behavior of this or that: metals, ceramics and graphites at the Battelle Memorial Institute, fiberglass insulation at Owens-Corning Fiberglas, and insulations and refractory metal alloys at the Oak Ridge National Laboratory where I am now a Distinguished R&D Staff Member. Along the way I obtained a PhD in condensed matter physics at the Ohio State University, with an experimental dissertation on the Kapitza thermal boundary resistance between metals and superfluid helium.

# Ed Eisele, PhD 1969, W. Fontaine and W. Leidenfrost

I did my heat transfer research at the Ray W. Herrick Laboratories and at that time there was research work on heat transfer also going on at the M E Annex, the Jet Propulsion Laboratories and in a number of other nooks and crannies in the M E building. Despite the geographic dispersion we heat transfer types had a good sense of each other's projects and all took the same courses which kept us in touch. Professors also often had students in numerous university locations so that we all felt as if we were part of the same team. No one location was deemed to be superior to another, largely the result of the attitudes of the professors. If you were doing an experimental thesis the model shop in each area also had skills that could help you and we students were allowed to take advantage of those skills. I particularly enjoyed the multidiscipline environment at the Herrick Labs. All of the experimental work was done in one large bay. It was impossible to work there and not have people (students, staff and visitors) stop by to see what you were doing and likewise, when you were frustrated, you could stop by and see what others were doing. Funny how other people's problems often seemed more interesting than your own at times! We also had a "coffee room" where, during a break or after class, some of the best discussions occurred on on-going research. These discussions often got quite involved and the resident blackboard got quite a workout. Sometimes the discussions became mini oral defenses of a research topic. Many of us quickly found out that the best and most profound questions were asked by people who were not working in your field! Over the years I have set up many engineering organizations worldwide and have always worked to have not only an open office and laboratory architecture, but also to have some meeting places where informal but very meaningful discussions could take place. As a result of my Purdue experience I am a firm believer that multidisciplinary solutions to problems are the best. I have also always felt that my work ethic and management style were largely shaped during my years as a graduate student at Purdue. Thank you Purdue for a stimulating, exciting and enjoyable educational experience.

#### William O. Barsch. PhD 1970. E.R.F. Winter

After graduation I accepted a position at Youngstown State University in Ohio as Coordinator of Mechanical Engineering Technology. This position required teaching and curriculum development in a much broader area than just heat transfer. I subsequently lead the program in the development of a 4 year curriculum, ABET accreditation, and later became the Chairman of the entire Engineering Technology Department encompassing 15 full-time faculty and over 1500 student majors. My training in Purdue's

classrooms, both as a student and later as a graduate instructor in the Heat Transfer Lab, gave me the tools to succeed. As a college Professor, I tried to emulate the effective teaching methods of Professor R.J. Schoenhals in Heat Transfer and Professor R. Fox in Fluid Mechanics. Now retired, I think fondly of the time I spent with my office mates, Al Wen and Alex Wong, in the Heat Transfer Annex building. Thank you Purdue.

# L. M. Clark, BSME 1973, MSME 1974, D.P. DeWitt

Purdue provided me opportunity when I needed it the most. Whether I deserved the help is arguable but in my time of need the University helped immeasurably.

I was initially awarded a Purdue scholarship and a national scholarship, chose Purdue over Michigan, was selected for the engineering honors program (the courses with H's added). After 2 years of pursuing non-scholarship activities and not learning much of anything, the University declined to allow me to continue. Almost 4 years later and after service in a volunteer unit in Viet-Nam, I was readmitted. The road back was very tough. On paper I had 3 semesters of credit but without any knowledge from the courses, essentially starting from scratch as a sophomore. It actually took years to get back up to the intellectual level comparable to when I left high school. Redevelopment of learning habits and analytical skills that had rusted away never fully returned until graduate school. But with understanding and encouragement, I graduated and was accepted for a research assistantship in heat transfer. Dave Dewitt was my supportive advisor. Ray Viskanta was on my committee (from him I learned about non-Fourier effects) as was Ray Taylor from TPRC. No need to say more except to add that over the years heat transfer and thermal sciences have served as excellent grounding for all the engineering science areas I have worked. And having also gone to Rice University which is an excellent school, I have nothing but praise and gratitude for the Purdue University Mechanical Engineering School and its faculty.

