## Incorporating Dynamic Simulation into Chemical Engineering Curricula

**Goals:** Although dynamics are critical for understanding most chemical processes, its coverage is limited in most chemical engineering curricula. Even then, coverage is usually limited to mathematical techniques and analytical solutions rather than physically motivated, industrially relevant problems. A typical problem statement might provide a process transfer function and request students to calculate the poles to determine whether the transfer function is stable. While students often end up with a set of mathematical skills that can be used to solve idealized textbook problems, they often are not able to apply these skills to realistic problems in an operating plant. To address these concerns, this workshop describes computer-aided tools for producing graduates with skills of value to the process industry. The workshop will be especially useful for instructors who want to integrate dynamic simulation into their courses but who are not control engineers.

We feel that chemical engineering is best taught by having the students actively employ realistic dynamic simulations of industrial processes, that is, which include such phenomena as nonlinearities, constraints, disturbances, and uncertainties. A typical class period may include presentation and discussion of a motivating industrial problem and time for the students to solve the problem using analytical techniques and simulation using MATLAB/Simulink.

The session provides instructors with specific chemical and biological engineering examples for use in various courses within the chemical engineering curriculum to motivate students to learn different modeling, analysis, and control techniques and to have the students engaged in authentic learning experiences. The expected outcomes are that participants are exposed to practical engineering problems, implement solutions in MATLAB/Simulink or Python, and discuss the effects of nonlinearities, disturbances, and design changes.

**Scope and Content:** After a brief overview of how to set up a blending problem, the instructors discuss some challenging problems for which MATLAB/Simulink or Python software implementations are available.

The ASEE Session includes 3 demo applications with Blending, a Hot Air Balloon, and an Arduino heat transfer and energy balance simulation. In the remainder of the session, participants gain hands-on experience with the MATLAB/Simulink or Python modules[1] that implement a variety of practical industrial problems, which participants select from

- Aspirin Crystallization
- Automobile Cruise Control
- Batch Distillation
- Continuous Distillation
- Continuously Stirred Tank Reactor
- Diabetes Blood Glucose Control with Insulin
- Drilling Automation (Oil and Gas)
- Gravity Drained Tank

[1] All MATLAB modules will be accessible via links at the CACHE Teaching Resources website and the websites of the instructors.

- Grid-energy system
- And others

Attendees who do not have MATLAB already installed on their laptops will be able to run the software on NC State's Virtual Computing Laboratory where MATLAB/Simulink is available. Python is freely available from Python.org or continuum.io (Anaconda with IPython).

**Method of Delivery:** The actual session is taught in a similar fashion as a typical lecture/discussion class. The session participants are exposed to specific chemical processes with nonlinear dynamics, constraints, and other realistic behavior, and asked to build process models, analyze process dynamics, and make design recommendation. The instructors are experts in the process control problems and the associated dynamic simulations implemented in MATLAB/Simulink and Python. Participants who are more interested in exploring multiple hands-on activities are allowed to do so.

**Take Home Materials:** The take-home materials will be links to relevant materials accessible on the web, the MATLAB/Simulink and Python files provided before and during the session, project assignments, student handouts, and example student presentations.

- Introduction to Dynamic Modeling (YouTube Playlist): https://goo.gl/G9KdYG
- Nonlinear Dynamic Model Library: http://www.hedengren.net/research/models.htm
- Process Control Course with Python: http://apmonitor.com/pdc
- Process Control Course with MATLAB: http://apmonitor.com/che436

**Presenters:** Martha Grover, John Hedengren, and Thomas Badgwell, whose bios are attached.

**Timing:** Two hours, with the breakdown in the Scope and Content section.

**Specific Logistical Needs:** Wireless internet access, provided by the host site. The participants should bring or be given laptops so that they can run the software and have the most benefit. Attendees who do not have MATLAB already installed on their laptops will be able to run the software on NC State's Virtual Computing Laboratory where MATLAB/Simulink is available. Python is freely available for download and installation is recommended before the session.

