The Evolution of Computing in Chemical Engineering: Some Perspectives and Future Direction

by

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Outline

- Introduction
- Driving Forces for Evolution of Computing in Chemical Engineering
- Case Study: The Adoption of Process Simulation
- Value Proposition for Application of Information Technology
- Future of CACHE

Driving Forces for Evolution of Computing in Chemical Engineering

Advances in Application of Computing

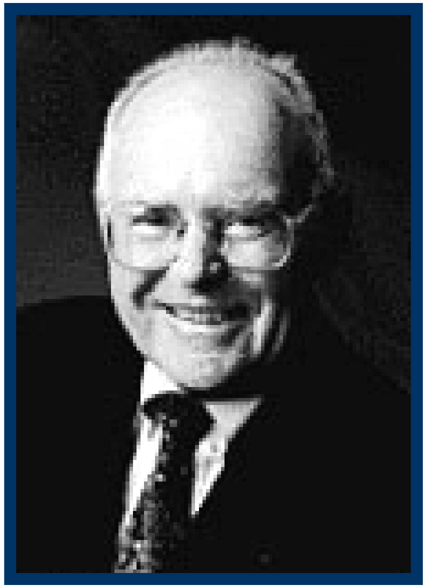
Advances in the application of computing are driven by:

- Relentless increase in computing power
- Improvement in our ability to model the physical and chemical world
- Opportunity to bring economic value

Relentless Increase in Computing Power

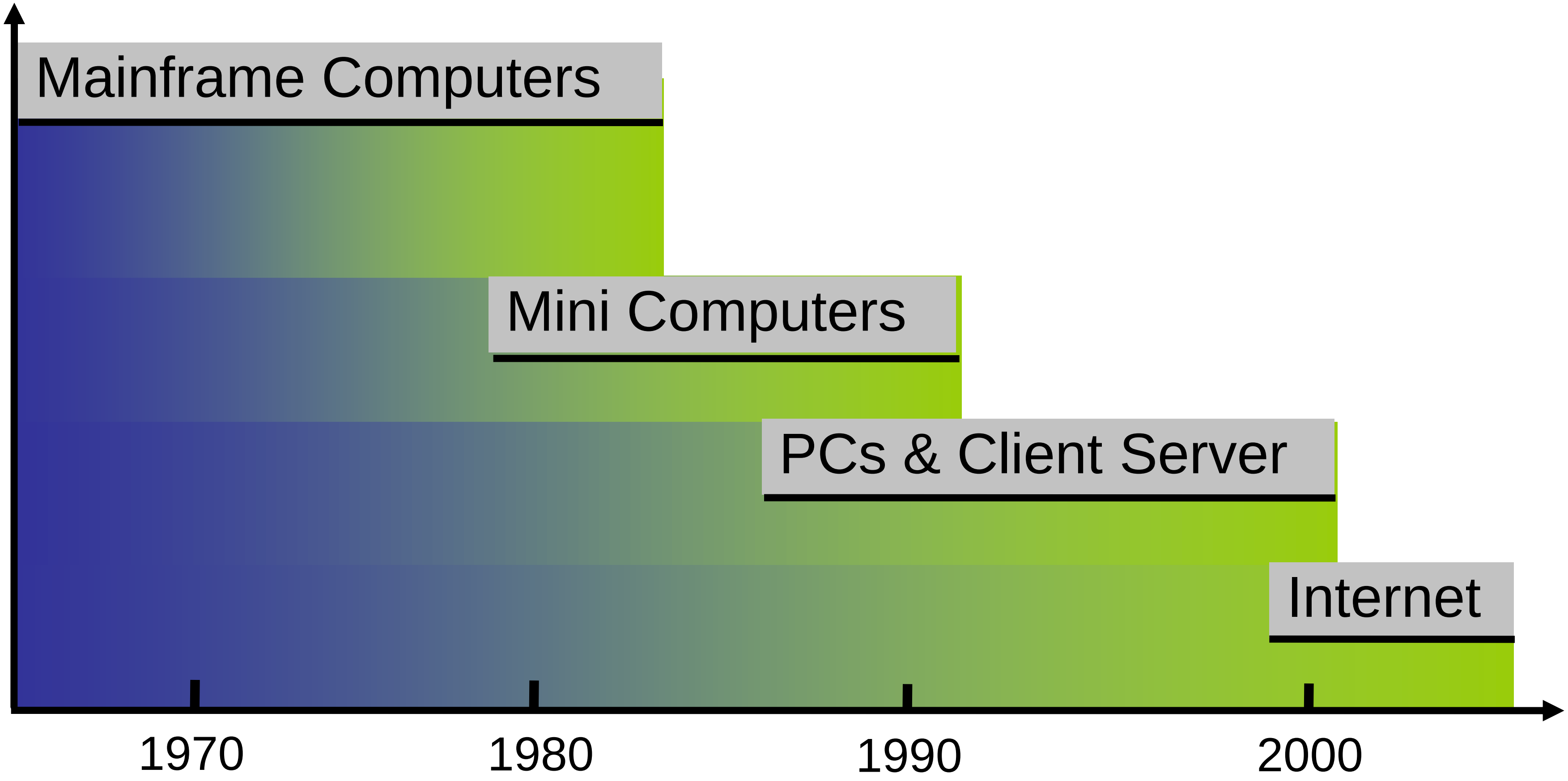
"Computing power per unit cost doubles every 24 months"