Thermosyphon apparatus for studying thermal-

buoyancy driven flows (1984).



Instrumentation center for recording data on the energy-efficient demonstration house (1985).



# Ray Chupp, PhD 1973, R. Viskanta

In my association with Purdue, I have two unique distinctions. First, I was in the very first group of four-year undergraduate students from GMI (now Kettering University) to attend Purdue and receive a Masters Degree with the thesis also counting toward GMI's Bachelor degree. In fact, I received the MS six months before the BS. Second, I had the honor of being associated with Purdue's graduate school as a student for ten years. This was one of the "benefits" of doing the thesis work in absentia. Ten years was the maximum time (at least at that time) that the course work would be credited toward the degree. So I tied the record maximum time in Purdue graduate school (that is without taking any courses over again). With so much time at Purdue, I collected many fond memories. I remember the professors who were outstanding and challenging; the staff who were courteous and helpful; the other graduate students with whom I learned and had enjoyable times; and the exciting sporting events including the home football games during the season that Purdue went to the Rose Bowl. I distinctly remember the quantifying and thesis exams because they showed me that I had mastered a few things but had a lot yet to learn (and still do). Ray Viskanta was an excellent major professor, advising me on both my MS and PhD thesis efforts. I appreciate his guidance and his compassion. He especially demonstrated the latter as I was approaching the ten-year "statute of limitations." He arranged for funding for me to return to campus to complete my thesis work. The education, experiences, and degrees from Purdue have been invaluable. My 35+year career has spanned four major companies and I believe I have made significant contributions in all four-a major part due to Purdue. I trust that the Mechanical Engineering Celebration of Purdue Heat Transfer is a very memorable event.

# Tim Craig, MSME 1982, F.P. Incropera

University life in West Lafayette, and in particular, the study of Heat Transfer at Purdue, was located close to an old smoke stack in 1976. Just as it served as the Schools Of Engineering locator beacon, the Red Bricked ME building was a beacon to the study of the Thermal Sciences for me. Undergraduate course work in Heat Transfer was centered on a draft version of what is now the benchmark text of Incropera and DeWitt. I continue to cherish the typed, double spaced and photocopied pages that contain the snippets of Prof. Incropera's insights noted in the margins. And, I keep my First Edition, hard cover copy of 'Heat Transfer' by Incropera and DeWitt, penned with Frank's wisdom, close at hand.

Seemingly as fate would have it, and once committed to graduate study under Frank Incropera, and assisted by Professors Viskanta and DeWitt, my path crossed with fellow students Ted Bergman and Mark Brosmer. With Frank's leadership, teaching and encouragement, the "stooges" team of Bergman, Brosmer and Craig flourished in that basement office that offered a bird's eye view of the ME building bike rack, a built-in chin-up bar and late night visits from the inhabitants of the buildings infrastructure that were stirred up during the renovation then underway. It is in retrospect that I fully appreciate the learning, creative and energetic environment that is Purdue's School of Heat Transfer as one that was highlighted by outstanding educators, first rate research and first class support staff, and one that I shared with what I am privileged to call friends. Thanks!

# Chie Gau, PhD 1984, R. Viskanta

As I recall, Purdue heat transfer had a sound and great team work. They had a very sound program in both teaching and research. The heat transfer lab. was well equipped. Students could get most recent information of research in the area of heat transfer from the weekly group seminar. Purdue also had a very good electronic shop and a machine shop to help to build necessary equipments and instrumentations for the experiments. Especially, people in electronic shop was very friendly and helpful. They were able to build most of the instrumentation you need, and provide useful information in electronics. I was very fortunate to be educated in the heat transfer group of Purdue and advised by Professor Raymond Viskanta. I have built a solid foundation in the area of heat transfer at Purdue. Especially, Professor Viskanta has given me a very challenging work of research and a great opportunity to achieve success. My achievement in the area of heat transfer is attributed mostly to the excellent research environment at Purdue and Professor Viskanta's guidance during my graduate study.

