

# **Computing and Systems Technology Division 2021**

Held at the 2021 AIChE Spring Meeting and 17th Global Congress on Process Safety

Online  
18 – 23 April 2021

ISBN: 978-1-7138-5340-4

**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© (2021) by AIChE  
All rights reserved.

Printed with permission by Curran Associates, Inc. (2022)

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](http://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](mailto:curran@proceedings.com)  
Web: [www.proceedings.com](http://www.proceedings.com)

## TABLE OF CONTENTS

The Digital Transformation Promises to Change Innovation in the Materials Industry. Will It?.....	1
<i>Andre Argenton</i>	
Digital Twins & Smart Manufacturing –Where Data Analytics Meet Modeling & Optimization.....	2
<i>Efstratios N. Pistikopoulos</i>	
Comparison of Statistical and Machine Learning Approaches for Fault Detection in a Continuous Catalytic Regeneration Unit .....	3
<i>Cagla Odabasi, Pelin Döloglu, Gizem Kusoglu, Omer Yurttas, Murat Kulahci, Ahmet Palazoglu</i>	
Data-Driven Identification of an Industrial Reverse Osmosis Membrane Process: Impact of the Feed Properties, Plant Variables and the Operating Window.....	4
<i>Pelin Döloglu, Fatih Gülmez, Hasan Sildir</i>	
Elucidating Diafiltration Membrane Cascade Design Rules with Superstructure Optimization .....	6
<i>Noah Wamble, Elvis Eugene, William Phillip, Alexander Dowling</i>	
Dynamic Modeling and Nonlinear Parameter Estimation of Nanofiltration Membranes .....	8
<i>Xinhong Liu, Jonathan A. Ouimet, Elvis Eugene, William Phillip, Alexander Dowling</i>	
Simulation and Dynamic Analysis of an Integrated Plant for the Production of Methanol from Natural Gas.....	10
<i>Md Emdadul Haque, Srinivas Palanki</i>	
Machine-Learning Enabled Optimization of Force Fields .....	11
<i>Bridgette Befort, Ryan S. DeFever, Garrett Tow, Ed Maginn, Alexander Dowling</i>	
Thermodynamic Modeling of Aqueous $\text{Na}^+$ - $\text{K}^+$ - $\text{Ca}^{2+}$ - $\text{Cl}^-$ - $\text{HCO}_3^-$ - $\text{CO}_3^{2-}$ - $\text{CO}_2$ Solution .....	13
<i>Sheik Tanveer, Chau-Chyun Chen</i>	

### Author Index