- Moore's Law



Dr. Gordon E. Moore,
Chairman Emeritus
Intel Corporation

Changes in Computing Environment



Improved Ability to Model Physical and Chemical World

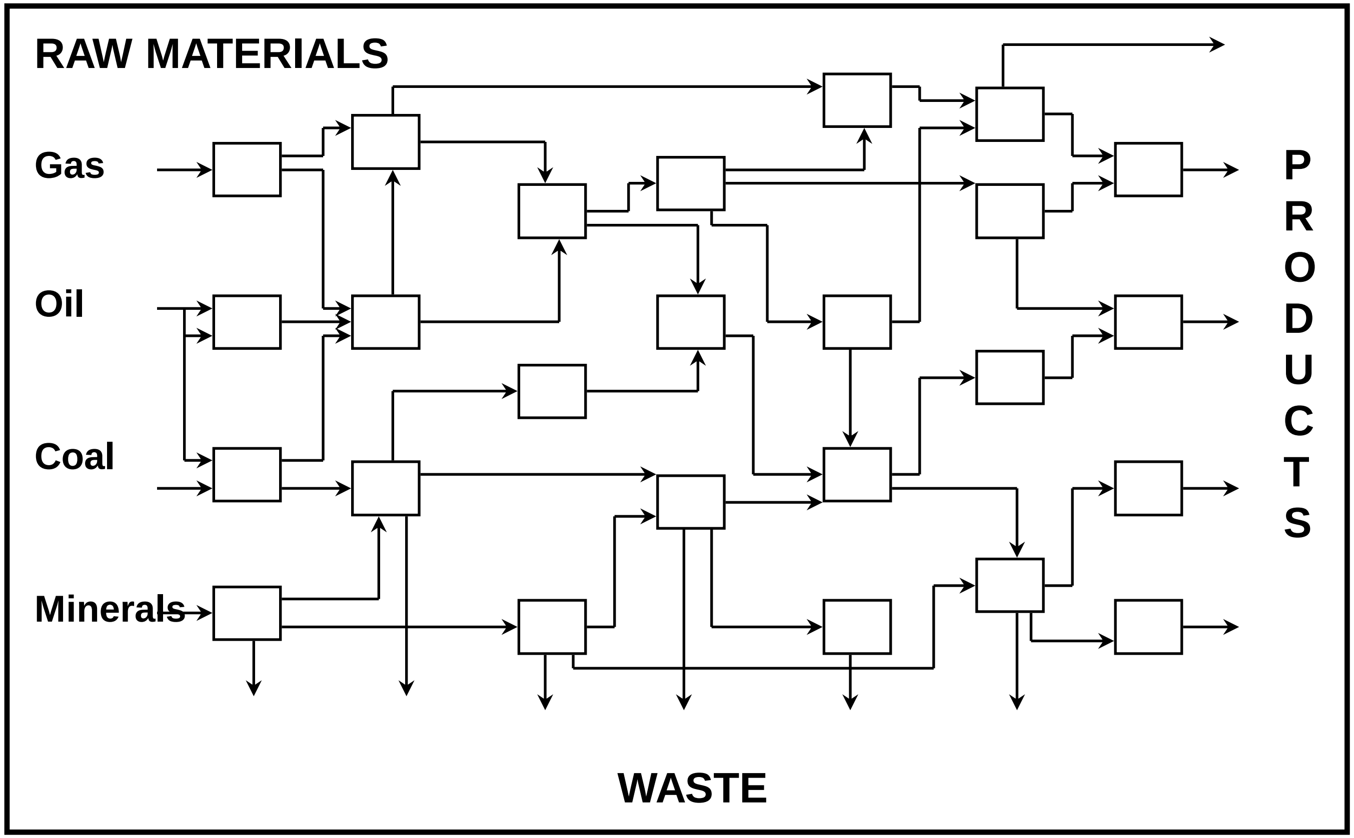
- Improvements have resulted partly from focus on mathematics in chemical engineering over the past several decades
- Result is better models to describe molecular dynamics, fluid mechanics, chemical kinetics and other physical/chemical phenomena
- Now being extended to the biological world
- Will ultimately extend to economic and social systems

