9th Asian Symposium on Process Systems Engineering (9th PSE Asia 2020)

4 – 6 November 2020

Taipei

An Asynchronous Webinar

Cheng-Liang Chen
Department of Chemical Engineering
National Taiwan University

PSE Asia Series

Kyoto (2000) Taipei (2002) Seoul (2005) Xi'an (2007)
Singapore (2010) Kuala Lumpur (2013) Tokyo (2016)
Bangkok (2019) Taipei (2020)

Welcome to The 9th PSE Asia 2020 Asynchronous Webinar

Official website: https://PSEAsia2020.org

On behalf of the Standing Committee (SC), the International Program Committee (IPC), and the National Organizing Committee (NOC), we would like to warmly welcome you to the **2020 9th Asian Symposium on Process Systems Engineering (the 9th PSE Asia 2020)**. We are delighted to have you here to share your experiences and to contribute to the theory and practice of Process Systems Engineering.

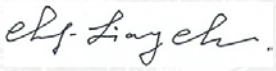
The **PSE Asia series** is a biennial international symposium in Asia bringing together researchers and practitioners to discuss recent developments in Process Systems Engineering. The areas of focus include, but are not limited to, Process and Product Design, Process Dynamics and Control, Process Integration and Optimization, Process Monitoring and Safety, Process Modeling and Simulation, Energy Systems Analysis, Artificial Intelligence and Big Data in Chemical Engineering, and other emerging issues. To encourage young researchers in the Asia area, each country can recommend one keynote speaker to share his/her excellent research results and future research planning. **PSE Asia 2020** is the ninth symposium following previous events at Kyoto (2000), Taipei (2002), Seoul (2005), Xi'an (2007), Singapore (2010), Kuala Lumpur (2013), Tokyo (2016), and Bangkok (January 2019). In 2016, the Standing Committee made a decision that starting from 2016, the **PSE Asia Symposium** will be held biennially. So the **10th PSE Asia** and the **11th PSE Asia** will be held in 2022 and 2024, respectively.

The **9th PSE Asia 2020** was converted into an asynchronous webinar due to the COVID-19 pandemic. However, we were determined to hold the symposium according to the original time schedule. We therefore established an asynchronous webinar system, canceled the poster session, and asked all presenters to upload presentation video(s). During the asynchronous webinar conference period (10:00 4th Nov – 17:00 6th Nov, Taipei time), all registered participants can go to the website and "attend" all sessions and watch all video presentations at any time. They can accelerate, playback, skip ahead

or repeat any part of any presentation. However, downloading or capturing of videos will be prohibited. Viewers can leave questions that presenters can answer immediately or later. The webinar server will periodically (say, at 9:00, 12:00, 15:00, 18:00, and 21:00) send an e-mail listing the number of questions asked for each presentation as a reminder to each presenter to answer questions posted about their presentations. The queries and answers will be open to all participants, but viewers may have to wait for a reply from the presenters. In this way, we hope the frequency and quality of discussion will be better than at conventional meetings. We also hope you will enjoy your visit and interaction with the **9th PSE Asia 2020** asynchronous webinar system.

Your participation and support will be the key to a successful conference. I would like to express my deep appreciation to all contributors and participants. Thank you very much.

Sincerely Yours



Cheng-Liang Chen, General Chair
9th PSE Asia 2020 Asynchronous Webinar
(10:00 4th Nov – 17:00 6th Nov 2020, Taipei Time Zone)
Dept of Chem Eng, Natl Taiwan University
CCL@ntu.edu.tw

9th PSE Asia 2020 Standing Committee

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25	Denny NG	Heriot-Watt Univ. Malaysia Campus	Putrajaya

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20	Wen-Shing Chang* (Assistant)	Natl Taiwan Univ.	Taipei
21	Chong Wei ONG* (Assistant)	Natl Taiwan Univ.	Taipei

9th PSE Asia 2020 Keynote Speakers

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1	Jui-Yuan LEE	Natl Taipei Univ. of Technology	Taipei
2	Lei ZHANG	Dalian Univ. of Technology	Dalian
3	Jinkuk KIM	Hanyang Univ.	Seoul
4	Yoshiaki KAWAJIRI	Nagoya Univ.	Nagoya
5	Setiyo GUNAWAN	Institut Teknologi Sepuluh Nopember	Surabaya
6	Xiaonan WANG	Natl Univ. of Singapore	Singapore
7	Babji Srinivasan	Indian Inst. of Tech. Gandhinagar	Gandhinagar
8	Kathleen B. Aviso	De La Salle Univ.	Manila
9	Viknesh Andiappan	Heriot-Watt Univ. Malaysia	Kuala Lumpur

9th PSE Asia 2020 Papers Categories

Total Accepted Submission: 136

9th PSE Asia 2020 Papers Categories

Keynote Speakers (9)

Chairs:

Raymond Tan (210077-210089)
Jinsong Zhao (210092-210110)
Renanto Handogo (210114-210121)

210077	Bayesian approaches for chemical process modeling	**Prof Yoshiaki Kawajiri**, (Nagoya University);
210084	QMaC: A Quantum mechanics/Machine learning-based Computational tool for chemical product design	**Dr Lei Zhang**, (Dalian University of Technology); Mr Qilei Liu, (Dalian University of Technology); Dr Linlin Liu, (Dalian University of Technology); Prof Jian Du, (Dalian University of Technology);
210089	Multi Stage of Batch-Wise Solvent Extraction Process for Separating Triacylglycerols from crude Callophyllum Inophyllum oil	**Dr Setiyo Gunawan**, (Institut Tek. Sepuluh Nopember); Prof Renanto Handogo, (Institut Teknologi Sepuluh Nopember); Dr Hakun Wirawasista Aparamarta, (Institut Teknologi Sepuluh Nopember);
210092	A Bi-Level Optimization Model for Optimal Green Technology Selection with Economic Incentives	**Prof Kathleen Aviso**, (De La Salle University); Prof Anthony Chiu, (De La Salle University); Prof Aristotle Ubando, (De La Salle University); Prof Raymond Tan, (De La Salle University);
210097	AI and machine learning through life cycle of energy and environmental systems	**Prof Xiaonan Wang**, (National University of Singapore);
210110	Performance Assessment of Operators in Process Industries using Wearable Sensing Devices	**Dr Babji Srinivasan**, (Indian Institute of Technology Gandhinagar);
210114	Application of Mathematical Programming to Process Integration and Energy Planning Problems	**Dr Jui-Yuan Lee**, (National Taipei University of Technology);
210119	Optimisation and Planning of Biomass Supply Chain for New and Existing Power Plants Based on Carbon Reduction Targets	Ms Nur Syahira Mohd Yahya, (Heriot-Watt University Malaysia); **Dr Viknesh Andiappan**, (Heriott-Watt University Malaysia);
210121	Process Design, Integration and Optimization of CO_2 Capture Systems	**Prof Jin-Kuk Kim**, (Hanyang University);

Keynote Speaker

9th PSE Asia 2020 Papers Categories

Process and Product Design (19)

Chairs:

J. Rafael Alcantara Avila (210003-210019)
Hao-Yeh Lee (210021-210060)
Xigang YUAN (210061-210098)
I-Lung Chien (210102-210135)

210003	Energy-efficient Design of Bio-butanol Purification Process from Acetone-Butanol-Ethanol Fermentation	Mr Tsung-Shi You (National Taiwan University); Prof Hao-Yeh Lee (National Taiwan University of Science and Technology); Prof Cheng-Liang Chen (National Taiwan University);
210011	Energy-Efficient Separation Design Aided by Liquid-Liquid Separation and Pressure Swing for Complicated Ternary System	Mr Meng-Lin Tsai, (National Taiwan University); Mr Kai-Yang Lin, (National Taiwan University); Mr Yin-Rui Zhang, (National Taiwan University); Prof I-Lung Chien, (National Taiwan University);
210017	Structure optimization considering multiple decanters in heterogeneous azeotropic distillation	Dr J. Rafael Alcantara Avila, (Kyoto University); Mr Keito Togami, (Kyoto University);
210019	Rigorous Simulation and Optimization of the Plant-wide Glycerol Carbonate (GC) Production Process through Transesterification	Prof Bor-Yih Yu, (Chang Gung University); Mr Wei-Jen Chen, (Chang Gung University);
210021	CO_2 Utilization Feasibility Study	Ms Tsai-Wei Wu, (National Taiwan University); Prof I-Lung Chien, (National Taiwan University);
210026	Optimization of extractive distillation processes with mixed solvents	Ms Hsin-Yu Hou, (National Taiwan University); Ms Yu-Feng Fang, (National Taiwan University); Dr Jeffrey Ward, (National Taiwan University);
210033	Methanol synthesis process modelling with exhaust gas	Mr JaeHun Jeong, (Seoul National University); Prof Won Bo Lee, (Seoul National University); Prof Myung-June Park, (Ajou University); Ms Yoori Kim, (Korea Shipbuilding & Offshore Engineering); Ms Se-Young Oh, (Korea Shipbuilding & Offshore Engineering);
210056	Model-based design of H_2O_2 decontamination processes in pharmaceutical manufacturing	Dr Keisho Yabuta, (The University of Tokyo); Ms Haruka Futamura, (Airex Co., Ltd.); Mr Koji Kawasaki, (Airex Co., Ltd.); Dr Hirokazu Sugiyama, (The University of Tokyo);
210060	Applying process simulation to life cycle assessment of cellulose nanofiber-reinforced plastics	Dr Yuichiro Kanematsu, (The University of Tokyo); Dr Yasunori Kikuchi, (The University of Tokyo);
210061	Simulation of cultivation processes in monoclonal antibody production towards the selection of operation modes	Ms Kozue Okamura, (The University of Tokyo); Prof Sara Badr, (The University of Tokyo); Prof Hirokazu Sugiyama, (The University of Tokyo);

