New Vistas for Process Systems Engineering: Integrating Physics Computation and Communication Networks for Better Decision Making

New Frontiers in Chemical Engineering:

Impact on Undergraduate Curriculum

Workshop, WPI May 7, 2004

B. Erik Ydstie Carnegie Mellon University

1. The Context (Industry/University/Grad. Research)
2. Challenges in UG graduation (Curriculum/Constraints/Proposal)
3. PSE Research (Case studies/Challenge)

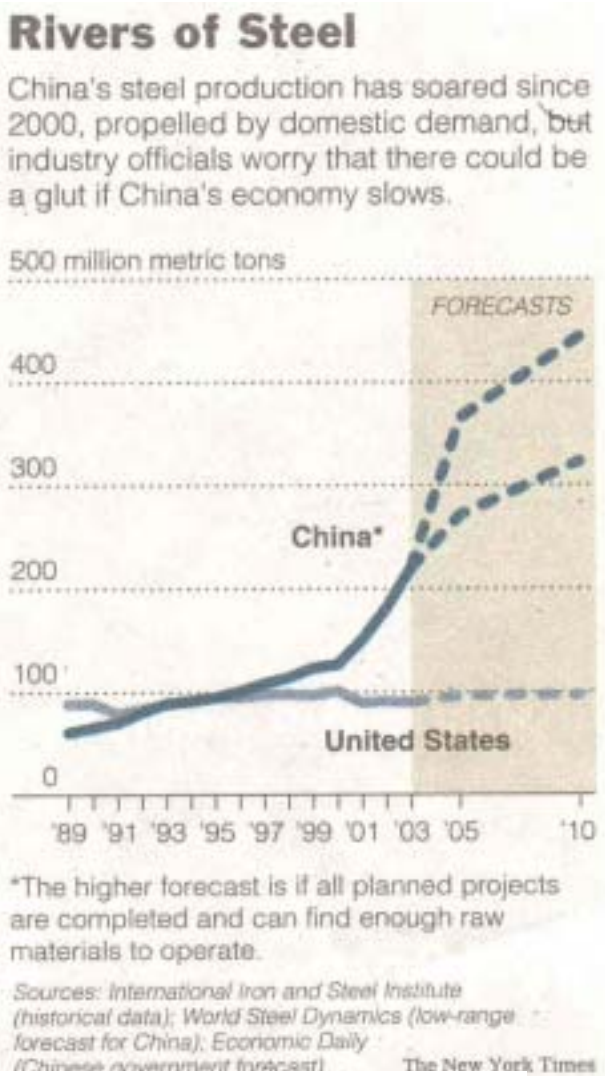
The Context: The Industries we Serve

Local	→	*Global, Flexible*
*Protected**		*Market Oriented*

Pittsburgh: Steel, Aluminum, Glass ++.

What about:

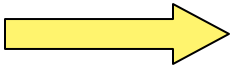
- *PetroChemicals?*
- *Micro-Electronics Manufacture?*
- *Software?*
- *What about Bio/Med-technology?*
- *Research and Development?*
- *++*



* *Proprietary technology, transportation, trade barriers, technology gap, know how,...*

The Context: The University

Specialization ("Excellence") and the Student as Customer

Local/National		*Global, Market oriented*
Canonical Programs		*Student choice, many options*
Fixed curriculum		*Flexible curriculum*

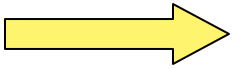
CMU:

$40M Univ Center.
$40M Performing Arts.
Programs in Greece/Calif./Quatar

Mission Statement: *A Carnegie Mellon education aims to prepare students for life and leadership. In a continually changing world, the most important qualities we can help our students develop are the ability to think independently and critically, the ability to learn, and the ability to change and grow.*

Context: University Graduate Research

Unit Process Design and control, petro-chemical processes, analytic and graphical solution to, transport, thermo, fluids and staged separation prblms,+++



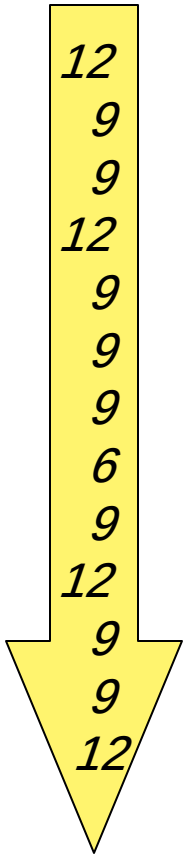
*Large scale computation, complex networks, molecular dynamics and design, quantum mech Biological systems theory, micro-electronics, complex fluids, self-assembly nano technology,…**

Chem. E. Research Programs have moved into new technologies and application areas. Dynamic and exciting! New Courses are being developed.

** Beyond the Molecular Frontier, CST-NRC Report, NAE/NAS, 2003*
Sessions at recent AIChE meetings

Chem Eng Curriculum: "The Pipeline Model"

1st year:	*Intro Chem Eng*	*12*
2nd year:	*Thermo 1*	*9*
	Fluid Mechanics	*9*
	Math Methods of Chem. Eng.	*12*
3rd year:	*Thermo 2*	*9*
	Heat and Mass	*9*
	Unit Operations	*9*
	Transport Lab	*6*
	Process Control	*9*
4th year	*Process Design*	*12*
	Reaction Engineering	*9*
	Unit Ops Lab	*9*
	Design Project/Optimization	*12*