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John Hedengren leads the Process Research and Intelligent Systems Modeling (PRISM) group at Brigham Young University. He teaches several undergraduate and graduate courses at BYU including Process Dynamics and Control, Computational Tools, Optimization, and Dynamic Optimization. His 500 videos on these topics are accessed over 100,000 times per month on YouTube. His courses include hands-on labs such as an Arduino-based heat transfer, modeling, and control lab. They also include simulation labs in MATLAB and Python such as a distillation column, diabetic blood glucose, exothermic tank reactor, gravity drained tanks, drilling, smart grid energy storage, and many others. He helped publish an online textbook on optimization (http://apmonitor.com/me575) and is developing content for the Python language in Process Dynamics and Control (http://apmonitor.com/pdc). He is a web editor for energy topics for AIChE, coordinates CAST division webinars, as well as the web editor for the Upstream Engineering and Flow Assurance (UEFA) division. He also serves as the web editor for the American Automatic Control Council (a2c2.org). Prior to BYU he worked as a consultant for Apache, ENI Petroleum, HESS, SABIC Ibn Zahr, and TOTAL on automation solutions and then full-time for 5 years with ExxonMobil supporting advanced control and optimization solutions. His area of expertise is in fiber optic monitoring, unmanned aerial systems, automation of production and drilling, and development of new technologies that monitor and control upstream infrastructure. His automation software has been applied to over 100 industrial applications worldwide. His modeling and automation software was cited in receiving the 2014 AIChE David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education.

## Education

| | | | |
|---|---|---|---|
| Brigham Young University | Chemical Engineering | B.S. | 2001 |
| Brigham Young University | Chemical Engineering | M.S. | 2002 |
| The University of Texas at Austin | Chemical Engineering | Ph.D. | 2005 |

## Teaching Honors and Awards

2014 AIChE David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education

## Academic and Industrial Positions

| | |
|---|---|
| 8/2011 – Present | Assistant Professor, Brigham Young University |
| 1/2007 – 8/2011 | Senior Engineer, ExxonMobil Chemical, Houston, Texas |
| 5/2005 – 1/2007 | Project Engineer, Plant Automation Services, Houston, Texas |
| 8/2002 – 5/2005 | Graduate Research Assistant, University of Texas at Austin |

## Selected Educational Publications

1. Hedengren, J. D., A Nonlinear Model Library for Dynamics and Control, Computer Aids for Chemical Engineering (CACHE) News, Summer 2008.
2. Hedengren, J. D. and Asgharzadeh Shishavan, R., Powell, K.M., and Edgar, T.F., Nonlinear

Modeling, Estimation and Predictive Control in APMonitor, Computers and Chemical Engineering, Volume 70, pp. 133–148, 2014, DOI: 10.1016/j.compchemeng.2014.04.013.

## Research Supervision

*Graduate*: Supervised 7 PhD and 3 MS theses, currently supervising 4 PhD students and 2 MS students
*Undergraduate*: Approximately 85% of students in the BYU Chemical Engineering department have an opportunity to do research and many are authors on publications. I supervise about 25 to 35 undergraduate researchers each semester.

## Courses Taught

Below are course websites with representative homework, video tutorials, exams, project descriptions, and examples of flipped classroom content.

ChEn 263 – Computational Tools
- Course Website: http://byu.apmonitor.com/che263
- Project: http://byu.apmonitor.com/che263/index.php/Main/CourseProjects

ChEn 436 – Process Dynamics and Control
- Course Website: http://byu.apmonitor.com/che436
- Project: http://byu.apmonitor.com/che436/index.php/Main/PhysicalLab

ME 575 – Design Optimization
- Course Website: http://byu.apmonitor.com/me575
- Homework: http://apmonitor.com/me575/index.php/Main/TwoBarTruss
- Project: http://apmonitor.com/me575/index.php/Main/ApplicationProject

ChEn 693R – Dynamic Optimization
- Course Website: http://byu.apmonitor.com/do
- Project: http://byu.apmonitor.com/do/index.php/Main/ProjectLab

## Past ASEE Summer School Experience

Attended the Chemical Engineering ASEE Summer School in 2012 in Maine as a new faculty member.

**Martha A. Grover**
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## Professional Preparation

| | | | |
|---|---|---|---|
| University of Illinois at Urbana-Champaign, IL | Mechanical Engineering | B.S. | 1996 |
| California Institute of Technology, Pasadena, CA | Mechanical Engineering | M.S. | 1997 |
| California Institute of Technology, Pasadena, CA | Mechanical Engineering | Ph.D. | 2003 |

## Appointment

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, Professor (2015–Present)

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, Associate Professor (2009–2015)

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, Assistant Professor (2003–2009)

## Awards

NSF CAREER Award (2004)

W. David Smith Graduate Publication Award, AIChE Computing and Systems Technology Division (2005)

Outstanding Young Investigator Award, AIChE Computing and Systems Technology Division (2011)

## Graduate and Postgraduate Advising

Supervised 13 PhD theses, 1 MS thesis, and 6 postdoctoral researchers

## Courses Taught

Undergraduate: Process Control Lecture, Process Control Lab, Thermodynamics I, Numerical Methods

Graduate: Mathematical Modeling and Analysis of Chemical Processes

## Educational Materials

- Produced ten screencasts for undergraduate process control, following a single process (the blending process) through key aspects of introductory dynamics and control: http://grover.chbe.gatech.edu/teach.htm
- Created design projects based on case studies for the undergraduate process control lab, including a project on aspirin crystallization that was adapted for use in Spring 2016 and Fall 2016.