# Stuart Olstad, MSME 1984, D.P. DeWitt

What I recall most about the Heat Transfer department at Purdue is the individualized attention that I received. While I was there, many of the faculty such as Professors DeWitt, Incropera and Viskanta, were at the mid-point of their professional careers. Though already established in the discipline, they were about the difficult task of still furthering their reputations and that of the School. Yet they always seemed to put my interests as a student front and center-not only with regard to classroom and research matters, but also with respect to matters attendant the full post-graduate experience. My advisor, Professor DeWitt, was instrumental in helping me network, attend symposia, and in finding exceptional employment upon graduation. Such individualized attention got me off to a great start.



A flow visualization experiment that will consider the effect of orientation relative to gravity on the solidification of crystals in annular cavities used for thermal management of very large scale integration (VLSI) circuits (1986).



Jet impingement studies with application to the cooling of primary metals processing. Heater and temperature measurement module are developed for monitoring local heat transfer to an impinging liquid jet (1987).

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# M. Pinar Mengüç, PhD 1985, R. Viskanta

I remember Purdue nights more than any other thing. Particularly, the yellow-orange scattered light from the smokestack, which is long gone, is really in my memories. It seems that that smokestack was like a magnet, or a beacon, as we traveled back and forth between our homes and the ME Building all the times.

# Brent W. Webb, PhD 1986, R. Viskanta

My time at Purdue was truly an enriching experience. I appreciated the camaraderie of other graduate students with whom I associated, both day and night in the Lab. We shared ideas (both technical and other), took joy in each other's success and offered encouragement in challenges. I have fond memories of friendships with my graduate student contemporaries. I am not surprised to see that they have excelled professionally.

Nearly two decades following my departure from Purdue, I note that much of who I am professionally I trace to my training and the interaction with world-class faculty there. I recall vividly the trust I felt in my technical work from my advisor Professor Viskanta. From him I learned not to be afraid to try to do my best work to place my trust in students even if they don't yet merit such. In him I saw the excitement of discovery long after it has faded for so many. I saw his concern for his students, providing wise counsel and support in areas well beyond the discipline we studied. A paper submitted to him for review at 5:00 pm was back on my desk at 7:30 am the next morning, replete with feedback in red. His wife insisted on entertaining us once a year, and we enjoyed her personable complement. She once quipped that even though her husband was known the world over for his work in heat transfer, he couldn't grill a hamburger without burning it. Other Heat Transfer faculty left their mark on me as well. Because of a conflict in scheduling my thesis defense, Professor Incropera, a member my thesis advising committee, spent two hours with me giving feedback on my thesis, almost page by page. From him I learned to be thorough. I remember Professor Ramadhyani sharing unselfishly his modeling expertise with me. I still aspire to his organized, methodical approach, and he helped to instill in me a love of numerical modeling. I recall Professor Mudawar's frequent trips to the laboratory working closely with his students. Like him, I have been drawn to the lab where the action is. Even after Professor Leidenfrost had retired, he came regularly to the office. It seemed he could not stay away. I hope to have such enthusiasm for the work at that stage in my career. Other faculty there taught me the importance of rigor in the classroom. I am deeply appreciative the investment Purdue made in me, and I hope to be able to pass it on.



Experimental facility for mixed-convection heat transfer studies (1988).

# Christoph Beckermann, PhD 1987, R. Viskanta

My Purdue heat transfer experience has enabled me to become a successful researcher and teacher at The University of Iowa for the last 15 years. My time as a graduate student was also personally very fulfilling. None of this would have been possible without the guidance of Professor Viskanta. He made me perform at a high level as a student and is still my most important role model as a professor. What also defined my experience at Purdue were the excellent graduate students in the heat transfer area during the mid-1980s. Among them are Bill Bennon, T.H. Song, Pinar Mengüç, Dave Zumbrunnen, Ted Bergman, Brent Webb, Dave Vader, M.K. Moallemi, A. Ungan, J.A. Weaver, F.Wolff, S. Chellaiah, and others. During the 4 years from 1985 to 1988 alone, Professor Viskanta and his students published 79 papers in archival journals. As of January 2003, these 79 papers have been cited almost 1,500 times (source: Science Citation Index). These numbers exceed what many professors accomplish in their entire career. I believe that the interactions among the graduate students were crucial in achieving these results and they had perhaps the greatest impact on my experience at Purdue.