Models represent a combination of first principles and statistical models

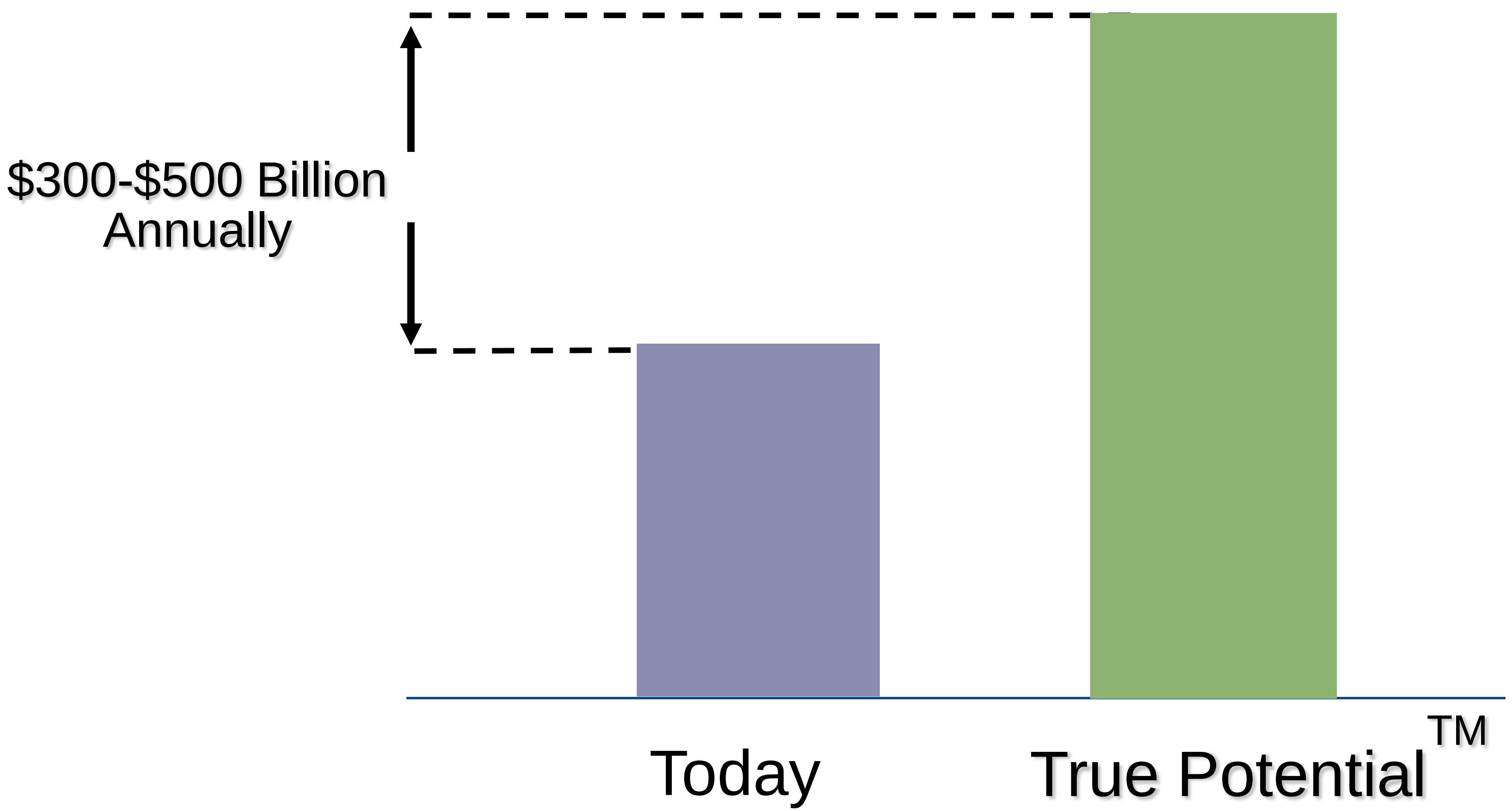
Opportunity to bring Economic Value Process Industries

