

Industry 4.0 Topical Conference

Topical Conference at the 2023 AIChE Spring Meeting and 19th
Global Congress on Process Safety

Houston, Texas, USA
12-16 March 2023

ISBN: 978-1-7138-7935-0

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2022) by AIChE
All rights reserved.

Printed with permission by Curran Associates, Inc. (2023)

For permission requests, please contact AIChE
at the address below.

AIChE
120 Wall Street, FL 23
New York, NY 10005-4020

Phone: (800) 242-4363
Fax: (203) 775-5177

www.aiche.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

ANALYTICS AND AI - INDUSTRY PERSPECTIVE

149a Exploiting Knowledge When Learning Reaction Rates with Neural ODEs from Experimental Observations.....	1
<i>Farshud Sorourifar, You Peng, Ivan Castillo, Linh Bui, Juan M. Venegas</i>	
149b Rapid Capability Analysis Using Discrete-Rate Simulation.....	2
<i>Scott J. Bury, Andrew Moeller</i>	
149c External Risks Created By Reliance on Open-Source Artificial Intelligence Libraries.....	3
<i>Joshua Holtz</i>	

ANALYTICS AND AI PLENARY

17b Towards a Discipline of Industrial Process Analytics: From Case-Based Problem Solving to a Systematic Body of Knowledge	4
<i>Marco Reis</i>	
17a Leveraging Data Driven Connected Worker Technologies to Empower Your Workforce and Drive Operational Excellence.....	5
<i>Constantyn Chalitsios</i>	

ANALYTICS AND FUNDAMENTAL MODELING

28a A Hybrid Modeling Approach for Catalyst Monitoring and Lifetime Prediction	6
<i>Linh Bui, Ivan Castillo, Birgit Braun, You Peng, Mark Joswiak, Ailene G. Phillips, Jin Yang, Justin Rose, Daniel Hickman</i>	
28b Physics-Informed Deep Learning for Prediction of Thermophysical Properties: Normal Boiling Point	8
<i>Mohammad R. Babaei, Frank Mtetwa, Ryan Stone, Thomas Knotts IV, John Hedengren</i>	
28c A Hybrid Approach for Fouling Monitoring and Forecasting with Application to an Industrial Heat Exchanger	9
<i>Joel Sansana, Ricardo Rendall, Ivan Castillo, Luc de Bruijne, Jonathan Huggins, Ailene G. Phillips, Marco Reis</i>	

CYBERSECURITY IN THE CHEMICAL INDUSTRY I

85a Cyber Risk Assessment Methodologies - Compare and Contrast Different Approaches ISA 62443, INL Cce	11
<i>Marco Ayala</i>	
85c Cyber Security Visibility in OT: The Active Approach	12
<i>Randy Conner, Rutger Hendricks</i>	

DATA ANALYTICS AND SMART MANUFACTURING II

70a Development of Advanced Image Analysis Algorithms for Quantitative Evaluation of Exterior Coating Degradation.....	13
<i>Xingyu Zhou, Michael Linsen, Stephanie Long, Sun Hye Kim, Kevin Henderson, Jonathan DeRocher, Yicheng Hu</i>	
70c Solubility Prediction of Industrial Chemicals: Feeding Graph Neural Networks with Physics-Based Simulations Data.....	14
<i>Ravindra Aglave, Shikha Mallick, Francesca Boioli, Panos Petris, Peter Mas</i>	
70b Deep Learning Applications in Advanced Analytic Approaches of Big Data	15
<i>Manuel Rodriguez, Ismael Díaz Moreno, Hamed Aardakani</i>	

DATA ANALYTICS AND STATISTICS

103a Total Dissolved Solids Forecast and Risk Assessment in Midland Wastewater Treatment Plant	17
<i>Caterina Rizzo, You Peng, Shane Bennett</i>	
103b Application of Functional Data Analysis (FDA) for Process Optimization.....	18
<i>Swee-Teng Chin, Joel Sansana, Ricardo Rendall, Matthew Malloure, Ivan Castillo, Zhenyu Wang, Jinyang Chen, João P. L. Coutinho, Brian Clark</i>	
103c Analysis of Foaming in Batch Fermentation Processes Using Observation-Wise and Batch-Wise Unfolding Partial Least Square (PLS) Approaches	19
<i>Xuan Dung James Nguyen, Niket Sharma, Y. Liu, Christopher McDowell</i>	

