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Reflections on 35 Years in Process Systems Engineering Research

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Main messages

- Importance of mentors and teachers

- Importance of having a “dream” in research

- Importance of focusing in research

- Evolution of Process Systems Engineering

- Lessons learned and things to avoid

- Acknowledgments

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Education

B.S. Universidad Iberoamericana (1974)

Ing. Alejandro Puron de la Borbolla

Mass and Energy Balances
Transport Phenomena
Differential Equations

Ing. Julian Castellanos

B.S. Thesis Mexican Petroleum Institute

"Simulation model of multipass exchanger for condensation of multicomponent mixtures with noncondensible gases"

Castellanos, J. and I. Grossmann, "Mathematical Modelling of a Vapour Condenser with Non-condensible Gases" (in Spanish), *Revista del Instituto Mexicano de Ingenieros Quimicos* **15**(5), 58 (1974).

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Imperial College London

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Prof. R.W.H. Sargent

Prof. Arthur Westerberg

M.Sc. and Ph.D., Imperial College (1977)

Ph.D. thesis:

"Problems in the Optimum Design of Chemical Plants"

Grossmann, I.E. and R.W.H. Sargent, "Optimum Design of Heat Exchanger Networks," *Computers and Chemical Engineering* **2**, 1 (1978).

Grossmann, I.E. and R.W.H. Sargent, "Optimum Design of Chemical Plants with Uncertain Parameters," *AIChE J.* **24**, 1021 (1978).

Grossmann, I.E. and R.W.H. Sargent, "Optimum Design of Multipurpose Chemical Plants," *Ind. Eng. Chem. Process Des. Development* **18**, 343 (1979).

Carnegie Mellon University

Met in Swansea at 4th IChemE Research Mtg.

Hired me to Carnegie Mellon

Introduced me to Design Research Center

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Carnegie Mellon interview slides (1978)

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OPTIMUM DESIGN PROBLEM

$$\min C = f^0(x^1, x^2, \ldots x^n, u, \hat{v}, v^1, v^2, \ldots v^n, t^1, t^2, \ldots t^n)$$

$$\text{s.t.} \quad \left.\begin{array}{l} f^k(x^k, u, v^k, t^k) = 0 \\ h_L^k \le h^k(x^k, u, v^k, t^k) \le h_U^k \\ \hat{v} \ge v^k \end{array}\right\} \quad k = 1, 2, \ldots n$$

$$s_L \le s(x^1, x^2, \ldots x^n, u, \hat{v}, v^1, v^2, \ldots v^n, t^1, t^2, \ldots t^n) \le s_U$$

IF VARIABLES ARE CONTINUOUS AND FUNCTIONS ARE CONTINUOUSLY DIFFERENTIABLE EFFICIENT NLP ALGORITHMS THAT DETERMINE LOCAL OPTIMUM SOLUTIONS CAN BE APPLIED

PARTICULAR FEATURES IN THIS NLP

1) REDUCTION OF DEGREES OF FREEDOM DUE TO THE PRESENCE OF VECTOR u

a) SPECIFY OUTPUT VARIABLES AS INEQUALITIES

b) MODIFY FLOWSHEET OF THE PROCESS WITH ADDITION OF BYPASSES, VALVES OR OTHER DEVICES

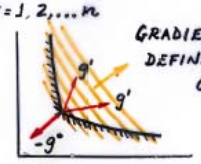
2) MONOTONICITY OF C W.R.T. $\hat{v}$ $(\partial C/\partial \hat{v} > 0)$

IMPLIES $\hat{v}_i = \max_{k=1,2,\ldots n} \{v_i^k\}$ IF $\hat{v}$ NOT BOUNDED

BETTER TO USE $\hat{v} \ge v^k \quad k = 1, 2, \ldots n$

IT IS MORE GENERAL

AVOIDS FAILURE OF KUHN TUCKER CONDITIONS



GRADIENT IS NOT DEFINED AT THE CORNER

CONSIDER MAXIMIZATION SUBPROBLEMS

FROM $f(w, z, \theta) = 0 \qquad z = \chi(w, \theta)$

$$\max_{\theta^L \le \theta \le \theta^U} g_i(w, \chi(w, \theta), \theta) \le 0$$