#### James Heidmann, MS 1988, F.P. Incropera and S. Ramadhyani

I came to Purdue in 1986, fresh out of undergraduate study. I didn't intend to pursue heat transfer - in fact, I was considering Purdue along with Illinois and Michigan, and really wanted to get into aerospace engineering. However, my meetings with Professors Incropera and Ramadhyani convinced me to work with them on convective cooling of electronic components - something I hadn't considered before. The education I received at Purdue, especially in the laboratory on my thesis work, prepared me very well for my future work - back in aerospace engineering at NASA Glenn Research Center. After my PhD qualifying exam a few years ago, the committee commented that my knowledge of heat transfer really carried me through (despite my weakness in compressible flows!). My time at Purdue was clearly the most beneficial educational experience of my life, and laid the groundwork for my work at NASA in turbine heat transfer.

# James Maughan, PhD 1988, F.P. Incropera

Nothing but good memories mark my time at Purdue, beginning with my February visit as a senior at BYU looking for a good fit in a graduate school and ending with my departure five years later for a GE job in New York with a 400 page thesis, a two year old kid, and an aging Chevy Citation. The one kid has now turned into four, the Citation has turned into a minivan,



Scanning electron microscope (SEM) for examining dendritic structure and measuring solute distribution is used to understand the relationship between microscopic and macroscopic transport processes during metal alloy solidification (1990).

and the thesis gathers dust on my office bookshelf, but I still think I could not have chosen a more suitable graduate school, program, or advisor.

Certain things still stand out: the challenging coursework, weekly seminars and advisor meetings, football games, Married Student Housing, long bike rides, the Sigma Xi contests, and my lab and office in the basement,#58, where after 4 years, I felt so attached I took the room number off the hallway wall and with me when I left. Purdue people with similar experiences are everywhere. I meet half of them when I point out the heat transfer text they have is from my professor, Frank Incropera.

What I miss most are the luxuries (I didn't fully appreciate) of endless hours at the library, building my own equipment, doing my own testing, having a purely technical focus, and pursuing something until I had a thorough understanding and had done my very best work. I don't suppose the specific coursework or my little study of mixed convection was of too much direct benefit to others or to the things I have done since and hope to yet do, but the approach I perceived at Purdue, namely not the problem and the math, but the physics, the principle, and the practical application of understanding, has made a huge difference. Learning that approach (and learning to pass it along to others) has been, I would say, my most important memory of my days at Purdue.

# Srinivasan Chellaiah: PhD 1988, R. Viskanta

Recollections by definition are reflections of the past in the present. My stay (Aug 1984 - Aug. 1988) at Purdue was as a doctoral student of Professor R.Viskanta. When you are among the best in your professional community and studying in a premier institution, one thing that stands out is the breadth of exposure that one receives. In addition, working with Professor Viskanta was truly a pleasure. I learnt a lot from him both professionally and personally. His dedication was par excellence. It could be a blizzard or brutally cold dry winds piercing your bones. Yet, he was there on a Saturday morning. He set high standards and demanded quality work, but he never gave up the human side. He was considerate and compassionate. I will always cherish my association with him.

My recollections cannot be confined to the reflections of the past; they have to include the influence of the past associations in my present endeavors. I owe my present capability to foray into new areas to the strong background (in both depth and breadth) that Purdue provided me. I admit that I realized this only after I left Purdue. The sense of discipline, the competitive spirit, the desire to achieve, the spirit to venture into new areas all have stemmed from my four years at the campus. I take immense pride in saying that when I mention that I am a "boilermaker", to the professional community at large, and heat transfer group in particular, I am put in a separate class. Is there anything more that one can expect from a graduate school?.

# Dave Zumbrunnen: MS 1984, PhD 1988, F.P. Incropera and R. Viskanta

I came to Purdue after serving in the United States Navy aboard submarines. I was accustomed to a work environment where excellence is pursued. The heat transfer group in the School of Mechanical Engineering had the right 'feel' to me. I found faculty members who were effective mentors and accomplished researchers. Research was fundamentally interesting but also of practical importance. I sensed then and still appreciate today an academic environment where educating students, delivering results for the benefit of society, and professional advancement of everyone involved was unified.