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210067	Design of Dual Pressure Reactive Distillation via Compressor with Intermediate Condenser for Silane Production Process	Ms Pitchaya Eiamsuttitam, (Natl Taiwan University of Sci. and Tech.); Prof Hao-Yeh Lee, (National Taiwan University of Science and Technology);
210083	A Comprehensive Numerical Procedure for Evaluating Flexibility Indices of Dynamic Systems with Piecewise Constant Manipulated Variables	Mr Shoeb Moon Ali, (National Cheng Kung University); Mr Shang-Wei Hwang, (National Cheng Kung University); Prof Chuei-Tin Chang, (National Cheng Kung University);
210091	Optimal Retrofit Designs of Multi-Plant Heat Exchanger Networks with Reasonable Benefit Allocation Plans	Mr Fang-Yi Lo, (National Cheng Kung University); Mr Ching-Hsiang Hsu, (National Cheng Kung University); Prof Chuei-Tin Chang, (National Cheng Kung University);
210098	Design of the Product Separation and Recovery Section of a Methanol-to-Olefins Plant	Mr Wen Hsieh, (Tamkang University); Prof Hsuan Chang, (Tamkang University);
210102	Two-step hybrid optimization of heat-integrated distillation columns	Mr Leonardo A. Chavez Diaz, (Universidad de Guanajuato); Mr Josue J. Herrera Velazquez, (Universidad de Guanajuato); Mr Fabián M. Zavala Duran, (Universidad de Guanajuato); Dr Julian Cabrera Ruiz, (Universidad de Guanajuato); Dr J. Rafael Alcantara Avila, (Kyoto University);
210118	Feasibility study on reactive distillation with double reactive sections in term of feed location and section total stage numbers	Mr Cheng-Yu Lin, (National Chung Hsing university); Dr Vincentius Surya Kur Adi, (National Chung Hsing University);
210124	Development of CAMD tools for the design of solvent additives to upgrade bio-oil	Ms Jia Wen Chong, (University of Nottingham Malaysia); Dr Suchithra Thangalazhy-Gopakuma, (University of Nottingham Malaysia); Dr Kasturi Muthoosamy, (University of Nottingham Malaysia); Dr Nishanth Chemmangattuvalappil, (University of Nottingham Malaysia);
210125	Novel Ethyl Lactate Production Process Design using Reactive Distillation and Membrane-Distillation Configuration	Prof Hao-Yeh Lee, (Natioanl Taiwan University of Science & Technology); Mr Yu-Yang Tsau, (Natioanl Taiwan University); Prof Cheng-Liang Chen, (Natioanl Taiwan University);
210135	Refrigeration System Synthesis based on Hybrid GA-PSO Method	Ms Danlei Chen, (Tianjin University); Prof Yiqing Luo, (Tianjin University); Prof Xigang Yuan, (Tianjin University);

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Process Dynamics and Control (13)

Chairs:

Yoshiyuki Yamashita (210023-210042)
Anikesh Kumar (210051-210066)
Jia-Lin Kang (210085-210140)

210023	Data-Driven Digital Twin Development for Chemical Plants Using Sequence-to-Sequence Approach and Rolling Training	Prof Jia-Lin Kang, (National Yunlin University of Science and Technology); Mr Yao-Chen Lee, (National Tsinghua University); Dr Yao-Cheng Chuang , (National Tsinghua University); Mr Marvin Frias , (National Tsinghua University); Dr Cheng-Huang Chou, (National Tsinghua University); Dr San-Jang Wang , (National Tsinghua University); Prof David Shan Hill Wong, (National Tsinghua University); Prof Shi-Shang Jang, (National Tsinghua University);
210024	Boiler Level Control Using Deep Deterministic Policy Gradient Model	Mr Jia-An Zhou, (Tamkang University); Prof Jia-Lin Kang, (National Yunlin University of Science and Technology); Mr Zi-Hung Yang, (National Yunlin University of Science and Technology); Prof Yih-Hang Chen, (Tamkang University);
210030	Enhanced microbial nitrogen removal by SHARON and Anammox (SHARON-AMX) integrated control strategies in wastewater treatment plants	Ms Paulina Vilela, (Kyung Hee University); Prof Chang Kyoo Yoo, (Kyung Hee University);
210042	Control of intensified distillation systems for quaternary mixtures	Mr Cristopher Villegas Uribe, (Universidad Autónoma de Nuevo León); Dr Salvador Tututi-Avila, (Universidad Autónoma de Nuevo León); Dr J. Rafael Alcantara Avila, (Kyoto University);
210051	Robust Imputation of Soft-Sensor Model Using Recurrent Neural Networks	Prof Jia-Lin Kang, (National Yunlin University of Science and Technology); Mr Wei-De Dai, (National Tsinghua University); Prof David Shan Hill Wong, (National Tsinghua University);
210055	A study on the epidemic model with periodic structure	Mr Jindong Dai, (Beijing University of Chemical Technology); Dr Jiali Ai, (Beijing University of Chemical Technology); Prof Chi Zhai, (Kunming University of Science and Technology); Prof Wei Sun, (Beijing University of Chemical Technology);
210058	Multi-loop PID Controllers Design Based on Frequency-Domain Direct Synthesis Method for Multivariable Interactive Processes	Prof Jyh-Cheng Jeng, (National Taipei University of Technology); Ms Yu-Yu Tseng, (National Taipei University of Technology); Dr Ming-Wei Lee, (China Steel Corporation);

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210066	Startup Operation Strategies of Styrene-Acrylonitrile (SAN) Copolymerization Process	Ms Yu-Chun Cheng, (Chang Gung University); Prof Bor-Yih Yu, (Chang Gung University); Prof Hao-Yeh Lee, (National Taiwan University of Science and Technology);
210085	Design of a PID controller with valve stiction	Mr Masaharu Daiguji, (JXTG Nippon Oil & Energy Corporation); Prof Yoshiyuki Yamashita, (Tokyo University of Agriculture and Technology);
210090	Process Control of a Sour Water Stripper Utilizing Feed Condition Estimator and Minimum Heat Duty Model	Mr Chao Ming Zhang, (Tamkang University); Prof Yih-Hang Chen, (Tamkang University); Prof Hsuan Chang, (Tamkang University);
210133	Data-based Digital Predictor Design for Processes Comprising Inverse Response	Dr Anikesh Kumar, (National University of Singapore); Dr Min-Sen Chiu, (National University of Singapore);
210140	Yield Conversion Improvement for Continuous Stirred Tank Reactor System using Output Frequency Response Function-based Analysis	Dr Nik Nor Liyana Nik Ibrahim, (Universiti Putra Malaysia); Prof Thomas Choong Shean Yaw, (Universiti Putra Malaysia); Prof Zi-Qiang Lang, (University of Sheffield);
210145	New PID Design Method for Under-damped Processes	Mr Thanh Tung Duong Huynh, (National University of Singapore); Prof Min-Sen Chiu, (National University of Singapore);

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Process Integration and Optimization (17)

Chairs:

Dominic Foo (210020-210046)
Santanu Bandyopadhyay (210057-210079)
Jeffrey Ward (210086-210106)
Jian DU (210122-210141)

210020	Circulating cooling water system optimization under varying parameters	Ms Bo Liu, (China University of Petroleum); Prof Yufei Wang, (China University of Petroleum);
210022	The coupling integration of ORC and compression-absorption refrigeration system for cooling and power cogeneration	Dr Xiaojing Sun, (Daliann University of Technology); Prof Linlin Liu, (Dalian University of Technology); Dr Yu Zhuang, (Dalian University of Technology); Prof Lei Zhang, (Dalian University of Technology); Prof Jian Du, (Dalian University of Technology);
210040	Rigorous Simulation and Techno-Economic Analysis of a Bio-Jet-Fuel Intermediate Production Process with Various Integration Strategies	Prof Bor-Yih Yu, (Chang Gung University); Mr Chang-Che Tsai, (National Taiwan University);
210046	A superstructure based approach to work exchange networks synthesis	Mr Yu-Ming Zhang, (National Chung Hsing University); Dr Vincentius Surya Kur Adi, (National Chung Hsing University);
210057	Optimal Design, Operation, and Scheduling of Membrane Cleaning for Stand-Alone Hybrid Membrane Osmosis Desalination Systems	Mr Hao-Chiun Lin, (National Taipei University of Technology); Prof Jyh-Cheng Jeng, (National Taipei University of Technology); Mr Shi-Yu Xu, (National Taipei University of Technology);
210070	Malaysian palm kernel shell (PKS) for biomass-power generation in Japan considering environmental feasibility of PKS life cycle	Dr Disni Gamaralalage, (The University of Tokyo); Prof Yuichiro Kanematsu, (The University of Tokyo); Prof Denny Ng, (Heriot-Watt University Malaysia); Dr Steve Foong, (Heriot-Watt University Malaysia); Prof Viknesh Andiappan, (Heriot-Watt University Malaysia); Prof Dominic Foo, (University of Nottinghan Malaysia Campus); Prof Yasunori Kikuchi, (The University of Tokyo);
210072	Structural Optimization of Reverse Osmosis Desalination System Powered by Photovoltaic and Pressure Retarded Osmosis	Mr Shi-Yu Xu, (China Steel Corporation); Prof Jyh-Cheng Jeng, (National Taipei University of Technology); Dr Ming-Wei Lee, (China Steel Company);
210079	Near-analytical optimization of seeded batch crystallization processes using optimal control theory	Mr Hao-Jen Pan, (National Taiwan University); Mr Ming-Chun Fang, (National Taiwan University); Dr Jeffrey Ward, (National Taiwan University);