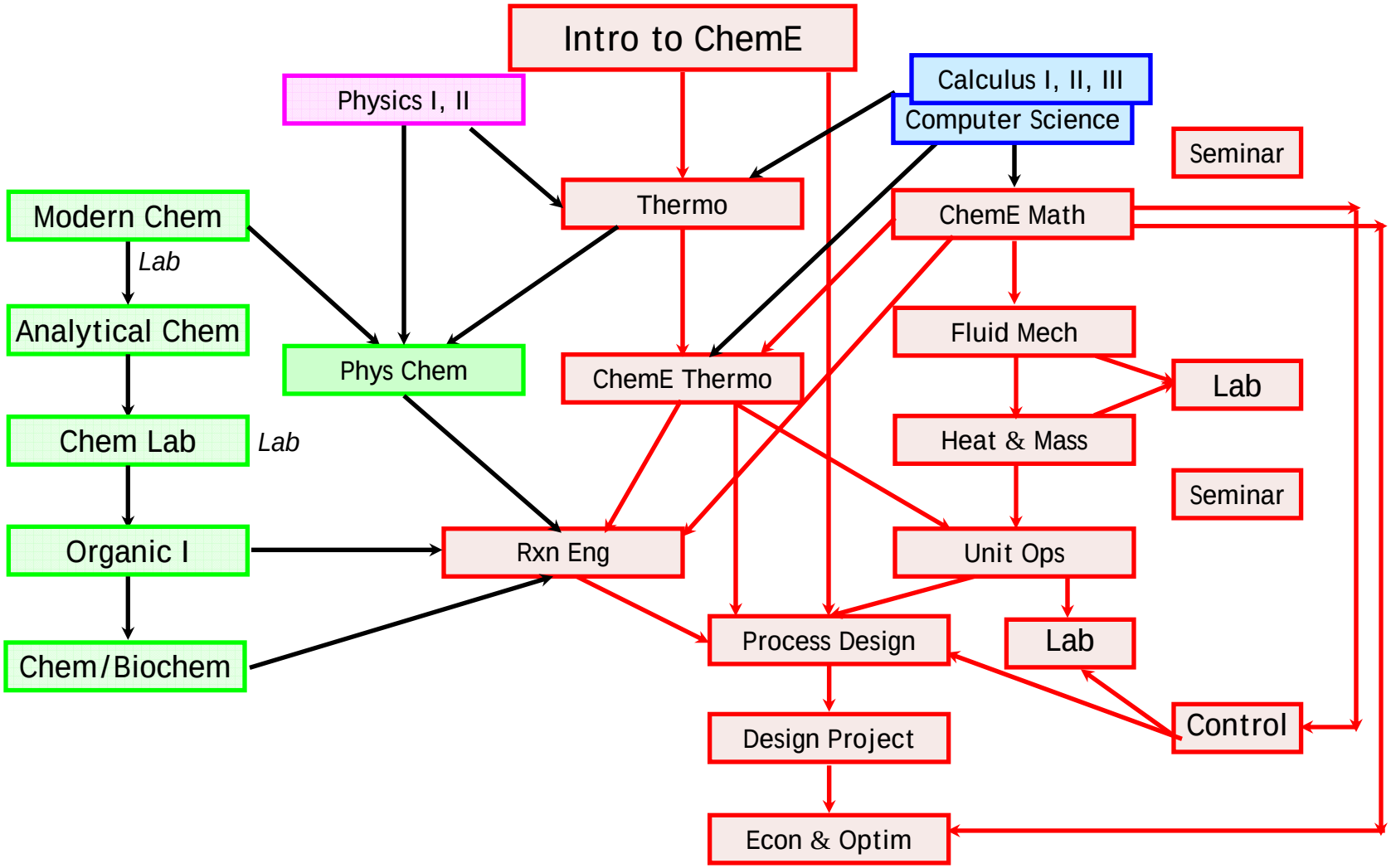
Static for 30+yrs

+ Basic Science and Math Gen. Ed., Tech Elect., Minors/Majors.

Curriculum

Class of 2004

http://www.cheme.cmu.edu/



Product Development

Process Engineering

The Result: Where Do CMU ChE Students go to Work?

BOC Gases
Air Liquide
Air Products & Chemicals

duPont
Dow Chemical
Exxon Mobil
Kodak
General Electric
Corning

Bristol-Myers Squibb
Merck
Pharmacia

Procter & Gamble
Johnson & Johnson
L'Oreal

U.S. Steel
PPG
Westinghouse

DOE
Navy
National Institute for Drug Abuse

Motorola
IBM
Seagate
Motorola
Xerox
Samsung Austin Semiconductor
Intel

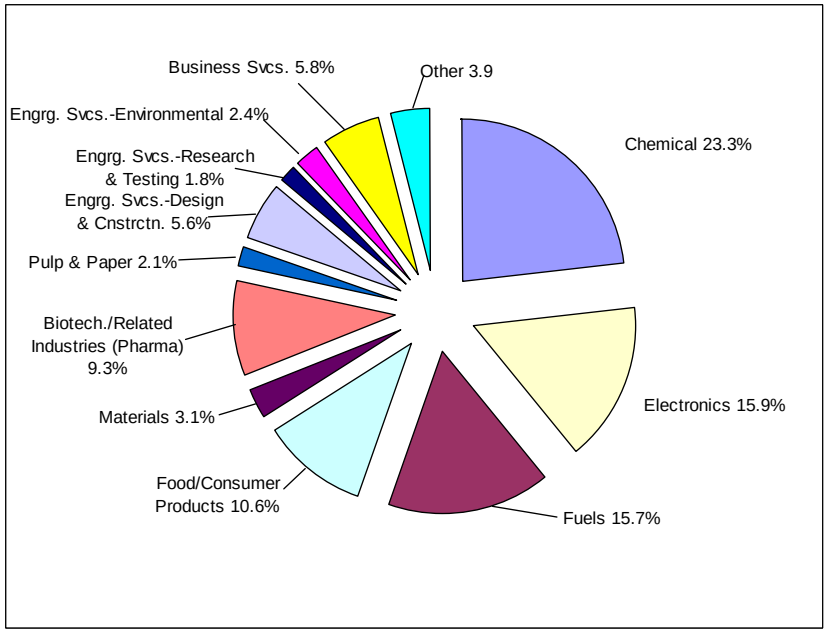
Aspen Technology
Ethicon
Aquatech
Cytec
Photocircuits Corp
International Fuel Cells.
Lexmark International

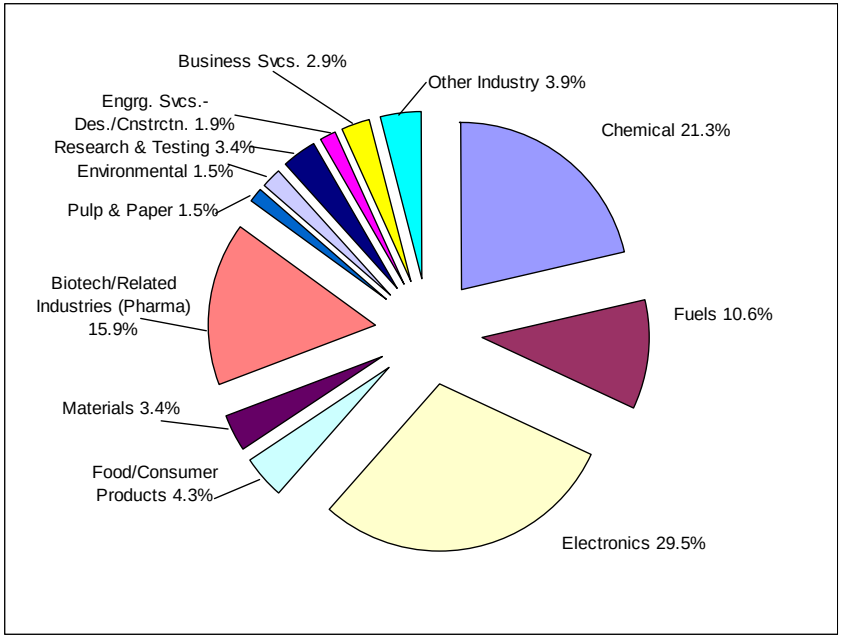
Andersen Consulting
Goldman Sachs
Deloitte and Touche
American Management Systems
Fuji Capital Markets
Banc of America Securities
Putnam Investments
Accenture