- Designed and recorded two course modules for an online Coursera MOOC on high-throughput materials characterization. Specifically, the modules focused on experimental design for high-throughput experiments (2016).

**Public Outreach**

- Science advisor and principal investigator for NSF-supported interactive theater production entitled "Group Intelligence" on molecular assembly and origins of life chemistry. The production premiered in Atlanta in April 2011 with five performances, and toured the east coast at science festivals during summer 2012. A high-school activity based on Group Intelligence premiered in 2014, with assessment conducted in 2015. A publication on this high-school activity is currently in review at the *Journal for Chemical Education*.
- Collaboration with Emory University Professor of Music Steven Everett, who composed a string quartet composition based on Grover's stochastic simulations of spatial-temporal organization. The world premiere was on March 4, 2012, with Grover narrating. The associated research publication was "Universal sequence replication, reversible polymerization and early functional biopolymers: A model for the initiation of prebiotic sequence evolution," S.I. Walker, M.A. Grover, and N.V. Hud, *PLoS ONE*, **7**(4) e34166 (2012).
- Faculty lead for Education, Outreach, and Diversity in the NSF/NASA Center for Chemical Evolution, 2013–present.

**Thomas A. Badgwell**
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Corporate Strategic Research
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Thomas A. (Tom) Badgwell is an Advanced Research Associate in the Data Analytics & Optimization Section, Corporate Strategic Research Department, at the ExxonMobil Research & Engineering Company in Annandale, NJ. Tom's career has focused on modeling, optimization, and control of refining and chemical processes, with past positions at SETPOINT, Fisher/Rosemount, Rice University, and Aspen Technology. He joined ExxonMobil in 2009, and came to CSR in 2012 following an initial assignment at the Baytown, Texas refinery. Tom is a Fellow of the American Institute of Chemical Engineers and received the Computing Practice Award from their Computing and Systems Technology Division in 2013. He is an Associate Editor for the Journal of Process Control and serves as an Industrial Trustee for the Computer Aids in Chemical Engineering Corporation.

## Education

| | | | |
|---|---|---|---|
| University of Texas, Austin, TX | Chemical Engineering | Ph.D. | 1992 |
| University of Texas, Austin, TX | Chemical Engineering | M.S. | 1990 |
| Rice University, Houston, TX | Chemical Engineering | B.S. | 1982 |

## Academic and Industrial Positions

| | | |
|---|---|---|
| 04/2015 – present | Senior Research Associate | ExxonMobil R&E, Annandale, NJ |
| 07/2012 – 04/2015 | Research Associate | ExxonMobil R&E, Annandale, NJ |
| 04/2009 – 07/2012 | Staff Engineer | ExxonMobil Chemical, Baytown, TX |
| 07/2007 – 04/2009 | Director, Technology | Aspen Technology, Houston, TX |
| 08/1999 – 07/2007 | Senior Principal Engineer | Aspen Technology, Houston, TX |
| 08/1993 – 08/1999 | Assistant Professor | Rice University, Houston, TX |
| 10/1992 – 08/1993 | Control Specialist | Fisher-Rosemount, Austin, TX |
| 08/1988 – 10/1992 | Graduate Research Assistant | University of Texas, Austin, TX |
| 05/1982 – 08/1988 | Project Engineer | SETPOINT, Houston, TX |

## Honors & Awards

2013 AIChE CAST Division Computing Practice Award
2011 Elected Fellow of the American Institute of Chemical Engineers
2010 ExxonMobil Shared Visions Award
2005 Control Engineering Practice Best Paper Prize
1998 Best Fundamental Paper Award, AIChE South Texas Section

## Graduate Student Advising

Supervised 4 PhD theses and 1 MS thesis

**Courses Taught**

Undergraduate: Process Design (6 times), Material and Energy Balances (1 time)
Graduate: Elements of Modern Control Theory (5 times)
Professional: Model Predictive Control Workshop, co-taught with James B. Rawlings (10 times)