# Abdulmajeed Mohamad, PhD 1991, R. Viskanta

Purdue molded my visions for research in heat transfer, particularly in the applications of heat and mass transfer. It was a pleasure and an honor to associate with Prof. Ray Viskanta. Ray was not only a teacher but also a great man. Ray's style of working influenced me throughout my career. Also, weekly seminars held by the heat transfer group broadened my understanding of different problems in heat and mass transfer.

I should mention that Satish Ramadhyani was a good teacher, who introduced me to the finite volume method. The time I spent at Purdue is full of memories and is unforgettable.

# Lubna B. Younis, MS 1991, R. Viskanta

Delightful inspirations always occur when Purdue University's name mentioned because of the special impact it has on my present study (PhD) at The University Of Calgary, Canada. Purdue faculty members at the School of Mechanical Engineering broaden my vision on the practical application in the area of heat and mass transfer through the open-ended assignments and projects. I will always be grateful to Prof.Viskanta for his valuable supervision, encouragement and advice. Prof.Viskanta was not only a great supervisor but also a great friend. Prof.Viskanta taught me a high standard and ethic in research that I will always cherish through my life. Last, I have to say that "Teachers open more than books they open minds".



Apparatus for determining the convection heat transfer coefficient for air flow through tubes imbedded in ceramic particles. This investigation provides an understanding of fundamental mechanism occurring in packed-bed type combustion heat exchangers (1991).



Research is underway to investigate fundamental processes involved in laser materials interaction, including energy transfer during femtosecond laser material interaction and near field, nanometer scale optical phenomena. Laser-based techniques are also developed for fabrication of micro and nanostructures, sensors, and bio-detection systems. The image shows an ultra-clean laser micromachining technique developed at Purdue.

# Patrick Prescott, MSME 1984, PhD 1992, F.P. Incropera

I have many fond memories of my experience as a graduate student in Purdue's Heat Transfer area in Mechanical Engineering. It was a period of great intellectual growth, facilitated by my advisor, Frank Incropera, who was always very kind to me. But there were many others who helped me enjoy those days. These included all of the Heat Transfer faculty, members of the technical and administrative staff, and most of all, my fellow students, who came from all walks of life. The camaraderie among the students was uniquely special, and the faculty did a fantastic job of nurturing this environment through their friendly interactions with students and one another. Indeed, the Heat Transfer area at Purdue is special.

#### Steve Slayzak, MS 1992, F.P. Incropera and R. Viskanta

Purdue provided a "best-of-the-best" culture of both peers and faculty. The experience defined for me the highest qualities of professionalism in research and continues to serve me profoundly well in hiring and contracting the best talent. I'm also thankful that Purdue's rigorous learning environment allowed me to pursue the physics as I was best able, to eventually describe a phenomena the equations did not.

#### Aaron M. Huber, PhD 1993, R. Viskanta

I enjoyed the opportunity to participate with the Purdue Heat Transfer Group. The range of ongoing research projects was fascinating to observe and learn from. The seminars were always something to anticipate. Besides the technical aspects, there were outstanding individuals to associate with in classes, seminars and around the water fountain. My time at Purdue has truly been very valuable to me throughout my career.