Americore
High Scool Education
Grad Schools

Major Trends in Chemical Engineering:

Increased diversity of jobs for chemical engineers





B.Sc. Placement
AIChE (2001)

40% chemicals/fuels

Ph.D. Placement
AIChE (2001)

32% chemicals/fuels

Mid-Course Conclusions:

Universities:	*Flexible, Market Oriented.*	
Chemical Industry:	*same*	*(new products/processes)*
Grad Research:	*same*	*(new areas bio/nano,..)*
Students:	*same*	*(diverse employment)*
UG ChE Curr:	*Static*	*("one size fits all")*

1. *Why are ChE's so adaptable?*
2. *Can we improve curriculum?*
3. *Make ChE relevant and attractive for high school students (what do Chem. E.s do?).*

-the best and the brightest are unlikely to choose chemical engineering in anything like the same numbers as in the past, and government and probably industrial funding will decline.

Prof. Herb Toor, (frmr.) Dean of Engineering CMU.

Why are Chem E's adaptable?

- *Broad base in science, analysis and engineering.*
- *Systems thinking promoted in control and design.*
- *Attracts a special kind of student.*

Can we/Should we improve curriculum

- *Yes*

What do Chem. E.s do (we are judget by the product)

- *petrochemical industry.*
- *research/teaching/government*
- *finance/consulting*
- *high tech*
- *software*
- *pharmaceutical/health care*
- *consumer products*
- *develop new materials*
- *environmental*

Must re-think our petrochemical (vap/liq.) focus

Constraints to Change 1: ABET and AIChE

PROGRAM CRITERIA FOR CHEMICALAND SIMILARLY NAMED ENGINEERING PROGRAMS (ABET)
Lead Society: American Institute of Chemical Engineers

Curriculum:

The program must demonstrate that graduates have: thorough grounding in chemistry and a working knowledge of advanced chemistry such as organic, inorganic, physical, analytical, materials chemistry, or biochemistry, selected as appropriate to the goals of the program; and working knowledge, including safety and environmental aspects, of material and energy balances applied to chemical processes; thermodynamics of physical and chemical equilibria; heat, mass, and momentum transfer; chemical reaction engineering; continuous and stage-wise separation operations; process dynamics and control; process design; and appropriate modern experimental and computing techniques.

Constraints to Change 2: The Textbooks

Fact: Easy to teach and learn when there is a good book.

1. *Process Control (Stephanopolous, Seborg et al., Bequette,..*
2. *Fluid Mechanics (3*W, BSL)*
3. *Thermodynamics 1&2, (Smith and Van Naess, Sandler,...*
4. *Process Design (Douglas, Grossmann, ...*
5. *Chem E Math (Kreyzig, diPrima,...*

The quality of the books range from superb to excellent. But -

1. *Contents (examples) too much focused on "ideal" vap/liq systems.*
2. *A lot of time spent to develop analytical/graphical solution methods.*
3. *The lead time from new research and technology to UG instruction can be very long.*

The Example of Process Control

Typical Course Contents:

Theory:

Dynamic Models
Laplace Transforms
Block Diagrams
Stability
Controller Design and tuning
PID control
Feedforward
IMC
Decoupling
Relative Gain Array
Predictive Control

Application:

Tanks
Reactors
Distillation
Bio-control
Batch Control
Plantwide control

Introduces students to Dynamics and Systems Thinking

What can be Done?

Enablers:

1. Academic freedom
2. Engaged faculty
3. Graduate research and courses
4. Industrial involvement in R&D
5. University backing
6. --

Desired Situation:

1. Dynamic curriculum.
2. Based on the "engineering science and analysis".
3. Technologies of current interest(bio/enviro/ molecular/petro-chem,...)

Current Situation:

1. Static curriculum.
2. Based on "engineering science and analysis" .
3. Weighted towards petro-chemicals (Cap-stone design).

Plan:

1. Review science core (now).
2. Introduce "selectives" (now).
3. Hire faculty in key areas.
4. Develop new courses.
5. New textbooks.

Modest Proposal: Non-Uniform Curriculum

Core: *(All Chem. E.'s, Backed up by Labs*)*

Math/Analysis/Computation
(Thermo 1 and 2?)
Chemistry/Bio Chemistry
Reaction Engineering
Heat/Mass/Momentum Transport
(Unit Operations? Process Control? Process Design 1,2,3?)
Process Systems Engineering

Selectives: *(Choose N out of following)*

Semiconductor processing
Atmospheric Chemistry Air Pollution and Global Change
Bio Technology and Environmental Processes
Bio Process Design
Principles and Application of Molecular Simulation
Physical Chemistry of Macro Molecules
Advanced Process Systems Engineering

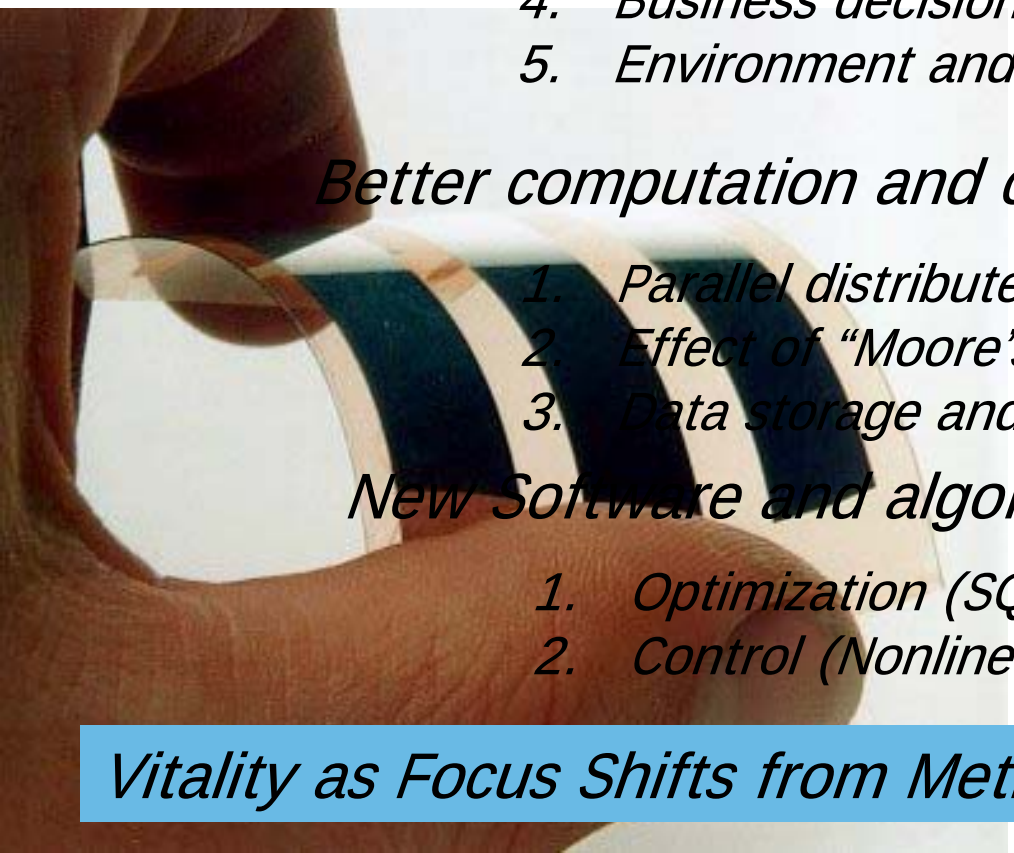
- *Computer Labs w. Adv. Software (CFD, Process Design, Math, Control,…)*
- *Physical Labs (measurement, analysis, process, procedure..)*