IF $g_i(w, \chi(w, \theta), \theta)$, $i = 1, 2, \ldots m$ IS MONOTONIC WRT θ SOLUTIONS OF THE SUBPROBLEMS MUST LIE AT THE CORNER POINTS OF $\theta^L \le \theta \le \theta^U$

MONOTONICITY OF THE CONSTRAINTS HOLDS FOR MANY TECHNICAL PARAMETERS IN THE DESIGN OF CHEMICAL PLANTS

SUFFICIENT CONDITIONS FOR THE MONOTONICITY OF THE CONSTRAINTS

ALL THE TERMS IN

$$\frac{\partial g_i}{\partial \theta_j} = \sum_{k=1}^{n} \frac{\partial g_i}{\partial z_k} \frac{\partial z_k}{\partial \theta_j} + \left.\frac{\partial g_i}{\partial \theta_j}\right|_z$$

MUST HAVE THE SAME SIGN

THIS HOLDS WHEN:

i) CONSTRAINTS ARE SPARSE AND MONOTONIC

EITHER $\frac{\partial g_i}{\partial z_k} = 0$ OR $\frac{\partial g_i}{\partial z_k}$ ONE SIGNED

ii) STATE VARIABLES ARE MONOTONIC WITH THE PARAMETERS

$\frac{\partial z_k}{\partial \theta_j}$ ONE SIGNED

Goal in Research: Develop Mixed-integer Programming Techniques and apply to the Design and Operation of Chemical Processes

Evolution from Mixed-integer Nonlinear Programming (MINLP) to Generalized Disjunctive Programming (GDP)

Driver: Towards integration of symbolic logic

Prof. Egon Balas

MINLP: Mixed-integer Nonlinear Programming

$$\begin{aligned} \min\ & Z = f(x,y) \\ s.t.\quad & h(x,y) = 0 \\ & g(x,y) \le 0 \\ & x \in R^n,\ \ y \in \{0,1\}^m \end{aligned}$$

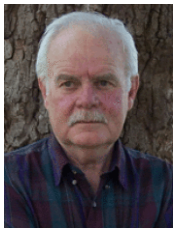
=>

GDP: Generalized Disjunctive Programming

$$\begin{aligned} \min\ & Z = f(x) \\ s.t.\quad & r\ (x) \le 0 \\ & \bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \end{bmatrix} \quad k \in K \\ & \Omega(Y) = true \\ & x \in R^n,\ Y_{jk} \in \{ true,\ false \} \end{aligned}$$

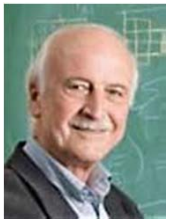
Evolution from Process Synthesis to Scheduling to Supply Chain

