

# FOCAPD 2019

## POSTER SESSION A

Monday, July 15, 2019 ♦ 8:00 p.m. to 10:00 p.m.

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### MAINGO – A DETERMINISTIC GLOBAL OPTIMIZATION SOLVER

**Dominik Bongartz**, Jannik Burre, Hatim Djelassi, Wolfgang R. Huster, Kaan Karacasulu, Jaromil Najman, Susanne Sass, Artur M. Schweidtmann and Alexander Mitsos  
(Paper ID 1)

### SYSTEMS ANALYSIS OF LIGHT ALKANE RESOURCES FOR CHEMICAL MANUFACTURING

Ioannis Giannikopoulos, Alkiviadis Skouteris, Yosuke Kimura, Sean DeRosa, Gary McGaughey, Elena McDonald-Buller, Thomas Edgar, David Allen, Michael Baldea and **Mark Stadtherr**  
(Paper ID 4)

### OPTIMAL SELECTION OF TESTS FOR ACTIVE FAULT DIAGNOSIS USING INTEGER PROGRAMMING

Kyle A. Palmer and **George M. Bollas**  
(Paper ID 8)

### PROCESS MODELING AND ENERGY EFFICIENCY ANALYSIS OF NATURAL GAS HYDRATE PRODUCTION BY CH<sub>4</sub>-CO<sub>2</sub>/H<sub>2</sub> REPLACEMENT COUPLING STEAM METHANE REFORMING

**Mengying Wang**, Xiaohui Wang, Chun Deng, Bei Liu, Changyu Sun, Guangjin Chen and Mahmoud El-Halwagi  
(Paper ID 11)

### ADVANCING AND ACCELERATING RELEASE ESTIMATIONS FOR CHEMICAL PROCESSES: OPPORTUNITIES FOR UNIT OPERATIONS, DATA MINING, AND MACHINE LEARNING

**Raymond Smith**, David Meyer, Gerardo Ruiz-Mercado, Michael Gonzalez, William Barrett and John Abraham  
(Paper ID 14)

### OPTIMIZATION OF REFINERY HYDROGEN NETWORK WITH PARAMETRIC UNCERTAINTIES

**Jian Liu**, Yeyang Zhou, Meiqian Zhu, Chun Deng and Jui-Yuan Li  
(Paper ID 19)

GENERATION OF DATA-DRIVEN MODELS FOR OPTIMIZATION UNDER  
UNCERTAINTY

**Joris Weigert**, Erik Esche, Christian Hoffmann and Jens-Uwe Repke

*(Paper ID 23)*

DEVELOPMENT OF DEEP LEARNING-BASED N<sub>2</sub>O EMISSION MODELLING USING  
BIG DATA FROM WASTEWATER TREATMENT PLANT

**Soonho Hwangbo**, Xueming Chen and Gürkan Sin

*(Paper ID 27)*

DECOMPOSING OPTIMIZATION BASED BOUNDS TIGHTENING PROBLEMS VIA  
GRAPH PARTITIONING

**Michael Bynum**, Anya Castillo, Bernard Knueven and Carl Laird

*(Paper ID 31)*

CONTROL OF SMALL-SCALE CHROMATOGRAPHIC SYSTEMS UNDER  
DISTURBANCES

Maria Papathanasiou, Baris Burbank, Justin Katz, Thomas Muller-Spath, Massimo Morbidelli,  
Nilay Shah and **Stratos Pistikopoulos**

*(Paper ID 34)*

OPTIMISATION OF ENERGY AND WATER SUPPLY SYSTEMS FOR THE DUBAI  
WATERFRONT

Thomas Bailey, Liu Pei and **Sandro Macchietto**

*(Paper ID 37)*

OPTIMAL PLACEMENT OF FLAME DETECTORS IN PETROCHEMICAL FACILITIES

**Todd Zhen**, Katherine Klise, Sean Cunningham, Edward Marszal and Carl Laird

*(Paper ID 40)*

DYNAMIC OPTIMIZATION OF NATURAL GAS NETWORK WITH RIGOROUS  
THERMODYNAMICS UNDER UNCERTAINTY

**Kai Liu**, Lorenz Biegler, Bingjian Zhang and Qinglin Chen

*(Paper ID 43)*

INTEGRATING A MICROTURBINE INTO A DISCRETE MANUFACTURING PROCESS  
WITH COMBINED HEAT AND POWER USING SMART SCHEDULING

Moriah Henning, **Derek Machalek** and Kody Powell

*(Paper ID 46)*

A NOVEL TOOL FOR COMPUTER-AIDED SUSTAINABILITY ASSESSMENT UNDER  
UNCERTAINTY: A DESIGN CASE OF NATURAL GAS OFFSHORE PROCESSING