Process Systems Engineering:

See the BIG Picture in the Small Pieces

Finding the right piece and seeing how it fits is the key.
Many may look attractive, but they may not answer to our current needs.

PSE Research: Integrating Physics and Computation



New application Domains

1. *Bio tech/med (modeling control, optimization)*
2. *Nano, self assembly, micro-structure*
3. *Micro electronic processing*
4. *Business decision making (PSE 2003)*
5. *Environment and energy.*

Better computation and communication tools

1. *Parallel distributed processing*
2. *Effect of "Moore's law"*
3. *Data storage and the web*

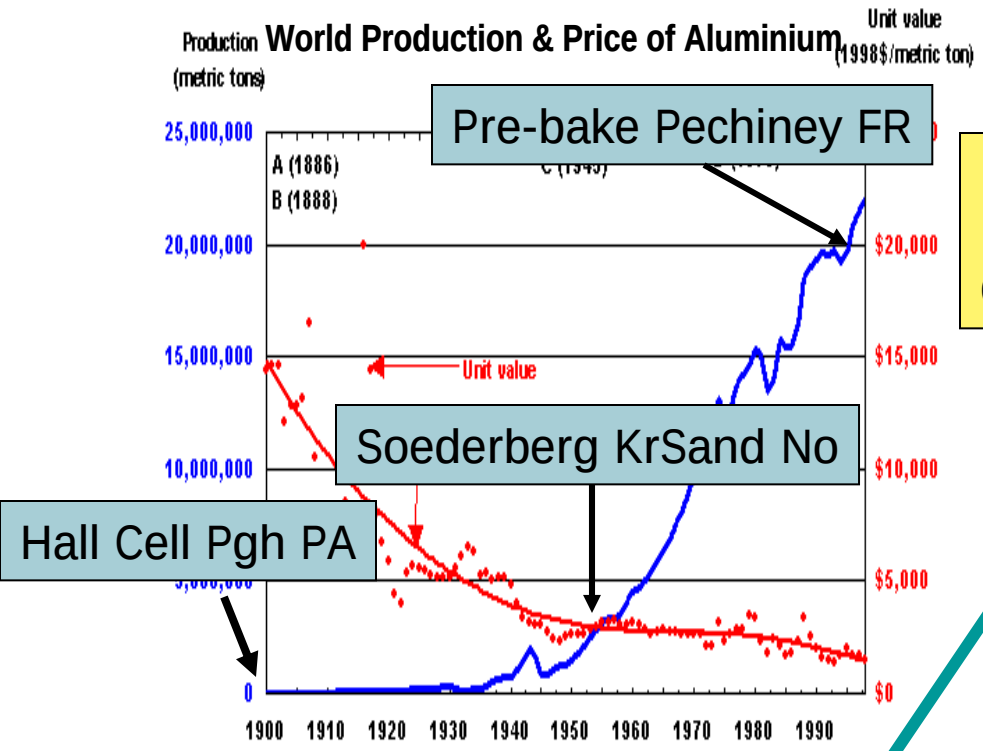
New Software and algorithms

1. *Optimization (SQP/MILP/MINLP…*
2. *Control (Nonlinear, predictive, hybrid,…*

Vitality as Focus Shifts from Methods to Applications

Case Study 1: Carbothermic Aluminum Production

(ALCOA Inc. $24B, Aluminum)

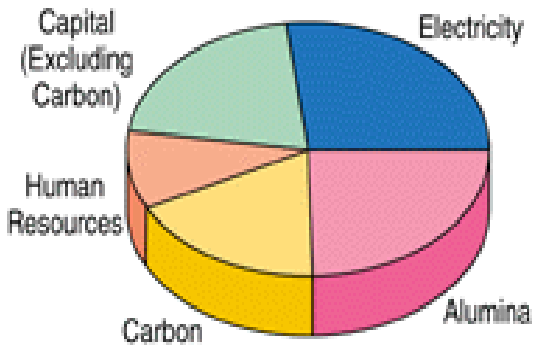


Competing processes:

Hall-Heroult	Al_2O_3 + C	=	Al + CO_2
Inert Anode	Al_2O_3	=	Al + O_2
Carbothermic	Al_2O_3 + C	=	Al + CO

PRIMARY Al: COST SECTORS

(WELCH, 1999)

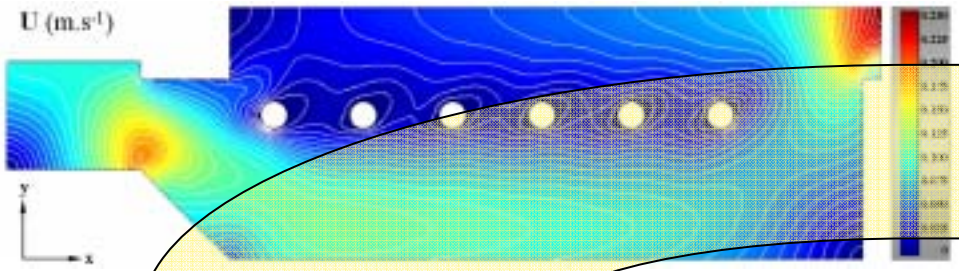


Hall-Heroult Process

Objective: Develop a better way (less energy and capital cost) for making Aluminum.