Drivers: From Design to Operations



Prof. Dale Rudd

Prof. Art Westerberg

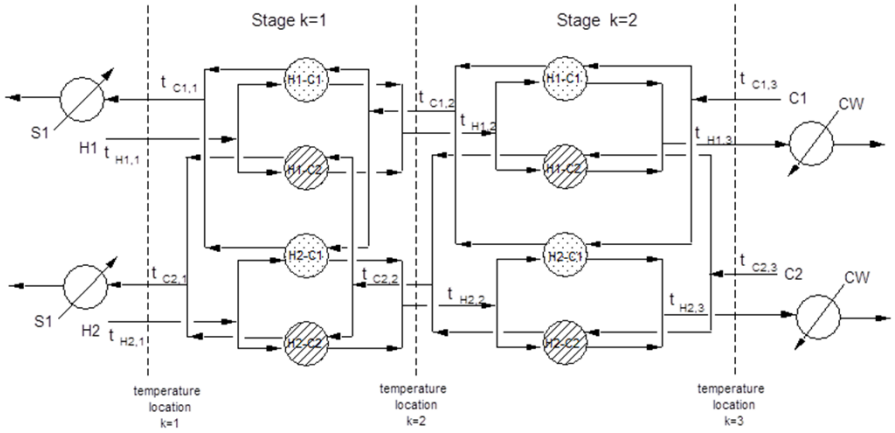


Prof. George Stephanopoulos

Prof. David Rippin

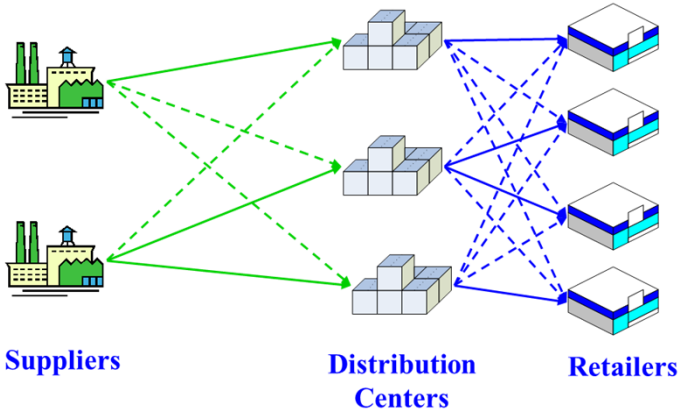
Prof. Rex Reklaitis

Heat Exchanger Network Synthesis



=>

Supply Chain Design



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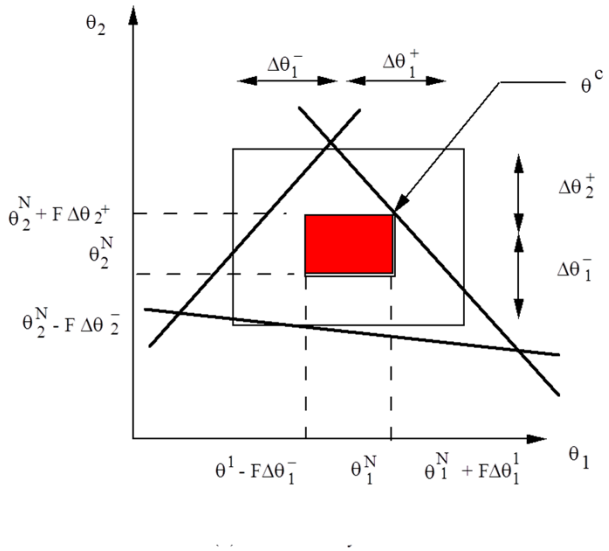
Evolution from Process Flexibility to Stochastic Programming

Driver: From Deterministic to Probabilistic Approaches for Uncertainty

Prof. Manfred Morari

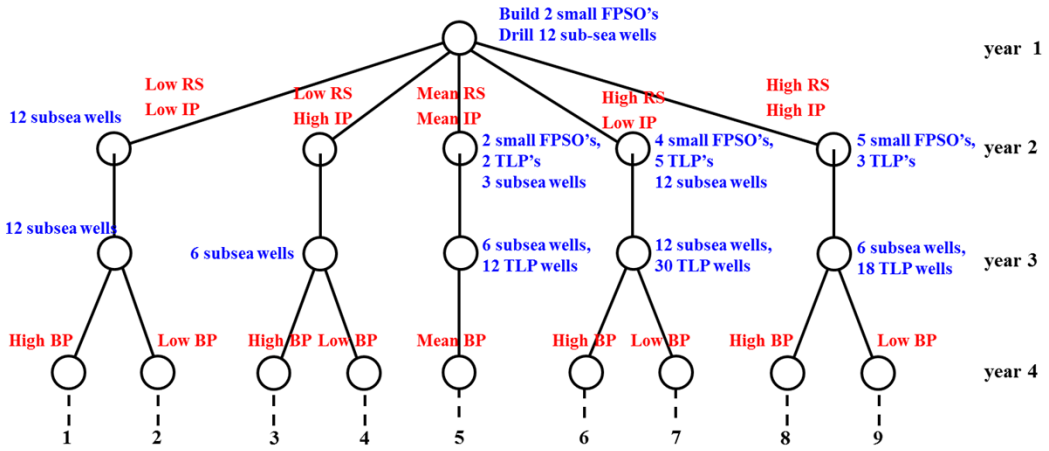
Flexibility Analysis



Critical Point

=>

Mutistage Stochastic Programming



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I. Mixed-integer nonlinear programming