- Process industries are huge
- Annual turnover exceeds $6 trillion
- Products are commodities
- Manufacturers must continually improve productivity

The Process Industry Network



Economic Potential

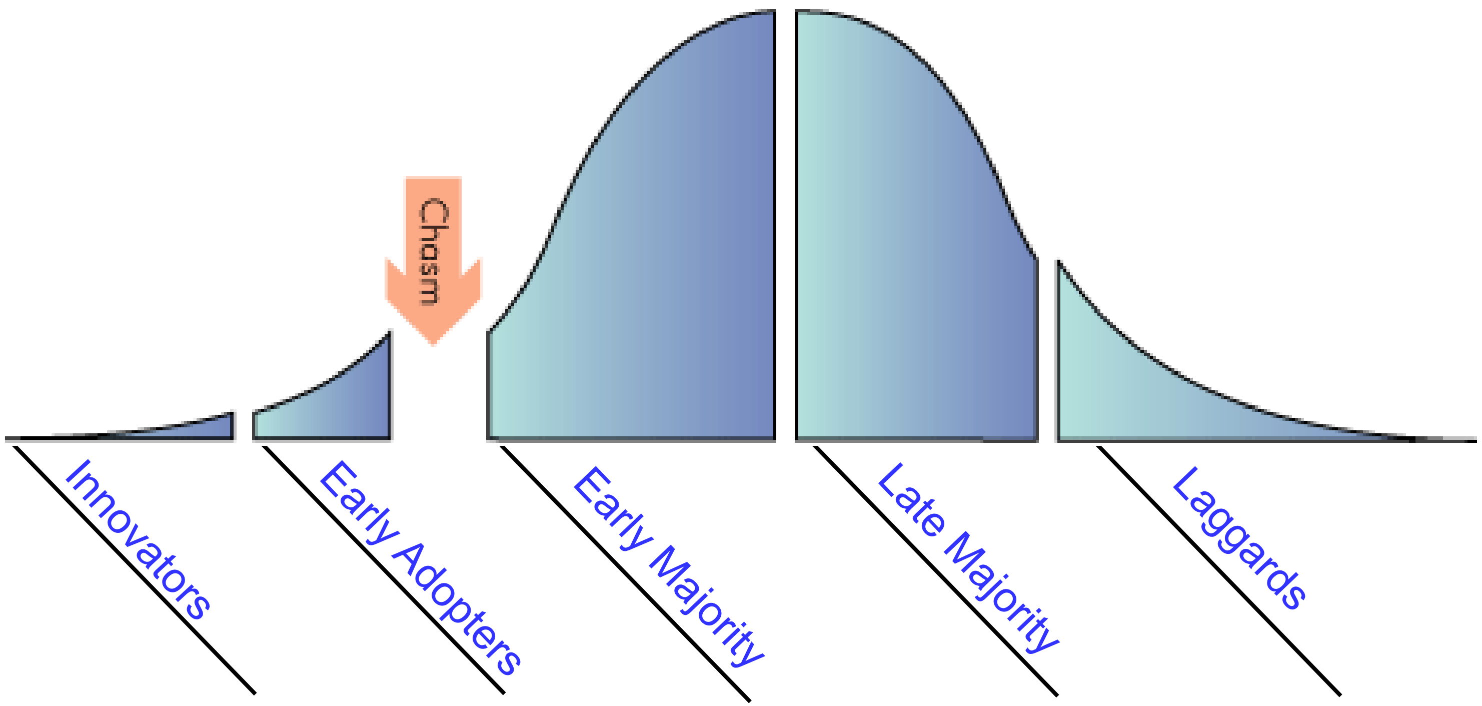


Technology Push vs. Market Pull

Increase in Computing Power	Technology Push
Improved Modeling Capability	Technology Push
Opportunity to Bring Economic Value	Market Pull

Geoffrey Moore: "Crossing the Chasm: Marketing and Selling High-Tech Products to Mainstream Customers"

Technology Adoption Lifecycle



Case Study:
Adoption of Process Simulation

Innovation Phase (1950 – 1975)

Early Innovators
- Paul Shannon, Purdue
- Rudy Motard, University of Houston
- Dick Hughes, Shell
- Bob Cavett, Monsanto

Development of Proprietary In-house Systems
- Specs (Shell)
- COPE (Exxon)
- IPES (Union Carbide)
- FLOWTRAN(Monsanto)
- and many others

Primarily used by experts

Creation of ASPEN at MIT (1975-1981)

- 1973 – the opportunity to develop a next-generation process simulator to be used by the entire industry
- MIT was a hotbed of activity in computer-aided problem solving:
  - Computer-aided civil engineering
  - Computer-aided mechanical engineering
  - Computer-aided electrical engineering
- The timing was right for a large-scale development
  - Country facing the first energy crisis
  - MIT Energy Laboratory established for interdisciplinary research
  - US believed it needed to develop large number of plants to produce “synthetic fuel” from coal to achieve energy independence