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210086	Negative Emissions Technologies for Carbon-constrained Energy Planning	Mr Purusothmn Nair Bhasker Nair, (University of Nottingham Malaysia); Prof Raymond Tan, (De La Salle University, Philippines); Prof Dominic Foo, (University of Nottingham Malaysia);
210096	Synthesis of Heat Integrated Water Regeneration Network with Optimum Process/Regeneration Temperatures	Ms Shweta Kamat, (Indian Institute of Technology Bombay); Prof Santanu Bandyopadhyay, (Indian Institute of Technology Bombay);
210103	Pinch Analysis approach for multi-objective segregated targeting problems with common resources	Ms Sheetal Jain, (Indian Institute of Technology Bombay); Prof Santanu Bandyopadhyay, (Indian Institute of Technology Bombay);
210106	Scheduling for Multipurpose Batch Processes-A Fuzzy Optimization Approach	Mr Piyush Kumawat, (Indian Institute of Technology, Patna); Dr Nitin Dutt Chaturvedi, (Indian Institute of Technology, Patna);
210122	Multi-objective optimization of an energy system and its reliability	Ms CHARLETTE cabral, (de la salle university); Dr Viknesh Andiappan, (Heriot-Watt University Malaysia); Dr Kathleen Aviso , (De La Salle University); Dr Raymond Tan, (De La Salle University);
210129	Heat integration design of alpha methyl ester sulfonate production process	Mr Kittawit Choptumdee, (Chulalongkorn University); Prof Paisan Kittisupakorn, (Chulalongkorn University); Dr Wachira Daosud, (Chulalongkorn University);
210136	Microalgae biofuel supply chain optimization under weather uncertainty	Ms Peiyao Li, (Tianjin University); Prof Xigang Yuan, (Tianjin University); Prof Yiqing Luo, (Tianjin University);
210139	Utilization of Process Network Synthesis and Machine Learning as Decision Making Tools for Municipal Solid Waste Management	Dr Nik Nor Liyana Nik Ibrahim, (Universiti Putra Malaysia); Ms Rabiatul Adawiyah Ali, (Universiti Putra Malaysia); Dr Wan Azlina Wan Abdul Karim Ghan, (Universiti Putra Malaysia); Prof Hon Loong Lam, (The University of Nottingham Malaysia Campus); Dr Nor Samsiah Sani, (Universiti Kebangsaan Malaysia);
210141	Process Systems Engineering (PSE) Applications In Semiconductor Manufacturing: Contact Pad Structure Design	Prof Chih-Yao Lin, (Tunghai University);

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Process Monitoring and Safety (12)

Chairs:

Rajagopalan Srinivasan (210010-210045)
Jong Min Lee (210053-210088)
Dongil Shin (210093-210116)

210010	Gated Recurrent Unit Applied to Fault Diagnosis in Chemical process	Mr Kuo-Yao Chiu, (National Yunlin University of Science and Technology); Mr Kuang-Yi Chu, (Tamkang University); Dr Jia-Lin Kang, (National Yunlin University of Science and Technology);
210029	Indoor air quality monitoring in an underground transportation facility using variational convolutional autoencoders-driven anomaly detection and sensor reconciliation	Mr Jorge Loy, (Kyung Hee University); Mr Shahzeb Tariq, (Kyung Hee University); Prof ChangKyoo Yoo, (Kyung Hee University);
210038	Fence line monitoring system optimization for detecting toxic gas considering spatio-temporal risk using gas detectors	Mr Dongho Kwak, (Myongji University,); Prof Dongil Shin, (Myongji University);
210045	Data Visualization and Fault Detection of Chemical Process Using UMAP	Mr Damdae Park, (Seoul National University); Mr Hodong Lee, (Seoul National University); Prof Jong Min Lee, (Seoul National University);
210053	Continuous Wavelet Transform with Neural Network for the Monitoring Chemical Process	Ms Chinatsu Ukawa, (Tokyo University of Agriculture and Technology); Prof Yoshiyuki Yamashita, (Tokyo University of Agriculture and Technology);
210063	Verification of ART-based Supervised Data Clustering Using Plant Simulation Data	Dr Yoshinari Hori, (Hitachi, Ltd.);
210065	CFD-based analysis of the effect on adjacent pipes in the event of pipe accident	Mr Cheolwon Eo, (Seoul National University); Mr Shikyung Yoon, (Seoul National University); Prof Jongmin Lee, (Seoul National University);
210088	Optimal Design and Maintenance Strategies of Multi-Layer Standby Mechanisms in Continuous Chemical Processes	Mr Sing-Zhi Chan, (National Cheng Kung University); Mr Cheng-I Tu, (National Cheng Kung University); Prof Chuei-Tin Chang, (National Cheng Kung University);
210093	Nonlinear Dynamic Processes Monitoring using Kernel CVA with Automatic Relevance Determination	Dr Karl Ezra Pilario, (University of the Philippines-Diliman); Prof Yi Cao, (Zhejiang University); Prof Shuang-Hua Yang, (Zhejiang University);
210100	Infrared Thermography-Based Statistical Process Control for Defect Detection in Vaccum-Assisted Resin Transfer Molding	Mr Hung-Pin Hsu, (National Tsing Hua University); Prof Yuan Yao, (National Tsing Hua University);

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210112	Improvement of Process Variable Selection Method for Fault Detection System using Negative Selection Algorithm	Mr Kazunori Tanihara, (Kyushu University); Ms Yuki Ichikawa, (Kyushu University); Prof Naoki Kimura, (Kyushu University); Prof Gen Inoue, (Kyushu University); Prof Yoshifumi Tsuge, (Kyushu University);
210116	Verification of Firefighters' Heuristics and Predictive Model Development through Big Data Analysis	Ms Sohyun Park, (Myongji University); Mr Yongbeom Shin, (Myongji university); Prof Dongil Shin, (Myongji University);

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Process Modeling and Simulation (35)

Chairs:

Manabu Kano (210002-210014)
Jin-Kuk Kim (210016-210034)
Denny Ng (210037-210049)
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210048	Safe Reinforcement Learning for Process Control	Mr Seishiro Kawamura, (Kyoto University); Prof Manabu Kano, (Kyoto University);
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210082	Developing Dynamic Soft Sensor Based Variational Autoencoders	Mr Dave Tanny, (Chung Yuan Christian University); Prof Junghui Chen, (Chung Yuan Christian University);
210104	Small Data Integration for Process Modeling by Feature Learning via Deep Convolutional Autoencoder	Mr Tzu-Tang Liu, (National Tsing Hua University); Prof Yuan Yao, (National Tsing Hua University);
210105	Investigating Factors Affecting Future Circularity with Machine Learning	Mr Ivan Henderson Gue, (FEU - Institute of Technology); Dr Pocholo James Loresco, (FEU - Institute of Technology); Prof Raymond Tan, (De La Salle University - Manila); Prof Aristotle Ubando, (De La Salle University - Manila);
210115	Real-time Intelligent Knowledge Service as Symptom-based Expert for Advanced Response to Chemical Hazards (SEARCH)	Ms Eunji Shin, (Myongji University); Prof Dongil Peter Shin, (Myongji University); Mr Moon-Soo Koh, (Anseong Fire Station);
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210128	Physics-Informed Neural Networks for Solving Polymer Self-Consistent Field Equations	Mr Danny Lin, (National Taiwan University); Ms Le-Chi Lin, (National Taiwan University); Prof Hsiu-Yu Yu, (National Taiwan University);
210137	A Machine Learning Method for Identifying Rules for Synthesis of Ternary-distillation Systems Based on Decision Tree	Ms Xili Chen, (Tianjin University); Prof Xigang Yuan, (Tianjin University); Prof Shengkun Jia, (Tianjin University); Prof Yiqing Luo, (Tianjin University);
210142	Big data analysis of chemical plant data	Dr Erqiang Wang, (University of Chinese Academy of Sciences);

Keynote Speakers

Bayesian approaches for chemical process modeling

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Abstract

Developing a chemical process requires a reliable mathematical model to predict the performance. To increase the predictability of the model, the data should be obtained carefully so that parameters in the models can be obtained efficiently and accurately. There exist many challenges in modeling complex chemical processes. Adsorption processes, for example, are intrinsically dynamic processes that do not have a steady state, where complex equilibrium as well as kinetics must be modeled carefully so that sufficiently accurate predictions can be given. Many experimental tests must be carried out so that the adsorption and mass transfer mechanisms can be observed.

To enable robust process design and operation, uncertainties in mathematical models should be quantified. However, uncertainty quantification can be challenging for many chemical processes. Model uncertainties are often ignored, or quantified approximately by linearizing the model. Such approaches may not guarantee sufficient robustness.

In this presentation, Bayesian estimation techniques are applied to estimate model parameters and quantify model uncertainties. By applying the Bayes' principle, model parameters are estimated as posterior probability distributions, utilizing prior knowledge as prior probability distributions. This quantification can be performed by sampling such as the Markov Chain Monte Carlo (MCMC) technique. Some case studies are presented including adsorption isotherms, as well as chromatographic processes. Flexibility of this framework is demonstrated, where multiple data sources are handled effectively in a hierarchical manner, while quantifying differences among data sets.

QMaC: A Quantum mechanics/Machine learning-based Computational tool for chemical product design

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Abstract

Chemical industry is focusing more on higher value-added materials compared to commodity chemicals. Chemical-based product design has now become a key topic in chemical engineering. A few computer-aided chemical product design platforms/tools, such as OptCAMD, have been developed to help design various chemical products. In this work, a Quantum mechanics/Machine learning-based Computational property prediction tool (QMaC) is developed for chemical product design, aiming to employ the Quantum Mechanics (QM) and Machine Learning (ML) techniques to better design organic small molecules, inorganic materials, fertilizers and pesticides, polymers, catalysts and other chemical products for human needs. The QMaC framework and its relationships with the database and OptCAMD are shown in Figure 1.