Outer-Approximation Algorithm: *Marco Duran (1984)*

Modeling-Decomposition: *Gary Kocis (1988)*

Linear Generalized-Disjunctive Programming (GDP): *Ramesh Raman (1992)*

LP/NLP Based Branch and Bound: *Ignacio Quesada (1993)*

Multiperiod MINLP: *Dimitrios Varvarezos (1994)*

Logic-Based Outer Approximation: *Metin Turkay (1996)*

Global Optimization NLP: *Juan Zamora (1997)*

Integration MILP and Constraint Programming: *Vipul Jain (1999)*

LOGMIP: *Aldo Vechietti (2000)*

Nonlinear Generalized Disjunctive Programming: *Sangbum Lee (2002)*

Logical Modeling Framework: *Ashish Agrawal (2006)*

Cutting Planes Linear GDP: *Nicolas Sawaya (2006)*

Convex Nonlinear GDP: *Juan Pablo Ruiz (2011)*

Automated Reformulation of GDP: *Francisco Trespalacios (2015*)

II. Process Synthesis

LP/MILP Transshipment: *Soterios Papoulias (1982)*

Integrated Refrigeration Systems: *Mark Shelton (1985)*

NLP Superstructure Heat Exchanger Networks: *Chris Floudas (1986)*

MINLP Model for Heat Exchanger Networks: *Terry Yee (1990*)

Hierarchical Decomposition/MINLP: *Mark Daichendt (1995)*

MINLP and GDP Superstructure Modeling: *Hector Yeomans (1999)*

MINLP and GDP Models Distillation: *Mariana Bartfeld (2003)*

GDP Model Reactive Distillation: *Jennifer Jackson(2003)*

Global Optimization Water Networks: *Ramkumar Karuppiah (2007)*

Optimal Design Integrated Gasification Combined Cycle: *Ravi Kamath (2012)*

Water management for shale gas production: *Linlin Yang (2014)*

III. Batch and Continuous Scheduling

Retrofit Design Batch Plants: *Jane Vaselenak (1985)*

Design & Scheduling Multiproduct Batch Plants: *Deepak Birewar (1989*)

Design of Multipurpose Batch Plants: *Vasilios Voudoris (1993)*

Cyclic Scheduling of Continuous Multiproduct Plants: *Jose Pinto (1995)*

Scheduling Tests for New Product Development: *Craig Schmidt (1998)*

Batch Scheduling with Uncertainty: *Jayanth Balasubramanian (2003)*

Continuous Time State-Task-Network Model: *Christos Maravelias (2004)*

Optimal Crude Oil Scheduling Operations: *Sylvain Mouret (2010)*

Scheduling of Fast Moving Consumer Products: *Martijn Elzakker (2013)*

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IV. Planning and Supply Chain

Lot Sizing Reformulation Long Range Planning: *Nick Sahinidis (1990)*

Bi-Level Decomposition Process Networks: *Ramesh Iyer (1997)*

Design and Planning of Offshore Oilfield Facilities: *Susara Van den Heever (2001)*

Dynamics and Control for Supply Chain Management: *Edgar Perea (2002)*

Integration Planning & Scheduling Continuous Multiproduct: *Muge Erdirik (2007)*

Design Responsive Supply Chains: *Fengqi You (2009)*

Design Reliable Integrated Chemical Production Sites: *Sebastian Terrazas (2011)*

Nonlinear Refinery Planning Model: *Abdul Alattas (2012)*

Demand-side Management Air Separation Plants: *Sumit Mitra (2013)*

Oilfield Development Planning under Endogenous Uncertainties *Vijay Gupta (2013)*

Design of Supply Chains under Disruptions: *Pablo Garcia-Herreros (2016)*

Multiscale Optimization for Production and Distribution Industrial Gases: *Qi Zhang (2016)*

Optimal Design and Drilling Operations for Shale Gas Production: *Markus Drouven (2018)*