- Warren Seider spent academic year 1973-74 on leave at MIT helping me write the proposal to the Department of Energy

Creation of ASPEN (Continued)

- Department of Energy funded the ASPEN Project at MIT with more than $5 million over five years.
- Recruited key staff members on loan from industry to work on the project:
  - Paul Gallier came from Monsanto as Project Manager
  - Herb Britt from Union Carbide as Associate Project Manager
  - Joe Boston from University of Toledo as Associate Project Manager
- Formed an Industrial Advisory Committee with more than 50 companies each provided $30K in funding
- Project completed in 1981, ASPEN source code delivered to Department of Energy, available free from the Argonne Code Center
- MIT owned the copyright, DOE had an unlimited right to use and distribute copies to others

Formation of AspenTech: the Early Years (1981-1986)

- AspenTech founded as private company in 1981
- Plan was to to offer a commercial version of ASPEN called ASPEN PLUS that would be supported and further developed
- Couldn’t raise venture capital, so we bootstrapped the company
- Goal: to develop ASPEN PLUS into a commercially viable product and get it adopted by the early adopters.
- In 1986 the company was still struggling, software used by a few experts in each of our customers//
- We hadn’t crossed the chasm into widespread use by the mainstream majority
- Company was dangerously short of cash
- In 1986 AspenTech raised $2.6 million in venture capital from Advent International