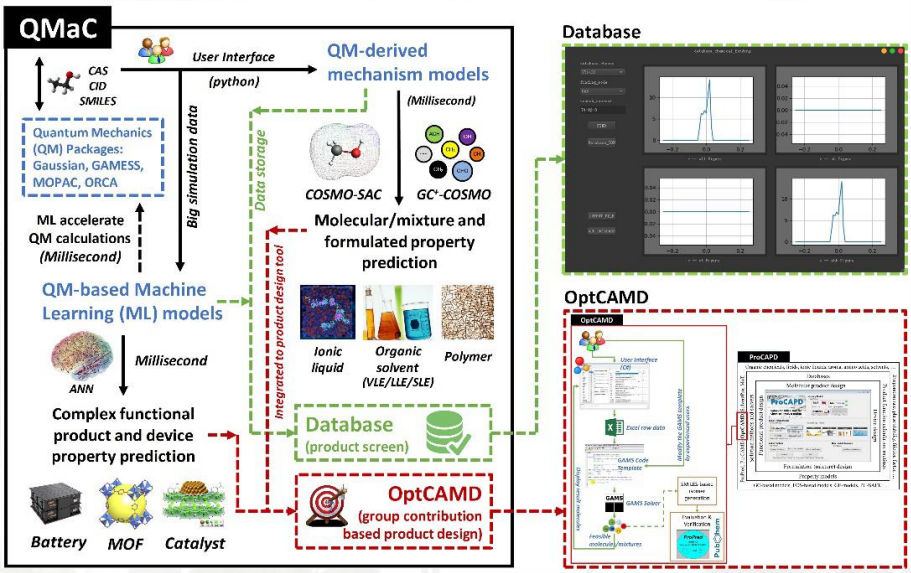

Figure 1. QMaC framework and its relationships with the database and OptCAMD.

The input data of QMaC is a set of molecules represented with SMILES (Simplified Molecular Input Line Entry Specification), CAS number or CID number (in PubChem database). QM calculation packages, e.g., Gaussian (Ochterski, 2000), MOPAC (Stewart, 2016), GAMESS (Schmidt et al., 1993), etc., are incorporated into QMaC as the execution module for molecular simulations. The functions of the execution module include molecular structure optimization, single point energy calculation, Gibbs free energy calculation, HOMO-LUMO calculation and all other functions that QM packages provide. Users can select QM packages, execution module functions and functional method/basis set parameters in QMaC interface. Case studies are given to demonstrate the validity of the developed product design tool.

Keywords: product design, computer-aided molecular design, quantum mechanics, machine learning, surrogate model.

Multi Stage of Batch-Wise Solvent Extraction Process for Separating Triacylglycerols from crude *Calophyllum Inophyllum* oil

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Abstract

Vegetable oils have a variety of uses as cooking aids and food constituents. They are usually refined before use. Crude vegetable oils are generally refined to isolate triacylglycerols (TAG) by either chemical or physical refining. Chemical refining is commonly accomplished by the use of caustic refining compounds, in which the free fatty acids (FFA) are removed by reaction with a sodium hydroxide solution. Physical refining is commonly accomplished by distillation neutralization, in which the free fatty acids are removed by water vapor. However, from both methods there are several stages of the process that are considered dangerous and produce contaminants in the refined cooking oil. The first contaminant issue is the presence of 3-monochloropropane diol (3-MCPD) Esters in cooking oil. 3-MCPD Esters have been proven to be carcinogenic compounds. They are mainly formed during the high-temperature deodorization process which is above 200 ^{o}C. They are formed from TAG, diacylglycerols (DAG), and monoacylglycerols (MAG) to form acyloxsonium ions which react with chloride ions to form 3-MCPD Esters. The second issue is the bleaching process, which is the process of removing the majority of the insoluble or colloidal dyes which give oil color. Bleaching usually requires materials in the form of activated carbon which can come from wood, coconut shell, or animal bones. Most of the vegetable oil industry abroad uses animal bones as activated carbon raw material because these materials are easily obtained at cheap prices. This is a serious issue for Muslims if the animal bones used are in the form of pig bones. From a Muslim point-of-view, the government must ensure that food and other products consumed are halal. “Halal” is an Arabic term associated with any products allowed to be consumed by Muslims according to Islamic law, known as Syariah Law. Another, bleaching earth used in the bleaching process has also the potential to be a source of chlorine ions, and is said to contribute to the formation of 3-MCPD Esters by 20-30% of the entire refining process. Therefore, it is necessary to find an efficient process for separating TAG from crude vegetable oil that free from the use of pig bones activated carbon and bleaching earth to ensure optimal taste, aroma, stability, appearance, and nutritional value while maximizing product quality, safety, and yield. In this work, the multi-stage of batch-wise solvent extraction process for separating TAG from crude *Calophyllum Inophyllum* oil was developed based on the polarity difference. Experimental work was also carried out to ensure the accuracy of the simulation. Simulation work was reported that TAG was successfully isolated in non-polar fraction with a purity of 100% after 8 stages. This result was proved by experimental work with an error of less than 3%

Keywords: Batch-wise solvent extraxtion; *Calophyllum Inophyllum* oil; Polarity; Triacylglycerols

A Bi-Level Optimization Model for Optimal Green Technology Selection with Economic Incentives

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Abstract

Government-industry interactions can be modelled using the Stackelberg (leader-follower) game framework. Such games involve optimization by two or more agents with potentially conflicting interests. Static Stackelberg games can be modelled using bi-level mathematical programming models consisting of nested optimization problems. In such games, the upper-level model represents the leader's interest; the lower-level model represents the follower's interest, and acts as an additional constraint in the leader's problem. The two levels interact because each agent's objective function is determined partially by the other agent's decisions. This modelling framework has been used for environmental engineering problems where government (acting as the leader) has a sustainability objective on behalf of the public good, while industry (acting as the follower) has a profitability objective. In such problems, the government may seek to influence industry decisions to align more closely with its own through economic incentives; for example, bi-level optimization has been used to calibrate incentives to induce water conservation measures in eco-industrial parks [Aviso et al., 2010].

In this work, a bi-level optimization model is developed for green technology selection with economic incentives. Both agents seek to select the best option from a set of alternatives rated based on a set of common criteria; however, in general, the leader and follower may assign different weights to these criteria, and thus prefer different optimal choices. It is assumed that the leader can change the economic rating of the alternatives, as seen from the follower's vantage point, via incentives. It is also assumed that the follower's overall preference is seen by the leader as an additional criterion of "technology acceptability." The leader's objective is to determine the minimum incentive needed to ensure that the follower's optimal choice of technology matches its own choice.

In this work, the bi-level optimization model is formulated as a mixed integer non-linear program (MINLP) with a bi-objective upper problem. It is then reformulated as a single-level, single-objective mixed integer linear program (MILP). A case study on the selection of negative emissions technologies (NETs) [Tan et al., 2019] is used to demonstrate the modelling framework.

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AI and machine learning through life cycle of energy and environmental systems

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Abstract

The recent rapid development of deep learning enabled artificial intelligence (AI) has brought tremendous new opportunities to many fundamental domains in energy, environmental, and engineering systems. Either existing machine learning (ML) methods applied in new areas such as renewable energy systems and material science, or novel ML methods originated from our knowledge of classic control/optimization theories can make significant contributions to this emerging interdisciplinary field. In this talk, I will give a state-of-the-art overview of the ML methods and illustrate how AI can help in many fields we have investigated recently to accelerate smart city and advanced manufacturing. Not only commonly used ML methods e.g., random forest, support vector machine, and neural networks, but the recent developments of ML-in-the-loop through active learning, reinforcement learning, generative adversarial networks etc. are also explored to combine expert knowledge with the data-driven models and automated systems. Furthermore, we have developed a series of interpretable approaches to understand "black-box" ML models and make it more favoured by domain engineers and scientists to achieve abundant findings of complex systems that may embed a huge amount of hidden information.

Our recent developments of ML models and data-driven optimization that can expedite smart systems engineering development will be demonstrated via a series of frontier case studies such as 1) design of global negative emission systems through biochar; 2) flexible clustering approach for large-scale urban energy-water nexus optimization; 3) multi-step ML-enabled optimized nanoparticles synthesis; 4) full-map ML of sensors development and performance predictions for soft robotic systems; and 5) demand forecasting of manufacturing systems and data-driven optimization for industrial symbiosis. Although promising opportunities are identified, many challenges exist at this early stage, such as construction of valuable and open datasets, lack of standard algorithms workflow and fully autonomous experimental platforms, which will be discussed as future directions. In spite of the challenges, it is promising to embrace the dawn of a new data-driven era, especially taking advantage of the closely relevant PSE expertise from our community.

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Performance Assessment of Operators in Process Industries using Wearable Sensing Devices

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Abstract

Today's operators are involved in monitoring tightly integrated complex processes with sophisticated control strategies where missteps can be very costly in terms of safety, availability, and profitability. Numerous studies have revealed that human errors is one of the major causes behind various incidents in process industries. This is further compounded by mobile, retiring and ageing workforce. Therefore it is critical to impart required knowledge to the operators and assess their performance periodically. Typically, such knowledge and skills are imparted to operators using operator training simulator (OTS) which offer a simulated environment of the real process. However, these techniques emphasize on operator's ability to follow standard guidelines while neglect the cognitive aspect of humans. Moreover, there is hardly any approach that allows for continuous assessment of operators in process industries. In this talk, I will provide an overview of a Human-In-The-Loop (HITL) framework to analyse the performance of operators in process industries. The proposed framework utilizes data from various biometric wearable sensing devices (such as eye tracking and EEG device) along with process information for development of an operator model for knowledge and capability assessment. I will also present a few results to demonstrate the practical utility of the proposed framework to process industries.

Application of Mathematical Programming to Process Integration and Energy Planning Problems

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Abstract

Process integration techniques have been recognised as an effective planning tool for energy savings and waste reduction in the process industries, providing valuable insights and decision support. The application of process integration techniques has been extended to large-scale energy systems. In particular, mathematical programming approaches have the capability to deal with complicated problems involving a large number of decision variables, detailed cost considerations, trade-offs between various design objectives, uncertainties and case-specific constraints. This presentation covers recent research works on batch heat integration, resource conservation network retrofitting, separation network synthesis, energy sector planning, and renewable energy system design using mathematical programming and optimisation. The model structure and formulation will be briefly presented, with case studies and results for illustration. Future research recommendations will also be discussed.