V. Design and Planning under Uncertainty

Optimal Design Flexible Chemical Plants: *Keshava Halemane (1982)*

Flexibility Analysis: *Ross Swaney (1983)*

Retrofit Design for Improving Flexibility: *Stratos Pistikopoulos (1988)*

Expected Stochastic Flexibility: *David Straub (1991)*

Two-stage Programming with Flexibility Constraints: *Robert Clay (1994)*

Linear Multistage Stochastic Prog. Endogenous Param.: *Vikas Goel (2005)*

Nonlinear Multistage Stochastic Prog. Endogenous Param.: *Bora Tarhan (2005)*

Generation of Scenarios from Historical Data: *Bruno Calfa (2015)*

Multistage Stochastic Progr. Exogeneous & Endogenous Param.: *Rob Apap(2016)*

Other

Optimization Models for Metabolic Networks: *Soumitra Gosh(2006)*

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Process Systems Engineering

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Core area in Chemical Engineering: *systematic analysis and optimization of decision making processes* for the discovery, design, manufacture and distribution of chemical products

Rich knowledge base *(multidisciplinary)*

Process Knowledge => Conceptual design => Process Integration

Numerical analysis => Simulation => Performance process-product

Mathematical Programming => Optimization => Synthesis/design

Systems and Control Theory => Process Control => Manufacturing

Computer Science => Advanced Computing => Efficient solution

Management Science => Operations/Business => Supply chain

Greatly expanded scope:
from process to molecular and from process to enterprise level

Greatly expanded capability: *solution of large-scale industrial models*

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Emerging challenges

Product and Process Design
Energy and Sustainability
Enterprise-wide Optimization

+

Continuing Challenges in Fundamentals

Modeling
Optimization
Process Synthesis
Process Operations
Process Control

Challenge for Process Systems community given Science vs. Engineering:
Communicate importance of area to rest of Chemical Engineering Community
PSE also Science-based and driven by Industrial Needs!!

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Lessons Learned

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1. It pays to dream and it pays to persevere; do not give up!

"The problems of the world cannot be possibly solved by skeptics or cynics whose horizons are limited by obvious realities. We need people who can dream things that never were." -John F. Kennedy

2. Be strategic: concentrate on few areas

"The essence of strategy is choosing what not to do. "
- Michael E. Porter

3. Surround yourself with good and *enthusiastic* people

- *Ph.D. Students*
- *Research Collaborators*
- *University colleagues*
- *Industry colleagues*

"You can't have a goal without determination, because without the determination the goal will die." - Patrick Turner

4. Do not compromise on quality and recheck as many times as needed

"It's not that I'm so smart, it's just that I stay with problems longer."
--Albert Einstein

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Lessons Learned

5. View industry as source of new research problems

"You may be theoretically rich but practically poor."
–Rupsah Rana

6. View teaching as a way of reinforcing the research and vice-versa

"It is the supreme art of the teacher to awaken joy in creative expression and knowledge. -Albert Einstein

To be avoided

- University (corporate) administrators: *view them with suspicion*
- University IP lawyers: *unless you really have to, ignore them.*

Greatest satisfaction is to see your students grow and succeed

Graduate Students (1980-1994)

1. Jennifer Davidson, M.S., 1980, Tektronix
2. Robert Drabbant, M.S., 1981, Taylor Instruments
3. Keshava P. Halemane, Ph.D., 1982, Karnataka Regional Engineering College
4. Soterios Paopulias, Ph.D., 1982, Momentive, New York
5. Ilan Avidan, M.S., 1982, City College New York
6. Ross E. Swaney, Ph.D., 1983, University of Wisconsin, Associate Professor
7. Marco A. Duran, Ph.D., 1984, ExxonMobil, Annandale
8. Jane A. Vaselenak, Ph.D., 1985, Shell Development Co.
9. Mark R. Shelton, Ph.D., 1985, Eastman Chemical
10. Christodoulos A. Floudas, Ph.D., 1986, Princeton University, Professor
11. Gary R. Kocis, Ph.D., 1988, ExxonMobil, Fairfax
12. Efstratios N. Pistikopoulos, Ph.D., 1988, Imperial College, London, Professor
13. Mohini Chatrathi, M.S., 1987
14. Sanjay Pradhan, M.S., 1987, Max Secure Software, India
15. Terrence F. Yee, Ph.D., 1990, Air Products, Hong Kong.
16. Deepak B. Birewar, Ph.D., 1989, Invenstys, Bombay, India.
17. Nikolaos Sahinidis, Ph.D., 1990, Carnegie Mellon University, Professor
18. David Straub, Ph.D., 1991, ExxonMobil, Houston
19. Ramesh Raman, Ph.D., 1992, Amyris, San Francisco.
20. Ignacio Quesada, Ph.D., 1993, McKinsey, Mexico City
21. Vasilios Voudouris, Ph.D., 1993, Vereniki Solutions, Sacramento
22. Dimitrios Varvarezos, Ph.D., 1994, Aspen Technology
23. Robert Clay, Ph.D. , 1994, Sandia National Lab, Livermore