DATA-DRIVEN AND HYBRID APPROACHES TO DEVELOPMENT OF NEW PRODUCTS I

116a Making the Most of Small Data.....	20
<i>Michael Heiber, Christopher Farrow</i>	
116b Leveraging Small Data for Better Chemistry	21
<i>Daniela Blanco</i>	
116c Guided Experimental Design for Modeling Reaction Rate Expressions	22
<i>Byanne Malluhi, Mamoun Al-Rawashdeh, Costas Kravaris, Hazem Nounou, Mohamed Nounou</i>	

DIGITAL TRANSFORMATION IN INDUSTRY 4.0 I

54b Capital Asset Lifecycle Management (CALM) for Chemical Industry.	23
<i>Chandra Siddamreddy, John Nixon, Mallik Manem</i>	
54c Lessons Learned about Digital Transformation from Experienced Industry Professionals!.....	24
<i>Jonas Norinder</i>	
54a Digital Transformation of Process Design, Scale-up, and Control: Serving the Purpose	25
<i>Nima Yazdanpanah, Thomas Eppinger, Jorge Lopez, Ravindra Aglave, Justin Hodges</i>	

DIGITAL TWINS, AUGMENTED REALITY, AND ADVANCED SIMULATION

132a Virtual Reality in the Context of Training Frontline Workers and the Process Industries	26
<i>Iiro Esko</i>	
132b Using Digital Utilities Twin Technology on a Refinery to Drive Carbon and Energy Reductions	27
<i>Joana Brito, Hugo Carabineiro, Kunpeng Guo, Lorena Fernanda Dos Santos De Souza</i>	
132c Executable Digital Twin: Automation, Physics Based Simulation and Machine Learning	28
<i>Ravindra Aglave, Iiro Esko</i>	

EMERGING TECHNOLOGIES IN DATA ANALYTICS

87a Hybrid Modeling for Managing Process Changes in Chemical Processing Industries	29
<i>Joel Sansana, Ricardo Rendall, Ivan Castillo, Caterina Rizzo, Birgit Braun, Leo Chiang, Marco Reis</i>	
87b The Future of Hazard Analysis and Big Data: With Big Data Comes Big Responsibility	31
<i>Alyse Keller, Sam Aigen, Elias Quinn, Scott Sanderson, Alison Ballon</i>	

INDUSTRY 4.0 / FUELS AND PETROCHEMICALS DIVISION JOINT PLENARY

3b The Importance of Carbon Intensity and Compliance to Meet Decarbonization Goals	32
<i>Kristine Klavers</i>	
3a Accelerating Green Hydrogen Via Digitalization - Optimization in Design, Operation and Profitability of a Fully Digitized Green Value Chain	33
<i>Jens Schmidt</i>	

INVITED TUTORIAL SESSION - APPROACHES IN DATA ANALYTICS I

133a Learn Data-Driven Engineering with Interactive Modules	34
<i>John Hedengren</i>	
133b Monitoring, Diagnosis and Prognosis of Industrial Processes: Past, Present and Future	35
<i>Marco Reis</i>	

POSTER SESSION: INDUSTRY 4.0/ANALYTICS AND AI

110a Security in Remote Offshore Wind-Integrated Green Hydrogen Production.....	36
<i>Ahmed Elkady, Md Tanjin Amin, Faisal Khan</i>	
110b A Novel Zone-Based Machine Learning Approach for the Prediction of the Performance of Industrial Flares	37
<i>Jian Fang, Helen Lou, Sidney Lin</i>	
110c Joint Angle Calculations Using Motion Capture and Deep Learning Pose Estimation for Safety Applications.....	38
<i>Luke VanKeersbilck, McGyver Clark, Iain Hunter, John Hedengren</i>	

110d How to Implement AI in a Data Lean Environment to Deliver Business Value.	39
<i>Forogh Askari</i>	
110f How the Start-Small Strategy Is Helping Chemical Companies Generate Millions in Savings and Drive a Sustainable Future.....	40
<i>Forogh Askari</i>	
110h Data Centric AI—How to Build the Software 2.0 Stack to Maximize ROI on Unstructured Data	41
<i>Michael Van Meurer</i>	

ROBOTICS, CYBERPHYSICAL, AND AUTONOMOUS SYSTEMS

139c Enabling Autonomous Operations	43
<i>Richard Clarke, Oleg Mikhailov</i>	

SENSORS AND ANALYZERS FOR ONLINE MEASUREMENTS

117a Trends in on-Line Gas Chromatography and Unmet Needs	44
<i>Eric G. Schmidt, Wayne Kubala, Rod Spitler</i>	
117c Use of TDLAS in Fired Assets to Aid in Decarbonization Efforts	45
<i>Ryan McSherry</i>	
117b Non-Contact Gas Spectroscopy Exploiting Tuning Fork-Based Light Detectors.....	46
<i>Angelo Sampaolo, Pietro Patimisco, Andrea Zifarelli, Giansergio Menduni, Marilena Giglio, Hongpeng Wu, Lei Dong, Vincenzo Spagnolo</i>	