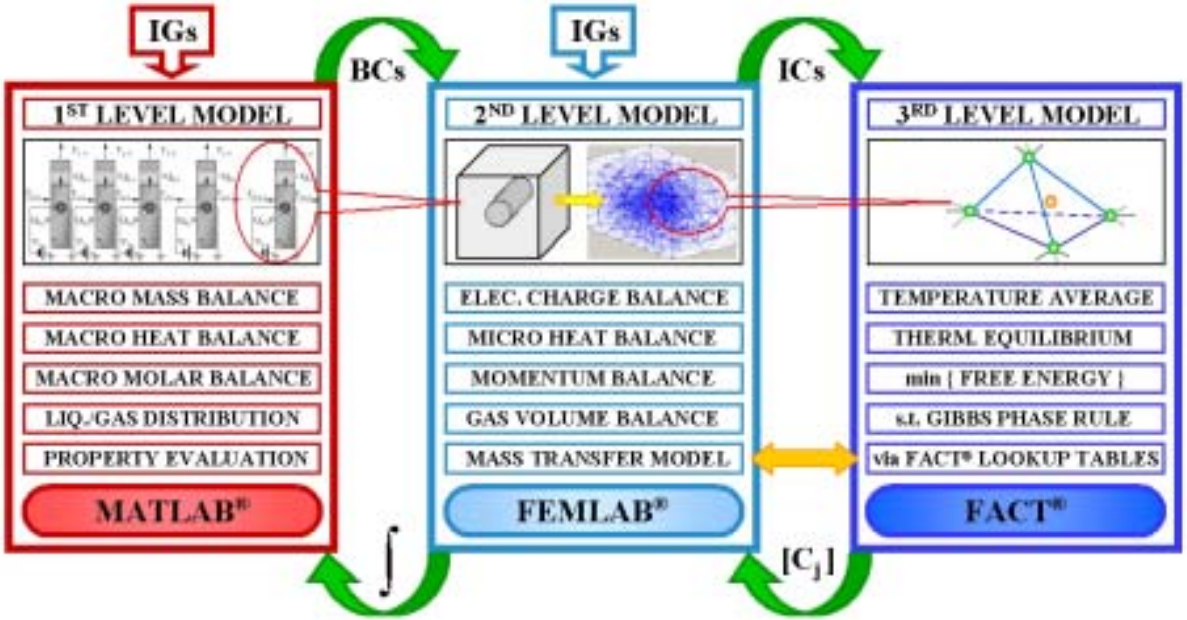
PSE Contribution: Multi-scale Modeling

(Integrate Physics and Computation for Concurrent Design - From Microstructure to Design and Control)



Complex Multi-Physics CFD models

Process optimization/control



Case Study 2: Automotive Windshield Manufacture *(PPG Inc. $20B, glass, coatings, chemicals)*

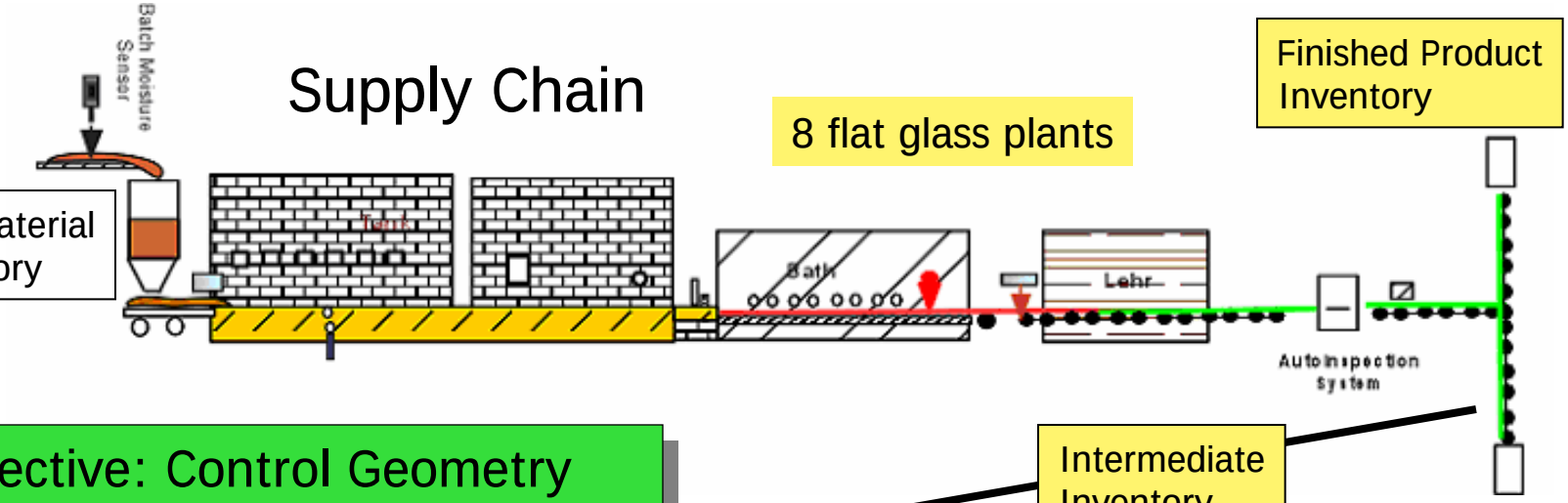
Architectural Glass

Supply Chain

8 flat glass plants

Raw Material Inventory

Finished Product Inventory



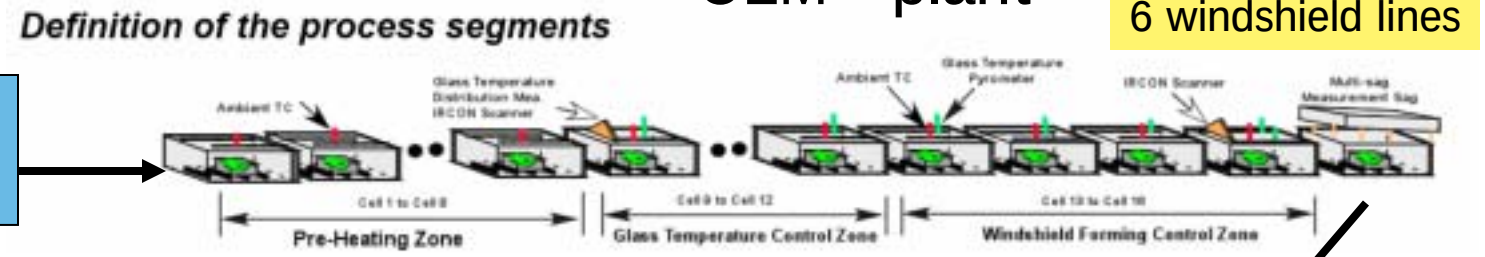
Intermediate Inventory

Objective: Control Geometry and Optical Quality of Finished Product. Improve yield, rate and reduce inventory

OEM - plant

6 windshield lines

High vacuum CVD coating



laminating

duPont

Finished Product Inventory

Automotive Manufacture
BMW, Ford, GM, Mercedes,..