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Optimisation and Planning of Biomass Supply Chain for New and Existing Power Plants Based on Carbon Reduction Targets

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Abstract

Biomass energy is a potential solution for reducing the effects of global warming. Unfortunately, the Malaysian biomass energy sector is not well established due to the high cost of implementation and lack of quantitative planning tools. To address these issues, this research developed a quantitative planning tool to optimise and plan biomass supply chains based on carbon reduction targets. The tool proposed in this work centres around three important stages; Carbon Emission Pinch Analysis (CEPA), mathematical optimisation and multi-stakeholder analysis. CEPA is used to determine the minimum amount of biomass based on a carbon reduction target. Then, mathematical optimisation is used to optimise the biomass supply chain. In addition to CEPA and mathematical optimisation, this work considered co-firing opportunities for existing power plants and importance of players in the optimal supply chain. The importance of players within the supply chain is identified using Shapley-Shubik Power Index. Shapley-Shubik Power Index determines the level of power held by each player (i.e., power plants) in the supply chain based on the number of times the players becomes pivotal in achieving a quota (i.e., power purchase agreement). Notable results from the optimised supply chain are the shortest total distance and boiler system are always preferred due to cheaper overall transportation cost and higher conversion factor respectively. Other than that, five tonnes truck is selected in every route as it has a cheaper hiring cost. From the multi-stakeholder analysis, it was observed that the player with a high power output will dominate the supply chain especially at lower quotas.

Keywords: CEPA, Supply Chain Optimisation, Shapley-Shubik Power Index, Co-firing

Process Design, Integration and Optimization for CO_2 Capture Systems

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Abstract

Capital investment and operating cost related to CO_2 capture heavily depends on characteristics of CO_2 emitters as well as capture technologies to be implemented. Due to complex design interactions and complexities in system-wide investigation, finding the most economic way of introducing CO_2 capture systems to process industries is not straightforward.

This presentation will address how techno-economic benefits can be maximized with the aid of computer-aided systems engineering tools. Discussion will be made to process design issues and their techno-economic impacts related to amine-based systems and membrane-based systems for post-combustion capture. The role of techno-economic analysis is explained not only to identify any economic bottleneck, but also to suggest technical gaps to be filled through R&D of materials and process scale-up.

With examples and case studies, it will be illustrated as the cost-effectiveness of CO_2 capture systems can be enhanced through systematic application of process design, integration and optimization methods.

Conceptual understanding as well as practical design guidelines gained from collaborative work conducted by author's research group with other researchers in the area of materials development, pilot test, process scale-up and FEED (Front-End Engineering Design) study, will be also discussed.

Acknowledgement

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Process and Product Design

Energy-efficient Design of Bio-butanol Purification Process from Acetone-Butanol-Ethanol Fermentation

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Abstract

Bio-butanol is an alternative fuel since its energy density is much higher than bioethanol and close to gasoline. Furthermore, it can cut down corrosion of the vehicle and is easy to mix with gasoline. The main target of this work is to design an energy-efficient process for separating high purity bio-butanol from the Acetone-Butanol-Ethanol fermenter. Acetone-Butanol-Ethanol Fermentation (ABE Fermentation) is a main production method of bio-butanol and can produce extra valuable bio-acetone and bio-ethanol. However, alcohol is toxicity for microorganisms. ABE fermentation must be operated in a dilution environment. Thus, the traditional process configuration is complicated with high energy consumption to obtain high purity bio-butanol.

This work proposes a novel design for purifying the bio-butanol from the ABE Fermentation. In the proposed innovative design, a distillation column is used to remove acetone in advance. The remaining stream at the bottom is sent to a decanter. The organic phase is sent to a stripper to purify butanol, and a second decanter is used to decrease water after removing water at the second stripper. The organic phase is sent to the third column to purify ethanol. Compared to the existing design, both total reboiler duty and TAC decreased by 30%.

A plant-wide control system is proposed finally. The novel control performance is approved by testing various disturbances, including the changes in throughput and input composition.

Energy-Efficient Separation Design Aided by Liquid-Liquid Separation and Pressure Swing for Complicated Ternary System

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Abstract

In this work, a new energy-efficient design flowsheet is provided for the separation of complicated ternary system with three binary azeotropes, one ternary azeotrope, three distillation regions and liquid-liquid envelope. Without adding foreign components into the separation, a new energy-efficient design flowsheet is proposed in this work with two main ideas. The first idea is using a decanter to overcome the limitation of the distillation boundary by taking advantage of the natural liquid-liquid separation in the system instead of only using distillation columns. The second idea is changing the operating pressure for the respective columns to move the pressure-sensitive distillation boundary in order to expand the operating distillation region and reduce the flow rate of overall recycle stream in the system.

We take the separation of the ternary mixture containing benzene, isopropanol and water as an example and compare our proposed design flowsheet with the partial heat-integrated pressure-swing distillation design scheme published in a recent paper [Cui et al., 2019]. The simulation results illustrate that 64.6% of the total operating cost and 56.4% of the total annual cost can be reduced by using our proposed design flowsheet. Doing heat integration by taking the heat removal of the condenser for the high-pressure column as the partial heat source of the reboiler for the low-pressure column can further reduce 9.3% of the total annual cost.

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Structure optimization considering multiple decanters in heterogeneous azeotropic distillation

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Abstract

The separation of heterogeneous azeotropic distillation can be easily done by combining a decanter and a distillation column to exploit vapor-liquid and liquid-liquid equilibrium driving forces [Julka et al., 2009]. The synthesis of heterogeneous azeotropic distillation processes involves a sequential procedure starting with the selection of structural conditions (i.e., the number of stages, feed stage(s), stream(s) connectivity between columns, choice of entrainers). Then, such a sequential procedure ends with the selection of operating conditions (e.g., pressure, reflux ratio, boil up ratio, decanter temperature). The above structural and operating parameters are estimated through guessing, extrapolation of existing separation systems, or by applying short-cut methods [Królikowski et al., 2011].

This research presents the synthesis problem for the separation of ternary mixtures that form heterogeneous azeotropes, which solved the problem the other way around: the interpretation of the optimal solution leads to the optimal distillation structure without any need of assuming a predefined structure or column connectivity. Furthermore, in this study, the entire liquid composition space was divided into a sufficient number of subspaces, and a representative liquid composition was chosen at each discrete subspace and assigned to a distillation module. Also, The entire vapor-liquid-liquid (VLL) region was divided into a sufficient number of subspaces, and a representative liquid composition of organic and aqueous phases falling along a tie line is chosen at each subspace, and it is assigned to a decanter module.

The distillation and decanter modules are included in a superstructure representation. Then, the superstructure is formulated as a linear programming (LP) problem. The optimization problem considers that a decanter can be located at any place in the distillation column. After finding the optimal solution, its interpretation is made. Finally, the interpreted solution is validated in the process simulator Aspen Plus. In this study, the ethanol-water separation considering benzene as entrainer was taken up. The interpreted optimal solution has one top and one bottom decanter, and it attained energy savings of around 37% in comparison with a conventional two-column process.

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Rigorous Simulation and Optimization of the Plant-wide Glycerol Carbonate (GC) Production Process through Transesterification

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Abstract

The spurring increase in bio-diesel production produces a large amount of glycerol as side product, which causes its over-supply. Hence, converting glycerol (GLY) into other value added chemicals would be a promising solution. In this work, the rigorous design and optimization plantwide glycerol carbonate (GC) production processe via transesterification reaction of GLY and dimethyl carbonate (DMC) is firstly proposed. The feasibility of using the reactive distillation technique to produce GC is discussed in detail. The process can be divided into a main section consisting of a reactive distillation column (RDC) and GC purification columns, and an extractive distillation section to separate the unreacted DMC and the side product methanol (MeOH). The research scope includes regressing the thermodynamic parameters suitable for representing both vapor-liquid and liquid-liquid equilibrium, correcting the kinetic parameters, developing process flowsheets, and optimization. In the current study, we found that the major economic trade-offs are resulted from two important variables, the RDC pressure (PRDC) and the molar excess ratio (ER). Through optimization, the cases operating at PRDC= 3 atm and ER= 2 is considered as the currently optimized one. Besides, further sensitivity tests are performed on this optimized case. We then found that designing the reactive trays in RDC with less catalyst loading would lead to possible improvement in the future.

CO2 Utilization Feasibility Study: Process Intensification of DMC Direct Synthesis Process

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Keywords: Dimethyl Carbonate, CO2 Utilization, Process Intensification, CO2 Emission Mitigation, DMC direct synthesis

Abstract

The urge to mitigate the greenhouse effect has risen in recent years. Other than CO2 capture and storage technology, research for CO2 utilization is also crucial. Among the candidate compounds of CO2 conversion, dimethyl carbonate (DMC) is one of the most promising material since it can be used as fuel additive, solvent for lithium ion batteries, building block for various organic synthesis, etc. Using CO2 as a feedstock to convert to other components is often challenging because of its stable chemical property. However, in this work, processes with intensified system were proposed to enhance the economic feasibility. DMC can be produced from a couple of routes. CO2 direct synthesis is the simplest route because it has solely one chemical reaction and includes less components. The weakness of the route, which is the low conversion of the reaction, can be overcome in this work. One conventional process (CDWC) and three intensified processes (DSR, RDSR and RDSRT) were developed and their total annual cost (TAC) and CO2 emission amount were compared. The three intensified processes were improved by a configuration including a column and a side reactor which is extremely helpful for reducing TAC because within it the reaction conversion can be enhanced from around 10% to nearly 100% and the cost for separation can be largely reduced. Further addition of EO as dehydration agent into the column can raise the separation efficiency because the hydration product EG increased the relative volatility in it. The results had shown that RDSR and RDSRT own great potential thanks to the most CO2 emission reduction amount and the lowest TAC, respectively.