Graduate Students (1995-2005)

24. Mark Daichendt, Ph.D., 1995, Air Products, Allentown
25. Jose Pinto Ph.D.,1995, Praxair, Dunbury; Polytechnic University, New York, and University of Sao Paulo, Brazil, Associate Professor.
26. Metin Turkay, Ph.D., 1996, Koc University, Istanbul, Professor.
27. Ramaswamy Iyer, Ph.D., 1997, GE, Cincinnati
28. Juan Zamora, Ph.D. , 1997, Universidad Autonoma Metropolitana, Mexico City.
29. Craig Schmidt, Ph.D., 1998, First Fuel Software, Boston
30. Vipul Jain, Ph.D., 1999, Bank of America, New York
31. Hector Yeomans, Ph.D.,1999, FEMSA, Mexico City.
32. Aldo Vecchietti, Ph.D., 2000 (Universidad Nacional Litoral, Argentina), INGAR.
33. Susara Van Den Heever, Ph.D., 2001, IBM, Nice, France.
34. Edgar Perea, Ph.D., 2002, PEMEX, Mexico.
35. Sangbum Lee, Ph.D, 2002, ExxonMobil, Fairfax.
36. Jennifer Jackson, Ph.D., 2003, Capital ONE, Washington DC
37. Jayanth Balasubramanian, Ph.D., 2003, ExxonMobil, Fairfax.
38. Mariana Barttfeld, Ph.D., 2003 (Universidad Nacional Litoral, Argentina), Chemical and Bioengineering Processes, University Erlangen, Germany.
39. Christos Maravalias, Ph.D., 2004, University of Wisconsin, Associate Professor.
40. Gabriela Garcia-Ayala, M.S. 2004, Universidad de Nuevo Leon, Ph.D. student.
41. Vikas Goel, Ph.D., Ph.D, 2005, ExxonMobil, Houston.
42. Soumitra Ghosh, Ph.D., 2006, Bayer Corporation, San Francisco.
43. Ashish Agarwal, Ph.D., 2006, Yale University, postdoc.
44. Nicolas Sawaya, Ph.D. 2006, ExxonMobil, Houston.

Graduate Students (2007-2014)

45. Muge Erdirik, Ph.D. 2007, Amazon, Seattle.
46. Ramkumar Karuppiah, Ph.D., 2007, ExxonMobil, Annandale.
47. Bora Tarhan, Ph.D. 2009, ExxonMobil, Houston
48. Fengqi You, Ph.D. 2009, Northwestern University
49. Sylvain Mouret, Ph.D. 2010, Artelys, Paris, France.
50. Ravindra Kamath, Ph.D., 2012, Bayer, Baytown
51. Abdularahman Alattas, 2012, Ph.D. Abu Dhabi NOC, Abu Dhabi
52. Juan Pablo Ruiz, Ph.D. 2011, Soteica, Austin.
53. Sebastián Terrazas, Ph.D. 2011, KBC Advanced Technologies, Houston.
54. Scott Kolodziej M.S. 2012, Shell Oil, Houston
55. Vijay Gupta, Ph.D., 2013, Shell Oil, Houston.
56. Sumit Mitra, Ph.D., 2013, A.T. Kearney, Dusseldorf
57. Ahmad Alothman, M.S., 2013, Saudi Aramco, Dhahran, Saudi Arabia.
58. Martijn Elzakker, Ph.D., 2013, Corbion
59. Linlin Yang, Ph.D., 2014, ExxonMobil, Fairfax.
60. Bruno Calfa, Ph.D. (expected 2015)
61. Pablo Garcia Herreros, Ph.D. (expected 2015)
62. Francisco Trespalacios, Ph.D. (expected 2016)
63. Qi Zhang, Ph.D. (expected 2016)
64. Robert Apap, Ph.D. (expected 2016)
65. Markus Drouven, Ph.D. (expected 2017)
66. Irene Lotero-Herrantz, M.S. (expected 2014)