**Cristiane São Bento Gonzaga**, Ofélia de Queiroz Fernandes Araújo and José Luiz de Medeiros

*(Paper ID 47)*

ENERGY CARRIER SUPPLY CHAIN OPTIMIZATION: A TEXAS CASE STUDY

**William Tso**, Doga Demirhan, Seungyeon Lee, Haneol Song, Joseph Powell and Efstratios Pistikopoulos

*(Paper ID 50)*

FRAMEWORK FOR SOLVENT RECOVERY, REUSE AND RECYCLING IN INDUSTRIES

**John Chea**, Amanda Christon, Vanessa Pierce, Julia Reilly, Maxim Russ, C. Stewart Slater, Mariano Savelski and Kirti Yenkie

*(Paper ID 54)*

ULTIMATE SELECTIVITIES AND SCREENING-LEVEL METRICS FOR CONCEPTUAL PROCESS DESIGN

**Jeffrey Frumkin** and Michael Doherty

*(Paper ID 55)*

DESIGNING FLEXIBILITY INTO A HYBRID SOLAR THERMAL POWER PLANT BY REAL-TIME ADAPTIVE HEAT INTEGRATION

Khalid Rashid, Kevin Ellingwood, Mostafa Safdarnejad and **Kody Powell**

*(Paper ID 60)*

MULTI-STAGE MEMBRANE SEPARATION DESIGN FOR LANDFILL GAS WITH UNCERTAIN FEED COMPOSITIONS

Jian Tao, Jianli Wang and **Lingyu Zhu**

*(Paper ID 66)*

TOWARDS OPTIMAL MIXTURES: INTEGRATING MIXTURE DESIGN INTO ORC PROCESS DESIGN USING PC-SAFT

**Johannes Schilling**, Marten Entrup, Madlen Hopp, Joachim Gross and André Bardow

*(Paper ID 69)*

DESIGN FOR ONLINE PROCESS AND BLEND SCHEDULING OPTIMIZATION

**Robert Eduard Franzoi**, Brenno Castrillon Menezes, Jeffrey Dean Kelly and Jorge Andrey Wilhelms Gut

*(Paper ID 73)*

USING ULTRAFILTRATION FOR FLOWBACK WATER MANAGEMENT IN SHALE GAS EXPLORATION: MULTICONTAMINANT CONSIDERATION

**Doris Oke**, Rajib Mukherjee, Debalina Sengupta, Thokozani Majozi and Mahmoud El-Halwagi

*(Paper ID 77)*

SYSTEMATIC METHOD AND TOOL FOR SUSTAINABLE PROCESS SYNTHESIS, DESIGN, ANALYSIS AND INNOVATION

**Anjan K. Tula**, Mario R. Eden and Rafiqul Gani

*(Paper ID 80)*

MODELING AND SIMULATION OF A WASTE TIRE TO LIQUEFIED SYNTHETIC NATURAL GAS (SNG) PLANT

**Avinash Shankar Rammohan Subramanian**, Donghoi Kim, Thomas A. Adams II and Truls Gundersen  
(Paper ID 83)

MATHEMATICAL MODELING AND OPTIMIZATION OF DIRECTIONAL SOLVENT EXTRACTION FOR SUSTAINABLE WATER DESALINATION

**Alejandro Garcadiago**, Tengfei Luo and Alexander Dowling  
(Paper ID 86)

DESIGN AND PLANNING SUPPLY CHAINS WITH BENEFICIAL SOCIETAL GOALS

Bruna Mota, Ana Carvalho, Maria Isabel Gomes and **Ana Paula Barbosa-Póvoa**  
(Paper ID 89)