Scalable Information Management: Compression, Representation, Modeling, Control Optimization

Enterprise

Division

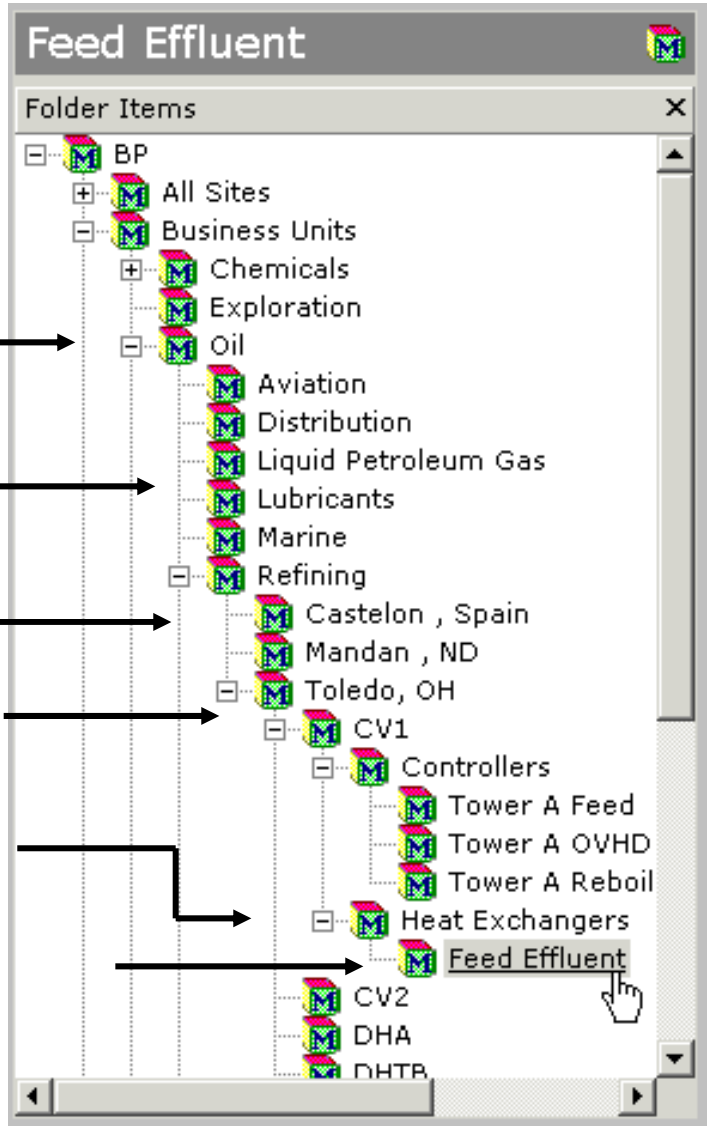
Department

Location

Unit

Equipment Class

Equipment



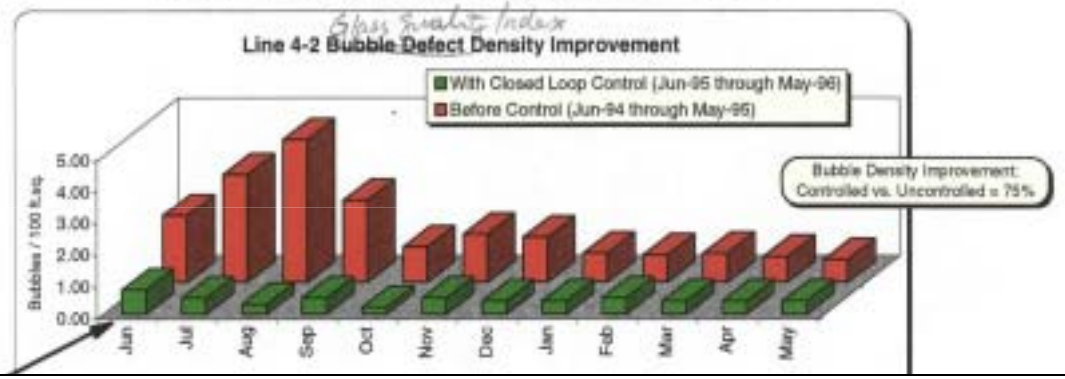
Information in relation to physical model, business model application model.

Adapted to end user
Specification
Appearance
Contents

Financial transactions
Inventory
Physical flow
Payroll
Plant data (T,P,C,..)
….

Results from On Line Trial:
Flat Glass Furnace Control

5% Higher Production rate in OEM:
Defect density 75% lower
Yield 8% higher



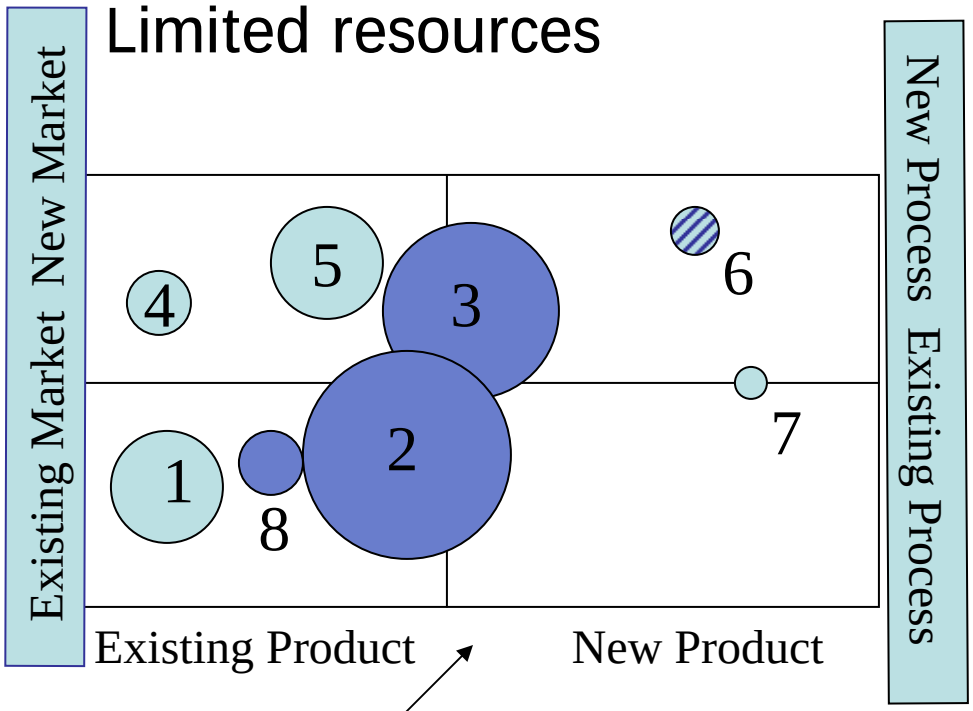
10% Higher Yield in Flat Glass Plant
Shorter Changeover time
Improve process capability to produce new products
Improve process consistency

Advanced control gives competitive advantage.
(Differentiation and ability to bid on and negotiate new contracts).