AspenTech Crossing the Chasm to Penetrate the Mainstream

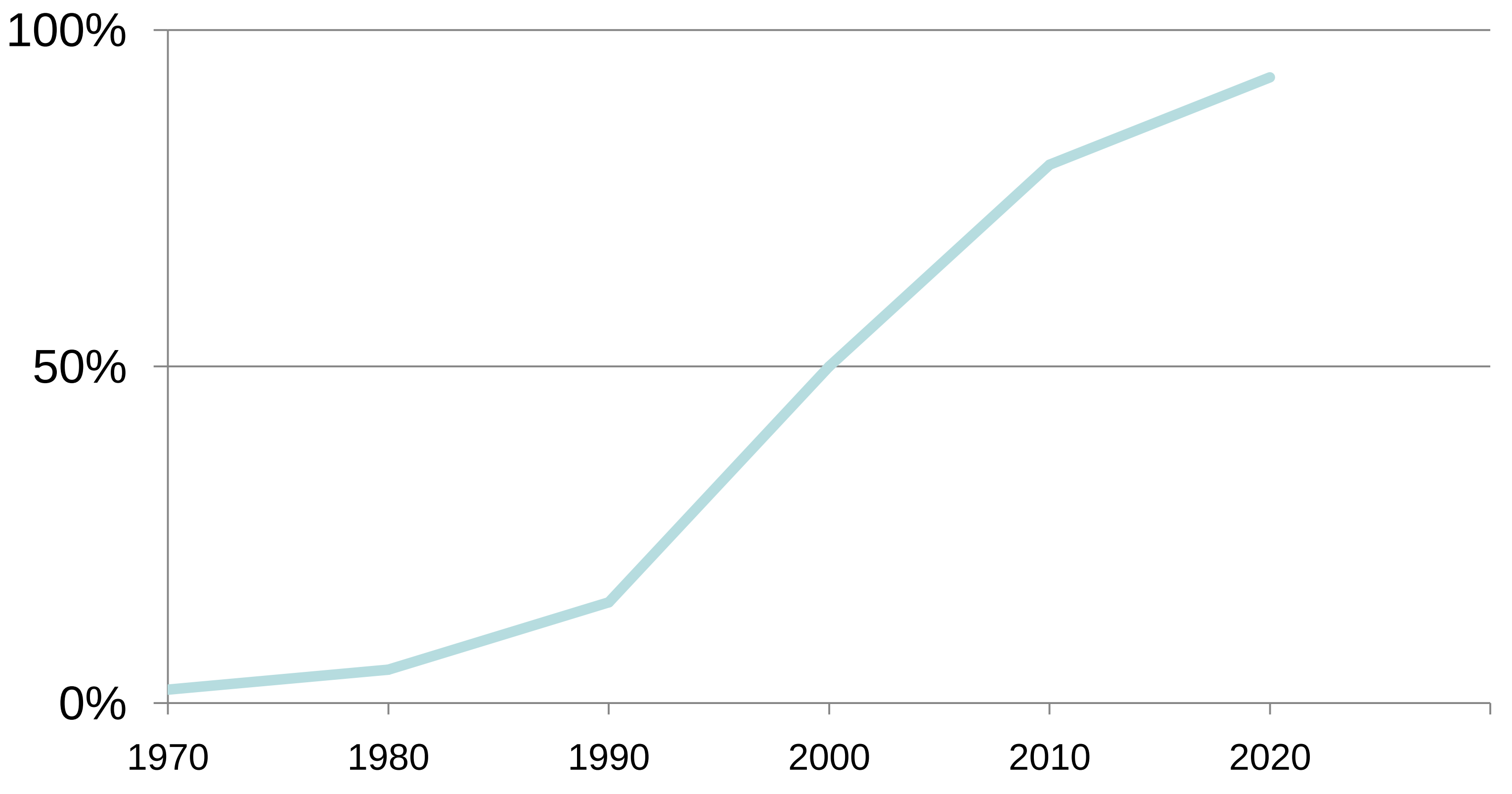
- During period 1986-1991 ASPEN PLUS began to penetrate into the mainstream
- Early adopters like MW Kellogg, Mitsubishi Chemical and Dow Chemical made a major commitment to use the software broadly in their company
- The mainstream adopters bought the software because of its economic value proposition
- By crossing this chasm AspenTech overcame a major hurdle.