Research Collaborators

Elvis Ahmetovic, University of Tuzla, Bosnia
Ana Barbosa Povoa, IST, Lisbon
Jose Caballero, Universidad de Alicante, Spain
Diego Cafaro, INTEC, Argentina
Pedro Castro, LNEG , Portugal
Jaime Cerda, INTEC,Santa Fe, Argentina
Soledad Diaz, PLAPIQUI, Argentina
Hongguang Dong, Dalian University of Technology, China
Sebastian Engell, Technical University Dortmund, Germany
Antonio Flores, Universidad Iberoamericana, Mexico
Berta Galan, Universidad de Cantabria, Spain
Gonzalo Guillen, Universidad Roviri e Virgili, Spain
Yongheng Jiang, Tsinghua University, China
Arturo Jimenez, Instituto Tecnologico de Celaya, Mexico
Zdravko Kravanja, University of Maribor, Slovenia
Ricardo Lima, LNEG, Portugal
Pablo Marchetti, INTEC, Argentina
Marian Marcovecchio, INGAR, Argentina
Mariano Martin, Universidad de Salamanca, Spain
Carlos Mendez, INTEC, Argentina
Aldo Vecchietti, INGAR, Argentina
Tapio Westerlund, Abo Akademi, Finland
Juan Zamora, Universidad Metropolitana-Iztapalapa, Mexico
Edwin Zondervan, Technical University of Eindhoven, Holland

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Visiting Researchers/Postdocs

Federico Andersen, PLAPIQUI
Lorena Bergamini, Universidad de Buenos Aires
Beatriz Bolio, Univ. Iberoamericana
Veronique Bizet, TotalElfFina
J.K. Bok, KAIST
Anna Bonfil, UPC
Eugenio Bringas, Universidad de Cantabria
Dirk Brusis, Technical University München
Elisabet Capon, UPC
Xuan Chen, Tsinghua Univ.
Pedro Copado, Roviri i Virgili
Daniela Drummond, University of Campinas
Macelo Escobar, Rio Grande do Sul
Sergio Frausto, Tecnologico de Celaya
Carlos Florensa, UPC
Drago Gajic, ABB
Berta Galan, Universidad de Cantabria
Gabriela Garcia, Universidad de Nuevo Leon
Marta Castilo Gomes, IST-Lisbon
Gonzalo Guillen, Universidat Roviri e Virgili
Truls Gundersen, NTNU
Hubert Hadera, ABB
Iiro Harjunkoski, ABB Corporate Research
Clara Heuberger, RWTH-Aachen
Martin Houze, TotalElfFina
Wang Jun, Tsinghua Univ.
Juan Reyes Labarta, Univ. Alicante
Heeman Lee, KAIST
Ricardo Lima, LNEG
Nancy Medina, Tecnologico de Celaya
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David Molina, Univ. Iberomericana
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Fabricio Oliveira, PUC-Rio de Janeiro
Francesca Palazzi, EPFL
Minhwan Park, Sangsum
Luisa Perez, ITESM
Jose Maria Ponce, Universidad Michoacana
Roger Rocha, Petrobras
Analia Rodriguez, INGAR
Ruben Ruiz, University of Alicante
Raquel Salcedo, University of Alicante
Edna Saucedo, U. Guanajuato
Mahdi Sharifzadeh, Imperial College
Arzu Turkay, Middle Eastern Technical University
Monica Valdez, Tecnologico de Celaya
J. Viswanathan, Engineers India
Lei Zhang, Tsinghua