High Management Visibility!!!

Case Study 3: New Process and Product.

Mergers and Acquisitions (Elkem ASA $3B, Materials)



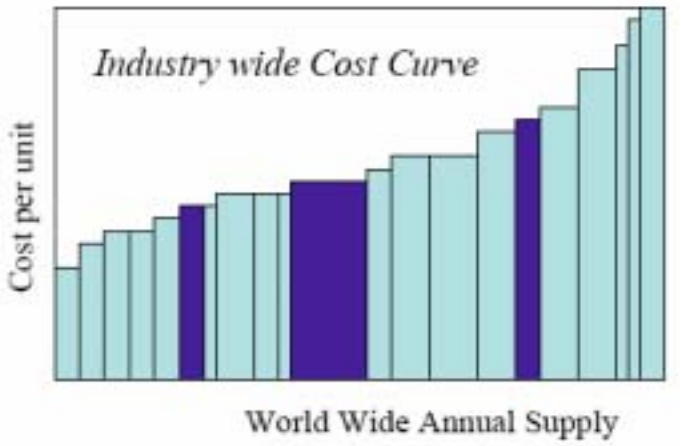
Objective: Grow Company and and expand product portfolio.

FeSi, Si, Al, C,SiO_2 commodities

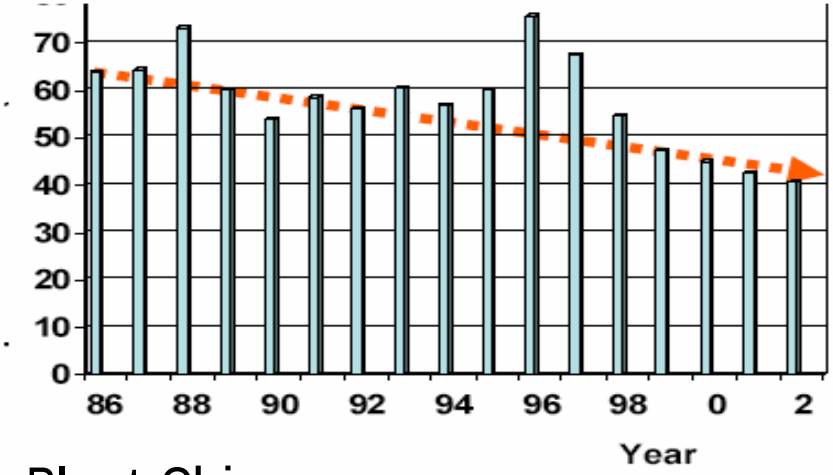
Organizational, technological, market, environment, human factors, legal, IP, culture, …

Si, SoG-Si, Al Products Advanced Materials and high value added products

The Systems Approach to Organisation



Silicon market



Geography/transporation/cost
- Buy Carbon Plant China
- Shut Down Plant in Norway

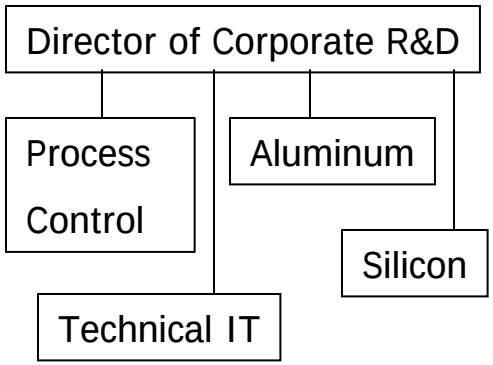
Technology (PSE) issues
- Buy Si Plant in Brazil
- Revamp Alloy Plant
- Large Scale Si Production in Salten

Supply chain
- Buy Aluminum Finished Products (SAPA)
- Secure energy supply through 2020

Result: Significant Change in Product Portfolio.

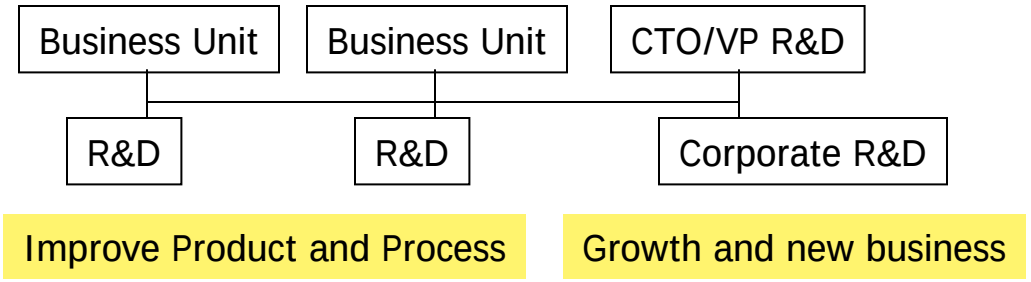
Higher Debt-Equity Ratio

Industrial R&D Reflects Company Structure



Centralized, Science Driven
In-house expertize

New Architecture for Industrial R&D



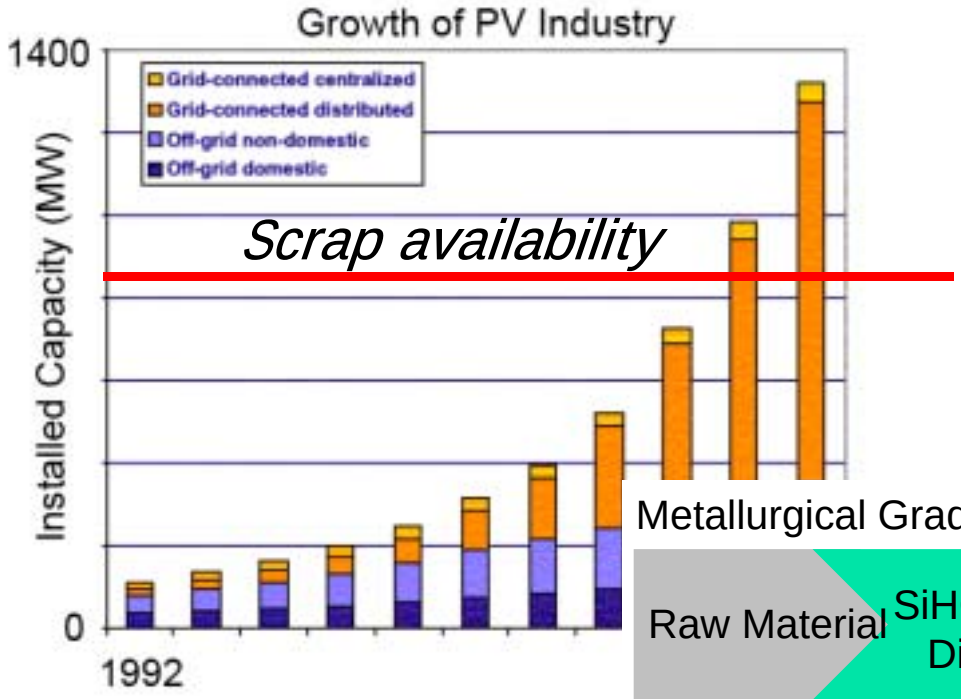
Decentralized and flexible market driven
Expertize brought in as needed

Strategic Business Units's (SBU) focus on projects with clear business impact in the areas of process and product improvements

Central R&D focus on growth, breakthrough technology and long term sustainability for the company. Involved in strategic decision making, mergers and acquisitions.