Optimization of extractive distillation processes with mixed solvents

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Abstract

Simulation-optimization was applied to determine nearly-optimal process designs in extractive distillation systems for the separation of azeotropic mixtures with mixed solvents. The separation of acetone and methanol [Sazonova et al., 2016; Yang and Ward, 2018], ethanol and water [Jaime et al., 2018; Zhao et al., 2017; Gil et al., 2014] and tetrahydrofuran, water and ethanol [Zhao et al., 2017] were considered. The performance of individual solvents and solvent mixtures was compared. Each column in the separation process was optimized and the total cost of the whole process was calculated. Due to the large number of variables, a stochastic optimization algorithm (simulated annealing) was combined with simulation in a commercial process simulator. The results suggest that mixed solvents are an attractive alternative to single-component solvents, but that it is important to screen candidates systematically because the best mixed entrainer is not necessarily composed of the two best single-component entrainers. The algorithm comprising simulation-optimization with simulated annealing was found to be feasible and attractive for solving the optimization problems for process flowsheets with a number of design variables between seven and thirteen.

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Methanol synthesis process modelling with exhaust gas

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Abstract

Exhaust gas contains approximately 10% of CO2, which is greenhouse gas. It would be good if CO2 in Exhaust gas could be reduced. Recently one of the possible applications to convert the exhaust gas into valuable products, dry reforming has received great attention to turn CO2 to syngas which can further be used for the synthesis of methanol. This paper study is about the modelling of total process, which consists of CO2 purifying, dry reforming and methanol synthesis process, for converse exhaust gas in to methanol. The purpose of a CO2 purifying unit is to separate N2 contained in the exhaust in large quantity using either membrane or acid gas removal unit(AGRU), among which the former showed low utility and equipment costs. All about process is designed using UniSim(Honeywell Inc.). Finally total process was used to evaluate the reduced amount of CO2 and economical analysis.

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Model-based design of H_2O_2 decontamination processes in pharmaceutical manufacturing

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Abstract

Hydrogen peroxide decontamination is the key technology to sterilize isolators or clean rooms to produce injectables using H_2O_2 as a decontaminant. Typically, injectables are manufactured batch-wise, where decontamination serves as the change-over operation between batches. Decontamination is known to be time-intensive, especially the aeration part to reduce the residual H_2O_2 to a target concentration (e.g., 1 ppm, or even lower). Decontamination is becoming relevant, along with the market growth of biopharmaceuticals/vaccines that are usually provided as injectables, and also with the trend of small lot-size production and frequent change-overs.

We present model-based approaches for designing decontamination processes. The presentation first introduces the time estimation model for the entire process including aeration, given the initial loading amount of H_2O_2 and the humidity in the isolator[1]. Experiments were performed to develop a regression-based model, which determines Pareto optimal conditions to minimize the negative impact on quality and to maximize the productivity. This model, dealing with one cycle change-over, was extended to multicycle change-over, in conjunction with the production scheduling[2], which is the second part of the presentation. Simulation was performed intensively to assess numerous combinations of scheduling options and process condition options from the quality and productivity objectives. The Pareto frontier was affected largely when tougher constraints were applied to the target aeration concentration, and the complexity in the product portfolio. Third part of the presentation shows an in-depth analysis on the sorption of H_2O_2 into the polymers in the isolator[3]. Experiments were performed to assess the sorption performance of five typical polymers used as materials/parts in sterile isolators. Furthermore, models were developed that can estimate the required duration of aeration, given the target H_2O_2 concentration and material specifications. Several polymers showed the tendency to require long duration for aeration, which suggests careful investigation in the design of isolators. The above three studies motivated more integrated development of pharmaceutical products, processes, and production equipment/facilities.

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Applying process simulation to life cycle assessment of cellulose nanofiber-reinforced plastics

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Abstract

Cellulose nanofiber (CNF) is one of the emerging technologies that can be produced from plant-derived renewable resources and have advantage of mechanical properties in lightness and strength. For the implementation of such emerging technologies into society, its environmental performance considering the life cycle should be examined with the options in process systems considering the future production scale. In this study, we applied process simulation to estimate energy and material balances in chemical preprocessing required in production of cellulose nanofiber-reinforced plastic and performed life cycle assessment (LCA) based on the estimated inventories.

We focused on a production method it can disintegrate the cellulose fibers by kneading the pulp with polymers, while various techniques for CNF production are currently under development. Paper pulp was selected as the raw material of CNF because of its high availability from existing market. The acetylation of paper pulp is effective for improving the chemical and mechanical properties and processing when CNF is used as the filler of composite with polymers, e.g. polypropylene, polyethylene or polyamide. Acetic anhydride is generally used as the reactant for the acetylation with the generation of acetic acid as byproducts and significant amount of unreacted acetic anhydride flows out from reactor. Although N-methylpyrrolidone (NMP) is used as the solvent in current lab-scale or pilot-scale reaction process, it can be replaced by excess amount of acetic anhydride. We conducted process simulation to investigate the effect of separation and recovery of excess acetic anhydride and the byproduct acetic acid, which had been treated as waste liquid in current lab-scale production. Multiple process alternatives for recycling chemicals were compared. The inventories of the mechanical kneading process were acquired through measurement of power consumption in demonstration plant, and discussed with CNF experts regarding its expected scale-up effects.

We specified the requirements of acetylation process that can mitigate life cycle greenhouse gas (GHG) through process simulation. Separation and recovery of excess acetic anhydride and the byproduct acetic acid was revealed to be mandatory. Process simulation can be used as strong tool for inventory estimation required for the LCA of emerging technology such as CNF.

Simulation of cultivation processes in monoclonal antibody production towards the selection of operation modes

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Abstract

Enhancing the production efficiency of monoclonal antibodies (mAb)s is becoming a high priority target of the biopharmaceutical industry to fulfill the increasing demand and to compete with emerging biosimilars[Gaughan, 2016]. Advances in the production process include improving host cell lines, as well as, optimizing feeding strategies and media. Additionally, different production modes are investigated and a move to continuous operation is assessed[Yang, et al., 2019].

This work presents a mechanistic model of the cultivation process, to be used for dynamic simulation applications. Batch, fed-batch and perfusion cultivation modes are modeled and explored in this work. Dynamic simulation of the process, taking into consideration cell-specific parameters and process conditions, is necessary for a more robust and transparent design and assessment of process alternatives. The model describes the rates of product formation, nutrient depletion and the production of major metabolites in the system. The employed model also takes into account process operability and product quality issues by including host cell proteins (HCP)s and DNA. Such components in the system may cause, for example, aggregation and increased difficulties in downstream purification processes. Experimental data from a Pilot facility in Japan are used for parameter estimation and model validation. A comprehensive assessment framework, which includes economic and operability indicators is presented to compare the various cultivation modes. A map of preferential operation modes is then presented for various production scenarios. This work offers a higher resolution model that can be used for a more practical and fairer comparison of process alternatives. The developed model offers increased insights into the system dynamics and impacts on product quality. Such a model is fundamental towards integrated design of upstream and downstream biopharmaceutical production processes.

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Design of Dual Pressure Reactive Distillation via Compressor with Intermediate Condenser for Silane Production Process

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Abstract

Reactive distillation (RD) for the production of silane is a process that requires a large amount of expensive refrigerant to condense top product due to its low boiling temperature (-112 oC). In this study, RD configuration is proposed as a base case and three other configurations are proposed to diminish the utility consumption cost; RD with an intermediate condenser (RD-IC), dual pressure reactive distillation (DPRD) and dual pressure reactive distillation with an intermediate condenser (DPRD-IC). The columns in all configurations are modeled using the RADFRAC module from Aspen Plus V10.0. To obtain the optimal designs, a simulated annealing algorithm (SAA) is applied to RD and DPRD configurations. The objective function is the total annual cost (TAC) which includes operating and capital costs. For RD configuration, five design variables need to be optimized. Since DPRD configuration is quite similar with HIDiC, it consists of a high-pressure column without reboiler and a low-pressure column without condenser and a compressor. However, there is no heat transfer from high pressure column to low pressure column. Based on this arrangement, seven design variables need to be optimized for this configuration. The configuration of RD-IC and DPRD-IC are adopted from the optimal RD and DPRD configurations, respectively. In RD-IC configuration, IC is installed into RD column to reduce the amount of expensive refrigerant supplied for a top condenser. The cheaper cooling media is used in IC because the temperature is higher than the top condenser. Meanwhile, the heating media consumption is slightly increased because the reboiler duty is increased. In DPRD configuration, the temperature of the bottom product is lower than RD because the operating pressure is lower. Therefore, the heating media is free of charge since quenched water can be used instead of low pressure steam. In DPRD-IC configuration, IC is installed into the HP column to obtain the advantage as in RD-IC. However, the increase of reboiler duty does not affect the heating media cost as mentioned in DPRD configuration. From the simulation results, compared to RD configuration, the operating cost saving of RD-IC, DPRD and DPRD-IC configurations are 39%, 10% and 56% and TAC saving are 38%, 4%, and 48%, respectively.

Keywords: intermediate condensers, reactive distillation, silane process.

A Comprehensive Numerical Procedure for Evaluating Flexibility Indices of Dynamic Systems with Piecewise Constant Manipulated Variables

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Abstract

Although chemical processes are traditionally evaluated according to economic criteria, it is still necessary to ensure the operational feasibility of a given process design. Many calculation methods for quantifying flexibility, e.g., the vertex method and the active set method, have already been proposed for the steady-state systems. However, none of them can be utilized to compute the dynamic flexibility index reliably and efficiently. The present work is aimed to develop effective numerical strategies for flexibility analysis of any unsteady process. In this study, manipulated variables have been assumed to be piecewise constant rather than continuous process. In the proposed computation procedure, the candidate vertices have first been reduced to narrow down the search scope and to facilitate convergence. Metaheuristic algorithms, namely the genetic algorithm and/or the truncated enumeration method, have been deployed for the above mentioned task, that is, to identify a probable region for the optimum. Subsequently, a comprehensive computation strategy has also been developed for accurately evaluating the dynamic flexibility index. A better probability of convergence and significant decrease in computational time for the dynamic flexibility index quantification can both be observed in the case studies. Two numerical examples are presented to demonstrate the effectiveness of the proposed methodology.