INVITED TUTORIAL SESSION - APPROACHES IN DATA ANALYTICS II

150b The Next Epoch of Model Predictive Control: Exploiting Machine Learning Methods for Approximation and Design.....	47
<i>Joel Paulson</i>	

VENDORS' PERSPECTIVE (SESSION SPEAKERS INVITED)

140a Benefits of Designing Product Development Experiments with AI.....	48
<i>Kristin Wallace, Marlene Cardin, Alexander Nguyen</i>	
140b Advanced Analytics Role in Technical Workforce Transformation	49
<i>Rupesh Parbhoo, Allison Buenemann</i>	
140c Moving Beyond Manufacturing Analytics to Knowledge	50
<i>Peter Guilfoyle</i>	

OPTIMIZATION AND MACHINE LEARNING IN CHEMICAL MANUFACTURING

104a Multi-Fidelity Surrogate Models to Generate Low-Fidelity Data for Data-Driven Branch-and- Bound Optimization	51
<i>Suryateja Ravutla, Fani Boukouvala</i>	

104b Considerations for Product Development Model Formulations in Constrained Optimization Problems.....	52
<i>Alexander Nguyen, Marlene Cardin, Kristin Wallace</i>	

104c Achieving Targeted Product Mix Using Web-Based Optimization Tool for Chemical Plants with Multiple Products	53
<i>Zubin Kuvadia, Xinjie Tong, David Koscielniak, Shachit Iyer, Jianping Zeng</i>	

DIGITAL TRANSFORMATION IN INDUSTRY 4.0 II

71a Data-Driven Transformations for a Sustainable Enterprise	54
<i>Stephen Reynolds</i>	

71b Impact of HTML5 and Web-Based Solutions for Frontline Plant Workers.....	55
<i>Iiro Esko</i>	

71c Safety Digitalization	56
<i>Abdulrahman Alamer, Wassam Alqahtani</i>	

CYBERSECURITY IN THE CHEMICAL INDUSTRY II

97a Cybersecurity Risk Assessment Strategies in Industrial Control Systems.....	57
<i>Timothy Gale</i>	

DATA ANALYTICS AND SMART MANUFACTURING I

53a Optimizing Petrochemical Manufacturing Processes with Deep Learning.....	58
<i>Roberto Linares</i>	

53b An Adaptive Framework for State-Based Prediction of Rotating Equipment Failures.....	59
<i>Maxwell Toothman, Birgit Braun, Scott J. Bury, James Moyne, Dawn Tilbury, Kira Barton</i>	

53c The Pros and Cons of Machine Learning Versus Physical Model ? Case Study on Hydrocracking.....	62
<i>Spagnol Adrien, Benoit Celse, Gabriel Ducret, Per Julian Becker</i>	

DATA-DRIVEN AND HYBRID APPROACHES TO DEVELOPMENT OF NEW PRODUCTS II

131b Applying Multivariate Modeling and Numerical Optimization to Two Product Development Datasets	63
<i>Marlene Cardin, Alexander Nguyen</i>	

131c Advanced Digital Data Capture and Analysis Tools Replacing Traditional Visual Performance Ratings of Coatings	64
<i>Yicheng Hu, Kevin Henderson, Jonathan DeRocher, Sun Hye Kim, Allyson Marianelli, Alicia Liew, Nipun Bisht, Maxwell Ingram, Michael Tran, Yang Liu, Ce Xi, Michael Linsen, Mathias Weeks</i>	

REAL-TIME APPLICATIONS OF DATA ANALYTICS AND MACHINE LEARNING I

143a A Perspective of AI, Machine Learning and Data Science Towards Industry 4.0.....	65
<i>Hong Zhao, Ashok Rao, John Campbell, Jason You</i>	

143b A practitioner’s assessment of Deep Reinforcement Learning for industrial process control applications..... 66
Thomas Badgwell, R Donald Bartusiak

143c Framework for Hybrid Machine Learning with Open-Source Python Seeq Sysid Package..... 68
Mohammad R. Babaei, Junho Park, Ashwin N. Venkat, John Hedengren

Author Index