Case Study 4: New Process and Product

Solar Grade Silicon *(REC SGS Ltd. $100M, Si, Wafers, Cells)*



Objective: Develop a Cost effective way to make Solar Grade Silicon.

Metallurgical Grade $3-5 per kg

Electronic Grade $40-60 per k

Raw Material → $SiHCl_3$ (TCS) Distillation → Decomposition → Crystallization → Wafers → C

10% Waste

Missing Link

Insufficient

Remelt/Cryst → Wafers → PV Cells

Solar Grade Aim: $15 per kg

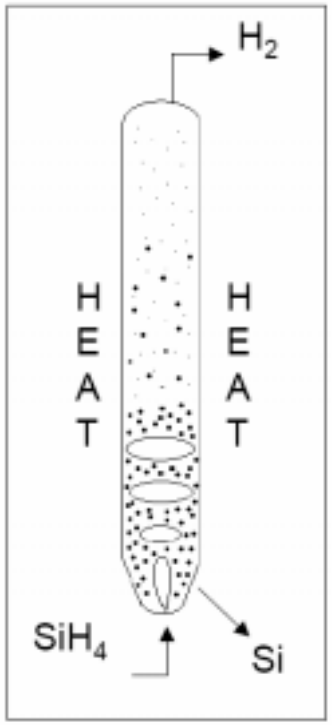
Many companies And technologies compete

PSE helps Concurrent Engineering: New Product and Process

Pilot

Demonstration

Production



Particulate process

Fluidization CFD

Multi-scale modeling

Optimization

Process Design

Process Control

New Sensors

Integrated Design to meet or exceed business expectations.

Prospect of reducing cost of producing PV electricity by a factor of 2-3 over the next five years looks promising.

R&D Team: SGS, PE Toronto, CAPD - CMU

The PSE Challenges and Opportunities in Research and Education (UG and Graduate)

Provide theoretical foundation, computational tools, educational methods and skilled personnel for:

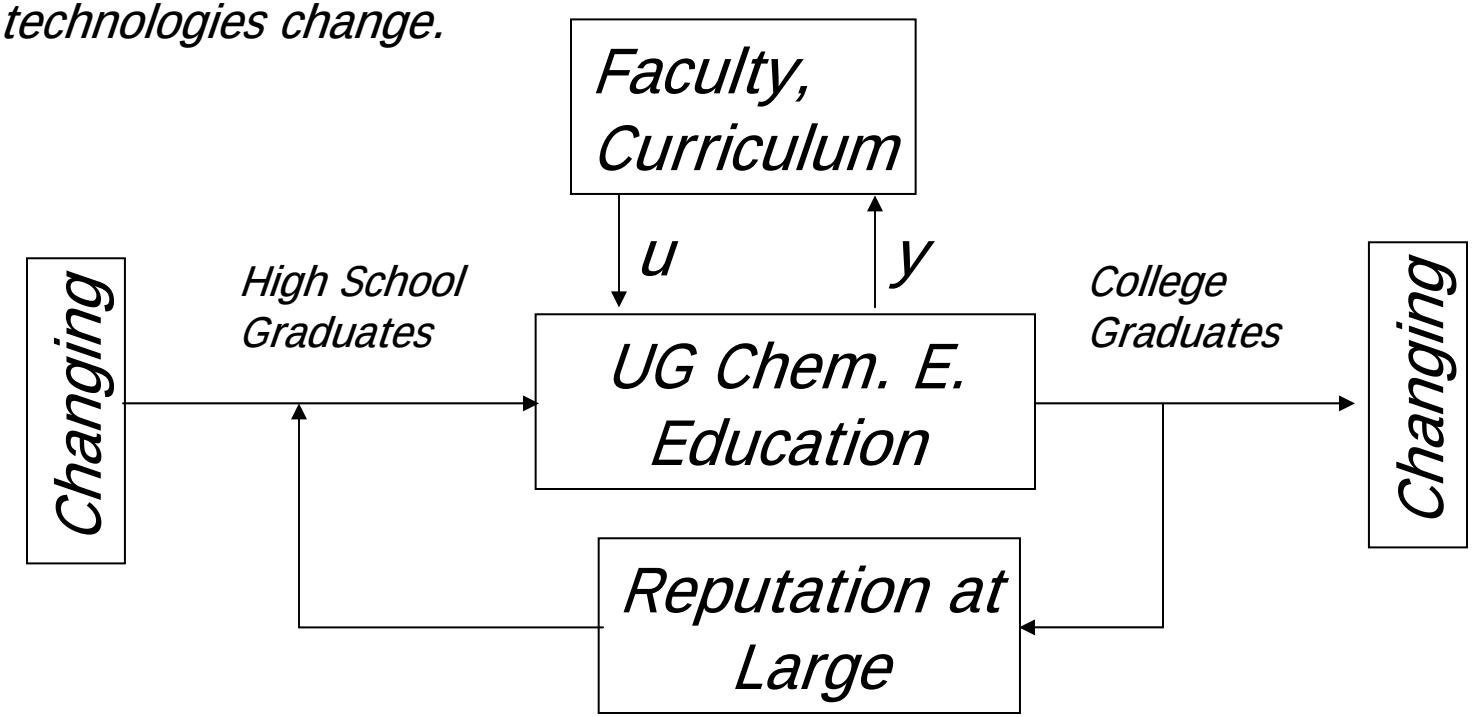
1) Designing and operating real time **decision support** systems for investment (management). These systems comprise physical processes, services, organizations and financial instruments. *(High Level Systems Thinking, Architecture design.)*

2) Automation of routine decision making in design and operation of complex **networks** of **embedded devices** for production and service. Optimization Design Control *(Algorithms, methods. Computation)*

3) Help advancing the frontiers of chemical engineering research in the application of computational tools to bio tech/bio med/nano tech/molecular, materials and drug design through interdisciplinary research. *(Expertise, Algorithms and Methods, Computational insight)*

The Challenge:

Derive a flexible curriculum that supports the complexity of the current market and adapts as the markets and technologies change.



1. *Envourage High School teaching as a career.*
2. *Quality <u>and</u> quantity.*
3. *Core+specialization*
4. *Include Bio in core*

→ *What goes out? More efficient?*