Keywords: dynamic flexibility index, unsteady state process, active set method, vertex method, genetic algorithm, exhaustive enumeration

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Optimal Retrofit Designs of Multi-Plant Heat Exchanger Networks with Reasonable Benefit Allocation Plans

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For the purpose of efficient heat conservation, several heat integration approaches have already been proposed for improving heat recovery in a single chemical plant [Yee and Grossmann, 1990]. During the last few years, the grass-root designs of multi-plant heat exchanger networks (HENs) have also been developed to achieve extra cost and energy savings [Hong et al., 2019]. Since the traditional model-based HEN synthesis strategies mostly focused on minimization of total annual cost (TAC) for the total site. The resulting integration scheme might be unacceptable to the participating plants since the total benefit may not be allocated fairly among all members. To resolve the benefit distribution issue, a two-stage computation procedure has already been developed to generate a practicable cost-sharing plan for any grass-root design in the spirit of cooperative game theory [Jin et al., 2018]. However, the chemical plants in an industrial park were rarely built at the same time and each existing plant must have already been equipped with its individual optimal HEN. Hence, the benefit allocation problem occurs mainly when a multi-plant HEN retrofit project is initiated for facilitating futher reduction in utility consumption.

Therefore, the research objective of present study is to develop a generic model-based multi-plant HEN retrofit method together with the corresponding benefit allocation scheme in the spirit of the cooperative game. It is also assumed that the interplant heat exchanges are facilitated indirectly through intermediate fluids. The actual financial profits distributed to the participating members are determined according to the risk-based Shapley values [Jin et al., 2018]. The feasibility of the proposed HEN synthsis and the benefit allocation methods are demonstrated with a simple example.

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Design of the Product Separation and Recovery Section of a Methanol-to-Olefins Plant

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Abstract

Light olefins, ethylene and propylene, are the most important basic raw material chemicals for the petrochemical industry. Different from the conventional petroleum-based production of olefins, the feedstock of methanol-to-olefins (MTO) technology[1] is methanol, which can be generated from renewable energy. Same as the conventional olefin plants, because of the sub-ambient and high-pressure operation conditions, the product separation and purification is the most energy consuming section of the MTO processes. For the UOP/Hydro MTO process[2], this study presents the design of the product separation and purification section, which includes several subsystems, namely a series of distillation columns, cold box, and refrigenation. For each column, an initial base design is determined using heuristics and further optimized by examining the column grand composite curve[3]. The cold box and refrigeration subsystems are designed by simultaneously considering heat and work integration and various options of refrigeration cycles, such as interevaporating, intercondensing, subcooling, and economizer[4,5]. The evolutionary design of the overall system is evaluated using ExPAnD procedure[6], which is based on the concept of exergy enegy.

Keywords: methanol-to-olefins, distillation, energy integration, sub-ambient, refrigeration

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Two-step hybrid optimization of heat-integrated distillation columns

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Abstract

Heat integration is one of the most used energy conservation methods in chemical processes, and it typically involves the heat transfer from the vapor stream entering a condenser and the liquid stream entering a reboiler. Nevertheless, this heat integration is done at the worst thermal condition because

Heat integration between stages exploits the idea of supplying heat at a temperature higher than that at the condenser in a high-pressure column and receiving it at a temperature lower than that at the reboiler in a low-pressure column [Alcántara-Avila et al., 2013]. The use of few heat integrations can outperform the typical concentric Heat Integrated Distillation Column (HIDiC) arrangement in terms of cost and energy consumption through the solution of a mixed-integer linear programming (MILP) problem [Alcantara-Avila, 2019]. However, since the proposed MILP is a linearized approach of the heat balance in HIDiC structures, there is a gap between the results in optimization and simulation. Therefore, this work proposes a two-step hybrid optimization procedure that combines deterministic optimization (i.e., MILP problem) and stochastic optimization (e.g., Simulated annealing) to take advantage of the strong points from each optimization technique.

Given a given number of stages and pressure in each section, the HIDiC structure with the best heat-integrated stages is obtained by solving the MILP problem at the first step. Then, the stochastic optimization finds the optimal amount of heat transfer at the second step. Therefore, the optimization is solved sequentially. The proposed hybrid optimization is applied for the separation of a binary mixture. The strong points in deterministic and stochastic optimization are combined to deal with complex intensified distillation structures with heat integration.

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Feasibility study on reactive distillation with double reactive sections in term of feed location and section total stage numbers

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Abstract

Reactive distillation generally has been known to save energy and equipment cost in chemical plants[1]. There have already been great number of patents and paper published on the application of reactive distillation columns[2]. Specifically, almost all of the studies performed so far had employed a reactive distillation column with a single reactive section (RDC-SRS) for the two-stage consecutive reversible reaction which is widely found in esterifications, acetalizations, trans-esterfifcations and aminations[2] that may take the forms as A + B ↔ C + D and C + B ↔ E + D. Since high conversion and high selectivity are much more difficult to be reached simultaneously in this kind of reaction, the RDC-SRS might not always be a good design options. Therefore, a different configurations of reactive distillation columns is worth exploring for the separations for this type of reaction [2]. In this work, a novel reactive distillation column with double reactive sections (RDC-DRS) is explored and evaluated.

There are many operating parameter that affect the efficiency of RDC (e.g., the number of stages in either reactive section and total stage of RDC)[3]. In this study, we would like to focus on the feed location and total stages in each sections while considering a spectrum of materials' relative volatility and equilibrium reaction constants [3].

It is expected that the design of RDC-DRS could initiate further works in this topic and save time in the design stage. Moreover, the issues on feed type, stage number distribution in each section under different equilibrium constants will be addressed to provide more insights on the design method of complex RDC-DRS.

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Keywords
Reactive distillation, double reactive section, two-stage consecutive reversible reaction

Development of CAMD tools for the design of solvent additives to upgrade bio-oil

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Abstract

Bio-oil from fast pyrolysis of biomass exhibits several undesirable attributes and storage instability which limits its direct application as fuel. Solvent addition is an approach used to upgrade bio-oil produced by fast pyrolysis. In this work, a computer-aided molecular design (CAMD) tool has been developed to identify the possible molecular structures of the solvents with desirable properties. ASTM D 6751 and EN:14214 standards of biodiesel are taken into account while defining the property targets. The developed CAMD approach can use property prediction models that incorporate different topological indices and group contribution models. The molecular signature descriptor is applied in the CAMD formulation to accommodate property prediction models of different indices via a multi-stage framework. After solvent candidates are identified, phase stability analysis is carried out to evaluate the stability and miscibility of the solvent-oil blend. Optimal solvent structures that match the target properties while having minimal environmental impact is generated.

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Novel Ethyl Lactate Production Process Design using Reactive Distillation and Membrane-Distillation Configuration

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Abstract

A novel process for producing ethyl lactate (L1E) is proposed in this study. The rigorous thermodynamic model is verified by experiment data (Vu et al., 2006 and Delgado et al., 2007). The overall process can be divided into two parts: the reaction and separation sections. For the reaction section, only one reactive distillation column is used to produce the target product, ethyl lactate, through a sidedraw flow. The heavy components recycle back to reactive distillation column itself to carry out the hydrolysis reaction. The distillate composed of water and ethanol is fed to separation section to recover high purity ethanol and recycle to the reaction section. For the separation section, a new hybrid separation configuration is composed of membranes in series and one distillation column. The purpose of membranes is to concentrate ethanol to high purity and recycle back to the reaction section., Moreover, one additional column is implemented to recover the loss of ethanol from the permeate of membrane. This hybrid separation arrangement can reduce a lot of energy consumption for ethanol recovery compared with the configuration by using a distillation first then membranes. Finally, ethanol feed concentration is changed from pure ethanol to azeotrope to elucidate its influence on the cost of the whole process. As a result, TAC of this novel process is \$211.45×103/y, and 57.9% of TAC reduction is compared to the previous work (Dai et al., 2019). The azeotropic ethanol feed can save the raw material cost around 69.8% of TAC to pure ethanol feed case.

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Refrigeration System Synthesis based on Hybrid GA-PSO Method

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Abstract

Refrigeration system is a common way to provide refrigeration at different pressure/temperature levels for chemical processes. The synthesis of refrigeration system often leads to a large-scale non-convex optimization problem, an effective modeling and solution of such a problem is still chalenging. In existing studies, simplifications were often made in order to confine the scale of the problem from being too large to be solved with available methods. For example, the workers either adopted fixed pressure levels [1], or discretized the temperature levels, or only considered the parallel structure of sub-coolers and expansion valves to avoid uncertain outlet temperature of sub-coolers [2], or did not consider the optimization of the number of temperature levels [3]. In our previous study [4], a more comprehensive model was proposed for the synthesis of a refrigeration system with single refrigerant. However, because of the difficulties in simultaneous solution of the large-scale problem by standard mixed-integer non-linear programming (MINLP)-solvers, a sequential optimization had to be performed: first, the pressure/temperature levels were optimized continuously, then, the refrigeration system was optimized on the basis of the obtained temperature levels.

In this study, to cope with the aforementioned difficulties, we formulate the simultaneous optimization of refrigeration system and its associated heat exchanging network as a MINLP problem. A two-layer hybrid solution method based on the genetic algorithm (GA) and the particle swarm optimization (PSO) is proposed for solving the problem. In an outer layer, the number of pressure levels for the refrigerant is initialy generated randomly and then evolved using the GA iteratively; in the inner layer, the corresponding continuous variables, including temperatures (or pressures) and flow rates for the refrigeration system with the given number of the pressure levels for the refrigerant, are optimized by the PSO to obtain the value of the fitness function for the GA, which is defined as the total annual cost (TAC) of the system. A main advantage of this method, thanks the random search nature of the stochastic algorithms, is that it does not need the gradient information and works on function evaluation alone, and thus is effective and robust for solving the large-scale non-convex optimization problem. The proposed methodology is validated by a case study on the optimal design of the ethylene refrigeration system in an existing plant.