AspenTech – the Rest of the Story

- Initial public offering in 1994
- Pursued strategy of going beyond engineers desktop into plant operations and supply chain management
- Goal was an integrated solution with same consistent models at each stage
- Acquired more than 20 best-in-class companies and integrated the software
- I stepped down as CEO in 2002

Purpose of the Case Study: Illustrate what is required to take a new application of information from an idea or technical curiosity into a successful commercial product

Penetration of Process Simulation



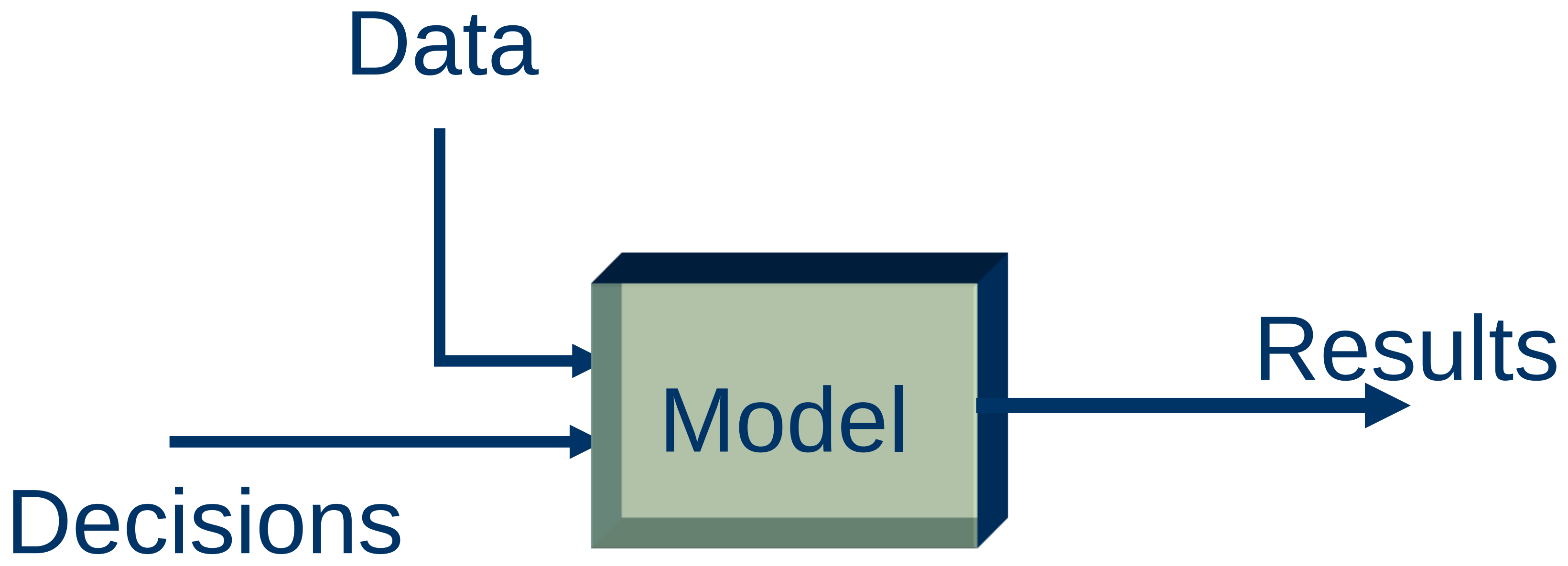
Delivering Value Through Application of Information Technology

The Value Proposition for Application of Information Technology

Information Technology delivers value by enabling individuals and organizations to make better decisions and implement these decisions consistently through automation