#### Benjamin K. Tsai, MSME 1990, PhD 1993, D.P. DeWitt

As I reminisce on my six years spent in ME at Purdue, I realize more and more how much the training and learning during that time has profoundly influenced my career and my life. Before graduate school, I already had set my goal to complete a doctorate degree before I started working for the primary reason of better preparing myself intellectually and mentally for the workplace. What I did not know a priori was that the preparation was also one of very intense emotional and physical training. My mind, it seemed, was constantly churning either with worrying about the Fluids homework or with thinking about how to solve the current laboratory crisis. Many a weekend was spent on finishing a paper to meet a deadline or preparing for class examinations. Although the Purdue graduate experience cannot be considered as a Disney vacation by any standard, I still hold many unforgettable memories to this day. The thrill of figuring out how to network all twenty Spark stations to run batch Monte Carlo simulations was very exhilarating. Creating exotic green fumes in our aluminum heater was a terrifying encounter at the moment, but now I can look back at the humorous event. I basked in the camaraderie of my then fellow graduate students, especially Duane Hill, Tom Habing, Charles Gibson, Lynn Zentner, and Mark Pellerin. During the few conferences which I was privileged to attend, I learned the basics of networking and giving proper presentations. Finally, the process of researching, writing, and defending the dissertations was a soul-searching but extremely valuable ordeal, one in which has helped me prepare to overcome obstacles and to begin to learn the basic ropes of a researcher. My infinite gratitude goes to Professor DeWitt, my graduate committee, my professors, and all those at Purdue, who have taught, influenced, and prepared me to be a better contributor in society. Happy Celebration of Heat Transfer at Purdue University, and thank you, Purdue!

#### David Wolf, PhD 1993, F.P. Incropera and R. Viskanta

I often reflect on my heat transfer training at Purdue and how it established a strong foundation for my career. When thinking of "training", it's tempting to gravitate to that which occurs in the classroom. While the classroom learning was first-rate, it was the environment at Purdue outside of the classroom that most shaped my learning. It was the expectation that the Purdue Heat Transfer Department produced only world-class results that elevated my investigative rigor to a new level. It was the intellectual stimulation from brilliant faculty and colleagues that broadened my thinking. It was the contagious work ethic that extracted everything I had to offer. Mostly, it was the gift of being able to work under the direction of two world-renown experts and gentlemen – Professors Frank Incropera and Ray Viskanta – that gave me the real education. They not only conveyed their technical knowledge, but also gave me the freedom to explore things on my own, which enabled unique learning experiences that have affected how I approach problem solving to this day. I am indebted to Professors Incropera and Viskanta and the Purdue Heat Transfer environment for imparting the learning experiences, formal and informal, that have enabled me to solve difficult technical challenges in my career.

#### Theodore (Ted) J. Heindel, MS 1990, PhD 1994, F.P. Incropera and S. Ramadhyani

I have very fond memories of the heat transfer community at Purdue University. One aspect of this community that used to be unique was that many faculty periodically collaborated with each other and co-advised students. Collaboration in now highly encouraged at many institutions, making Purdue and the Heat Transfer Area trend-setters. I had two co-advisors throughout my tenure at Purdue; this sometimes created more work for the student, like



A current research focuses on the feasibility study of targeted drug delivery for tumor treatment using thermal stimuli. In particular, we are investigating the microvascular endothelium permeability in a solid tumor to nano-particle drugs with the aid of heat treatment. The images show the condition of microtubules (pseudo-green) and nucleoli (pseudored) in endothelial cells before and after heat treatment at 43.5°C for 60 minutes, and their relationship with the cell morphology.



A wide variety of compact high-performance cooling technologies are being investigated in the Cooling Technologies Research Center, an NSF Industry/ University Cooperative Research Center at Purdue University, led by Professor Suresh Garimella. In this picture, graduate students Sydney Wait and Tolga Acikalin perform experiments on piezoelectric fans being developed in the Center in collaboration with Dr. Arvind Raman. The piezofans are small, low-power, noiseless devices for cooling portable electronics."

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when it came time for thesis or paper corrections (all of us remember the red ink). However, I feel that having two advisors made my graduate program much stronger because I could learn from two faculty that complimented their respective talents instead of one. I will always remember how well my advisors worked together and provided an excellent example of collaboration.

# Chris Essenburg, MSME 1996, J.T. Pearson and R.J. Schoenhals

I did my research work for Ford Motor Company and this involved system modeling of a fuel pump performance. I did an evaluation of the system and then compared my estimates to the actual results. I currently work as a mechanical engineer at Thermotron Industries. We manufacture environmental test chambers and I am involved with predicting the performance of test chambers. I have developed transient heat transfer models that predict how fast the chamber will transition between two temperature extremes with a given refrigeration system and product load. The refrigeration systems I work with include both cascade and single stage systems. I am able to develop performance specifications for new chambers without having to build and test an actual chamber. My research for Ford was very helpful in trying to apply engineering principles to explain the actual behavior of a system. I also served two semesters as a Teaching Assistant for the undergraduate Fluid Mechanics course. I encounter many situations in my job where flows through pipes and valves must be calculated. My experience in this position reinforced my knowledge of Fluid Mechanics. I also found the graduate level Heat Transfer course with Dr. Ramadhyani to be very helpful. Many of the homework problems forced us to apply heat transfer concepts to real-life situations.