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Process Systems Engineering Group

Center for Advanced Process Decision-making

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Larry Biegler

Chrysanthos Gounaris

Nick Sahinidis

Jeff Siirola

Erik Ydstie

U.S. and International Process Systems Community at Large

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Funding

National Science Foundation

Maria Burka

FULBRIGHT

Industrial Sponsors

Jeff Siirola-Eastman
Jerry Robertson-ExxonMobil
Marco Duran-ExxonMobil
John Wassick-Dow
Iiro Harjunkosky-ABB
Jose Pinto-Praxair

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reaching new frontiers
SK innovation
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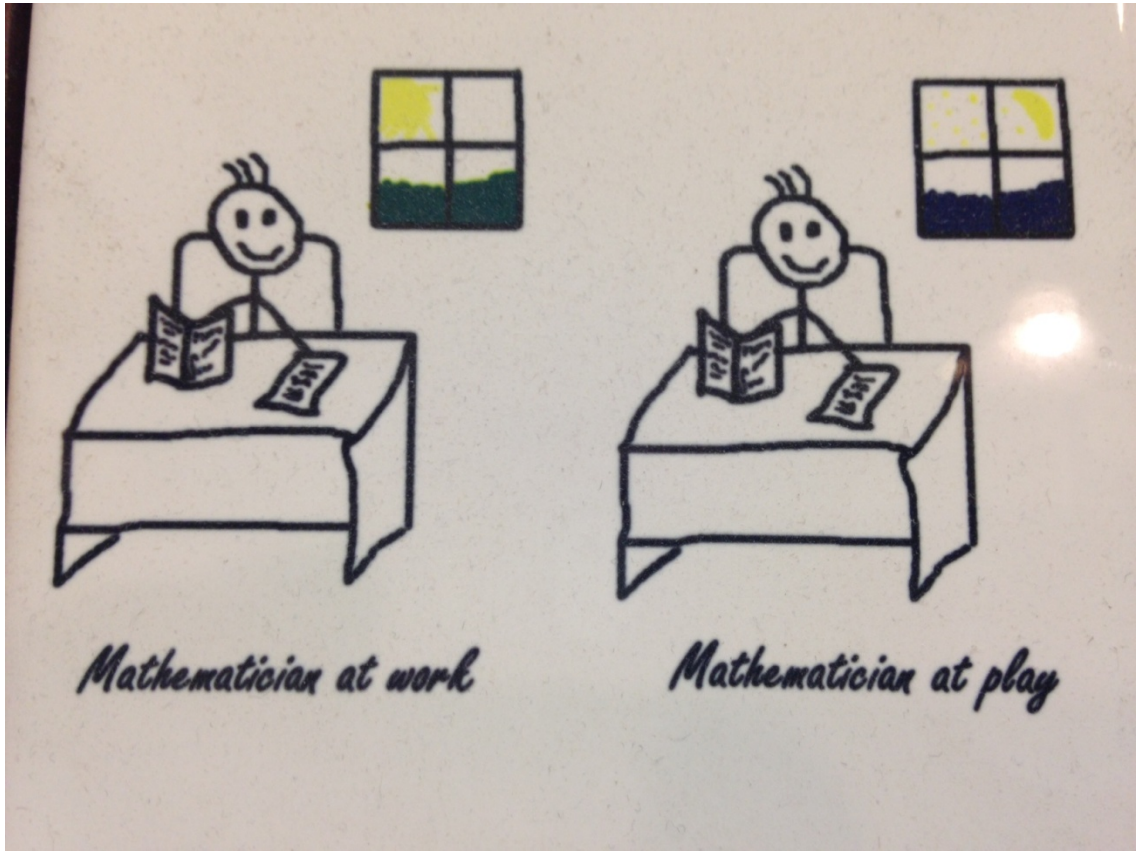
Unilever
United Technologies

From my daughter Claudia



My Parents

Donat Grossmann
(1920-1994)

Marie Louise Epper
(1929-2013)

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My Wife Blanca

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Our children: Claudia, Andrew, Thomas

Our grandchildren: Lucas, Oscar

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Many Thanks!