PROCESS AND MOLECULAR DESIGN INTEGRATION FOR THE SEPARATION OF HYDROFLUOROCARBON MIXTURES

**Bridgette Befort**, Edward Maginn and Alexander Dowling  
(Paper ID 92)

SYSTEMATIC PROCESS INTENSIFICATION INVOLVING ZEOTROPIC DISTILLATION

**Jianping Li**, Salih Emre Demirel and Faruque Hasan  
(Paper ID 95)

HYBRID MODELING FOR ROBUST PROCESS DESIGN AND EXTRAPOLATION

**William Terrill Bradley** and Fani Boukouvala  
(Paper ID 99)

DYNAMIC MODELING AND CONTROL OF A NATURAL GAS COMBINED CYCLE POWER PLANT FOR LOAD-FOLLOWING OPERATION

Yifan Wang, **Debangsu Bhattacharyya** and Richard Turton  
(Paper ID 102)

A BI-LEVEL FORMULATION AND SOLUTION METHOD FOR THE INTEGRATION OF PROCESS DESIGN AND SCHEDULING

**Styliani Avraamidou** and Efstratios Pistikopoulos  
(Paper ID 105)

TWO-STAGE LAND USE OPTIMIZATION FOR A FOOD-ENERGY-WATER NEXUS SYSTEM: A CASE STUDY IN TEXAS EDWARDS REGION

Yaling Nie, Styliani Avraamidou, **Xin Xiao**, Efstratios Pistikopoulos and Jie Li  
(Paper ID 108)

PROCESS BASED SCREENING METHOD AND SYSTEMS ANALYSIS FOR PRE-COMBUSTION CARBON CAPTURE USING IONIC LIQUIDS

**Omar Basha**  
(Paper ID 109)

DATA-DRIVEN SPATIAL BRANCH-AND-BOUND ALGORITHMS FOR BLACK-BOX OPTIMIZATION

**Jianyuan Zhai** and Fani Boukouvala  
(Paper ID 114)

OPTIMAL DESIGN AND OPERATION OF INTEGRATED SOLAR-ELECTROLYSIS  
SYSTEMS IN CALIFORNIA

**Mariya Koleva**, Omar Guerra, Joshua Eichman, Bri-Mathias Hodge and Jennifer Kurtz  
(Paper ID 117)

SUSTAINABLE PROCESS DESIGN ASSISTED BY FUZZY INFERENCE AND EMISSION  
ANALYTICS

Alexander Guzman-Urbina, Kakeru Ouchi, Hajime Ohno and **Yasuhiro Fukushima**  
(Paper ID 121)

ECONOMIES OF NUMBERS FOR A MODULAR STRANDED GAS PROCESSING  
NETWORK: MODELING AND OPTIMIZATION

**Qi Chen** and Ignacio Grossmann  
(Paper ID 125)

KIPET - AN OPEN-SOURCE KINETIC PARAMETER ESTIMATION TOOLKIT

**Michael Short**, Christina Schenk, David Thierry, Jose Santiago Rodriguez, Lorenz T. Biegler  
and Salvador Garcia-Munoz  
(Paper ID 134)

DEVELOPMENT AND DEMONSTRATION OF PARAMETER ESTIMATION  
CAPABILITIES FOR COAL-BASED POWER PLANTS

**Jaffer Ghouse**, John Eslick, Anthony Burgard, Miguel Zamarripa, Carl Laird, Debangsu  
Bhattacharya and David Miller  
(Paper ID 143)

PARTITIONING TO BORDERED BLOCK TRIANGULAR FORM FOR INITIALIZATION  
AND SOLUTION OF LARGE-SCALE EQUATION-ORIENTED MODELS IN IDAES

**Emmanuel Ogbe**, Andrew Lee, John Eslick, Anthony Burgard and David Miller  
(Paper ID 146)

pyomo.contrib.surrogates: A PYOMO-BASED FRAMEWORK FOR SURROGATE MODEL  
GENERATION

**Oluwamayowa O. Amusat**, John D. Sirola, Deb A. Agarwal and Dan Gunter  
(Paper ID 155)