# Rahul Mital, PhD 1996, J.P. Gore and R. Viskanta

Most of my research work was done at the Zucrow laboratories (formerly TSPC). Frequently I would need help from Purdue's Heat Transfer laboratories to make radiative property measurements or convective heat transfer coefficient measurements for the ceramic substrates I was testing. I am happy to say that Purdue's Heat Transfer labs had all the equipment I needed to collect this data. The students working in these labs were very helpful, friendly and knowledgeable. Outside Lafayette, I have noticed people hold Purdue's Heat Transfer in high regard primarily due to its well-known faculty. I wish Purdue Heat Transfer all the best in the future!

# Marcus V. A. Bianchi, PhD 1997, R. Viskanta

The years I spent at Purdue Heat Transfer have shaped me in many different ways. The privilege of working for Professor Ray Viskanta certainly generated the deepest impressions on me. His well-known outstanding professionalism and excellence in research have been an inspiration to me. Several times, when facing a difficult professional problem, I ask myself "what would RV do?" Parallel to his professional accomplishments, quantified by the remarkable number of publications and citations, RV impresses by his generosity, kindness, and humility. Other faculty members also contributed to my experience in West Lafayette. Professors Incropera and Ramadhyani always challenged me with difficult research questions and I had the opportunity of teaching undergraduate heat transfer with Professors DeWitt, Mudawar, and Schoenhals. The Heat Transfer faculty attracted first-class graduate students, who created a friendly atmosphere for collaboration. I learned more from them when they shared their fresh research findings in the Heat Transfer Seminar Series than in any formal class and I count many of them as friends. I will always miss and be grateful for those wonderful years.

# Andrei Fedorov, PhD 1997, R. Viskanta

There are hundreds of memorable moments of my six years at Purdue (1994-2000) which are all worth mentioning. However, I'd like to say a few words about the three stories which are perhaps the most memorable because of my current work as a faculty member at Georgia Tech. The first two stories are due to a unique experience working with my PhD advisor Ray Viskanta (or simply RV). His "always-open-door" policy always provided a mental support for me even in the hardest days for two reasons: it made me feel welcomed to stop by at any time to discuss whatever problems I may have and it also made me see RV always being so focused and working so hard an every single minute of the day that I couldn't feel tired or frustrated in my work. The second RV-related story is about the lesson that I learned for the rest of my professional life while I was working on my first journal paper with RV.I'm talking about going tirelessly through the multiple revisions of the manuscript and of the figures (the "more red than black" manuscript returning with RV's comments is the legend among his students). One day when I was about ready to give up, he probably sensed that and said briefly (I cannot guarantee the exactness of his words, but the essence is captured here):"When we prepare a paper, we should look at it through the eyes of the potential readers. That means we should do our best to make sure that the reader could obtain all necessary technical information in the shortest possible time and with the minimum efforts". The last few words or my third story is to acknowledge the fellow heat transfer graduate students of such diverse backgrounds and opinions on everything from food and drinks to the world politics with whom I spent long days and often nights, including most of the weekends, and which are still remember with warmth and smile. Cheers.



Prof. T.S. Fisher's work on novel carbon nanostructures focuses on enhancing electrical and thermal transport for improved direct energy conversion, power electronics, ion generation and pumping, thermal conduction through interfaces, and molecular electronics.



Prediction of silicon thermal conductivity in thin layers using Boltzmann Transport Equation (BTE) models accounting for phonon polarization and dispersion. Self-heating is a critical bottleneck in the performance of emerging microelectronic device technologies such as Silicon-On-Insulator (SOI). Accurate phonon transport models are being developed to better quantify the thermal performance of microelectronic devices at the 10-300 nm scale. (Inset courtesy IBM Corporation. Experimental data from Ju and Goodson (1999)).