- If there are no decisions to be made it is hard to find a way to deliver economic value
- The availability of models and data enable better decisions

Models Predict Performance



Application of Models

Application	Model	Decisions	Additional Data
Process Design	**Engineering Calculation**	**Sizing & Operating Conditions**	**Updated Cost Data and Design Constraints**
Production Planning	**Linear or Nonlinear Program**	**Amounts of Product at Each Facility**	**Prices and Availability of Raw Material**
Advanced Process Control	**Empirical Model from Plant Tests**	**Adjustments in Manipulated Variable**	**On-Line Measurements from Plant**

"If you can't model your Process, you don't understand it. If you don't understand it, you can't improve it. And, if you can't improve it, you won't be competitive in the 21st century."

– Jim Trainham, DuPont - 1994

DUPONT The miracles of science™

Observations About Using Models to Deliver Value

1. Technologies at the forefront of adoption today: (computational fluid mechanics, molecular modeling, and systems biology) are mostly at the innovation or early – adopter stage.
   - All of these applications are in a technology push mode driven by an improved ability to model the physical world
   - To achieve widespread adoption and large commercial success, they will need to deliver on a strong economic value proposition
   - We need to look at:
     - How these applications enable better decisions to be made
     - What models, data, algorithms and computer code are needed
     - How do we get these solutions used

Observations About Using Models to Deliver Value (Continued)

2. Big future applications will be driven by need to deliver value to companies and industries addressing societal problems
   - These applications will be in a market-pull mode driven by the need to make better economic decisions
   - Look at the big problems of society: such as Energy, Water, Food, Environment, Transportation, Health Care, Defense ….
   - Ask: How can Information Technology enable better decisions and deliver large economic value
   - Decide what models, data, algorithms, and computer systems will enable decisions to be made and implemented.

Observations About Using Models to Deliver Value (Continued)

3. There is a big premium on increased modeling accuracy

   – Accurate models important to give confidence to eliminate the column

   – A mistake could be a career limiting decision

Changing Paradigm Regarding Models

Old	New
Quick and dirty	**As accurate as possible**
“Know-How”	**“Know-Why”**
Get 80% of benefits for 20% of work	**Six Sigma Performance**

Observations About Using Models to Deliver Value (Continued)

4. The cost of the best tools is much less than the cost of the professional using the tools

- In the early days, companies hesitated to pay annual license fees of $10-20K per user for software
- But consider the economics
  - Cost of software: $10-20K
  - Cost of engineer using the software: $100-200K
  - Value of decision made by engineer: $10-20 million
- Therefore, provide the best most accurate tools available
- Instead of asking “How much does the software cost?” companies started asking “How good is it?” and “How can I get more of my engineers using it?”

Future of CACHE

CACHE Success Factors

- The core mission: to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession" has remained unchanged for almost 40 years.
- But, the activities within that definition have changed dramatically
  - From FORTRAN programs to hosting leading conferences and pioneering new applications of modeling
- CACHE bridged the gap between academia and industry by the addition of industrial trustees
- CACHE has found a way to add new trustees while still retaining a core of long-term trustees

CACHE Success Factors (Continued)

- CACHE has been entrepreneurial in adding new funding sources: government funding, supporting departments, industrial affiliates, sponsoring conferences, etc.
- CACHE has been at the forefront in many areas. The trustees are thought leaders in the use of computers; its products are well accepted; the people associated with CACHE are leaders of the profession; the CACHE conferences are prestigious.
- The structure of an independent, not-for-profit corporation has served CACHE well.
- A very important key to success as been the role of the University of Texas in hosting the executive office of CACHE and the dedication of people like Dave Himmelblau and Tom Edgar.

CACHE Opportunities for the Future

- There will be a continuing need to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.
- New technologies have the potential for changing the way:
  - University education is delivered
  - Research is published
  - Books are written
  - Continuing education is provided
  - Technical and professional meetings are held
- There will be a need for next-generation industrial computing tools to address the big problems of tomorrow – the innovative ideas need to come from university-industry-government cooperation

Thank You