Keywords: Process synthesis; Refrigeration system; Genetic algorithm; Particle swarm optimization; Hybrid algorithm.

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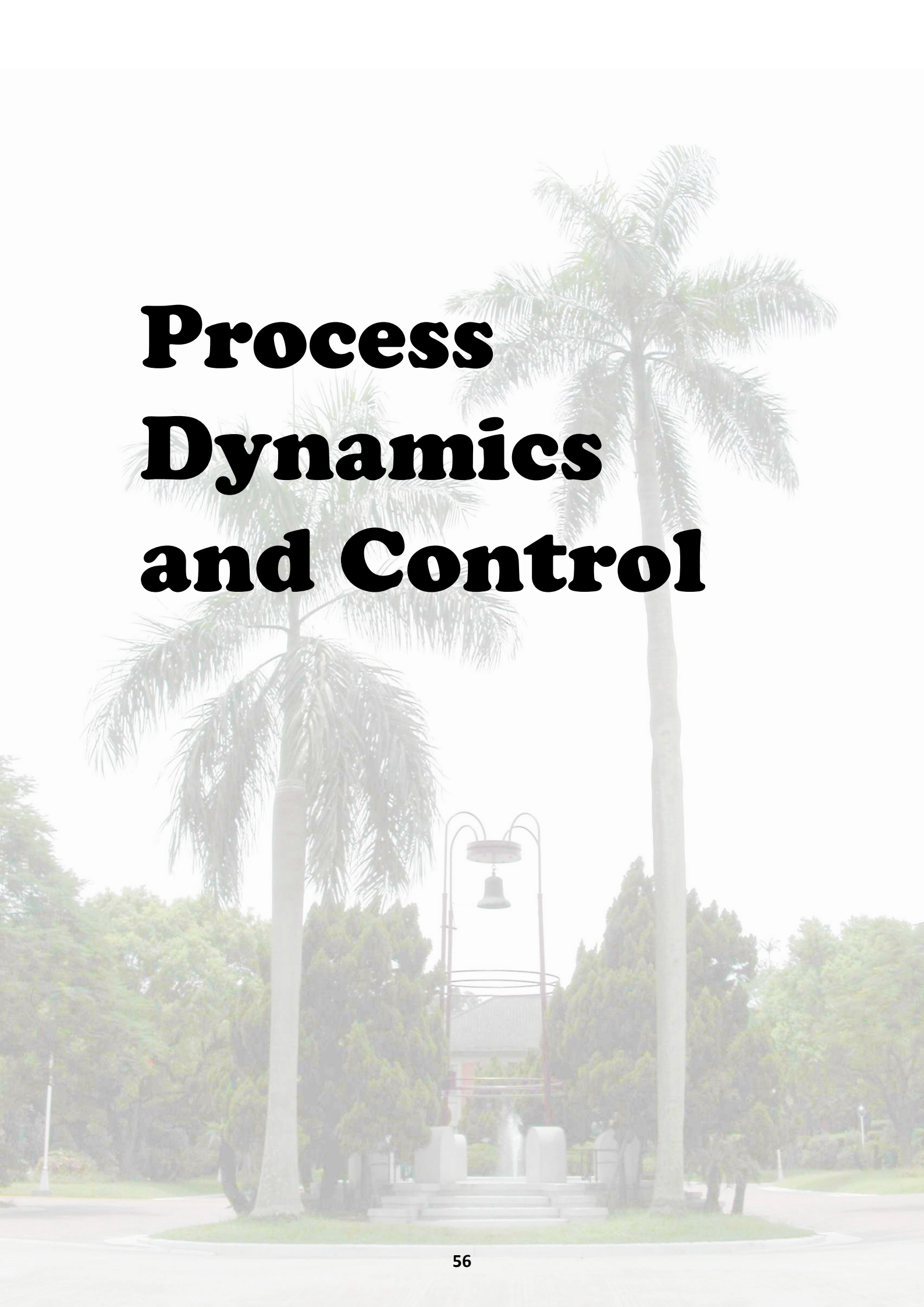

Process Dynamics and Control

Data-Driven Digital Twin Development for Chemical Plants Using Sequence-to-Sequence Approach and Rolling Training

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Abstract

A digital-twin can assist engineers in evaluating the benefits and safety of the control and operation strategies by interacting with the twin model before going online. A digital twin can be developed by the first principal model or by purely data-driven approaches. The former has the advantage of ensuring a physically reasonable process response. However, a lot of information may not be readily available. A lot of domain knowledge is required. The development cycle can be long, and the accuracy of the model may be limited. In recent years, advances in deep learning models invite a lot of interests in building purely data-driven digital twins. Since very little domain information about the process is used, there is no guarantee that the data-driven method is able to extrapolate beyond existing data. There are always doubts of whether such models can serve as true digital twins.

In our past work, a sequence-to-sequence observer model was proposed to model the behavior of a distillation column. The model used past sensor readings and manipulating variables as input to an observer to generate hidden states and use hidden states and future manipulating variables to predict future sensor responses. The model is able to give accurate short-term predictions with regular updates of actual sensor response. However, it was unable to provide long-term predictions such as the results of a step-test or evaluation of a novel control strategy with regular updates of actual sensor response. Hence it cannot be regarded a true digital twin.

In this work, a novel training algorithm was proposed to ensure that the model is able to generate long term rolling predictions. The procedure not only minimizes the output errors but also errors in hidden states prediction as we perform a rolling prediction without new sensor input. The concept was tested using data generated from ASPEN dynamic simulator of an industrial vapor-recompression distillation column. The results found that the model is able to predict dynamic responses over a near infinite horizon using various manipulation sequences that were not included in the training data, with only a very short window of observed data. In other words, the sequence-to-sequence model is a true data-driven digital twin of a physical simulator. Applicability of this approach to the real industrial processes will also be presented.

Boiler Level Control Using Deep Deterministic Policy Gradient Model

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Abstract

In the industrial process, the boiler was the main equipment for generating steam. In the boiler process, the sudden increase in steam usage caused the pressure in the boiler to decrease rapidly. At this time, the water in the boiler evaporates into steam and generate many bubbles and then caused the false liquid level. Therefore, many control methods were derived from controlling boiler with a false liquid level, such as Model Predictive Control (MPC) and Three-Elements control. However, the computational cost of MPC was high, and there was a long-term error in Three-Elements control. A novel method, reinforcement learning, can improve the disadvantages of traditional controls. However, reinforcement learning was not able to be accepted for industrial plants due to long-term interactive training requirements with real plants. Hence, this study proposed to use historical data to pre-train the deep deterministic policy gradient model (DDPG) model and then using the Priority Experience Replay training to accelerate the interactive training with plants. The backtracking multiple time steps were used to stably control boiler processes that contain delay and noise. The concept was implemented by a DDPG model with a boiler transfer function containing the inversed response curve. The results showed that compared with the traditional PI control and traditional DDPG, the method proposed in this study can be more stable and robust.

Enhanced microbial nitrogen removal by SHARON and Anammox (SHARON-AMX) integrated control strategies in wastewater treatment plants

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Abstract

Wastewater treatment problems have increased worldwide throughout the years, being essential to improve the design of wastewater treatment plants (WWTPs) and their policies, for adapting to better water reuse and nutrient removal. Nitrogen removal is essential in wastewater with a high concentration of organic loadings, being fundamental for meeting discharge limits and gaining further nitrogen reuse potential (Langone, 2013; Volcke et al., 2006). Thus, more efficient and cheaper technologies for enhanced nitrogen removal most be studied and developed. In WWTPs, the effluent discharge must hence meet the discharge standards for nitrogen concentration. Over the years, different N-removal methodologies have been implemented in WWTPs, such as the combined single reactor system for high activity ammonia removal over nitrite (SHARON) and anaerobic ammonium oxidation (Anammox) process which has shown a positive operational cost reduction in previous studies (Sri Shalini and Joseph, 2018). This technology has been utilized to develop better control strategies and monitoring of nitrogen removal, considering influential variables such as dissolved oxygen (DO), temperature, and pH in wastewater (Gut et al., 2006). However, the studies on different control strategies that could maximize the nitrogen removal potential of the combined SHARON and Anammox process are scarce. In this study, the combined SHARON and Anammox (SHARON-AMX) was implemented in the benchmark simulation model No. 2 (BSM2) of a WWTP. Control strategies were developed utilizing proportional-integrative-derivative (PID) controllers, and model predictive controller (MPC) to comparatively analyze different process control scenarios to maximize the nitrogen removal efficiency and reduce operational cost.

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Control of intensified distillation systems for quaternary mixtures

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Abstract

Distillation is one of the most energy demanding processes in the chemical and petroleum industry. It consumes between 40-50% of the total energy used in these industries [Isopescu, 2008]. Currently, the development of new technologies to reduce the environmental impact associated with the energy consumption that distillation columns need for their operation has gained interest. Energetically favorable alternatives to conventional separation sequences are the dividing-wall distillation columns. The use of the dividing-wall "Kaibel" type distillation columns with two side-draw flows to separate multicomponent mixtures in four products has been comprehensibly investigated [Olujić, 2009]. However, an improvement in economic performance has been reported with the addition of partition walls. One of the examples with multiple partition walls is called the "Satellite" column, which is built with two partition walls. The Satellite column has demonstrated to be more efficient in terms of energy consumption, with an 11.8% saving compared to the Kaibel column for the separation of a BTXH mixture [Tututi-Avila, 2017]. However, process control of these columns has been addressed in a few investigations.

This work aims to investigate control configurations for a Satellite distillation column and its dynamic comparison respect to a Kaibel column, considering only temperature controllers. Different temperature control configurations were studied, including the traditional, differential, and pressure-compensated control schemes. The dynamic study considers disturbances in the feed flow rate and the proportion of benzene in the feed. The results showed that the Satellite column had the best dynamic performance in the face of the disturbances by using a mixed differential temperature control scheme with conventional temperature control, leading to setpoint deviations less than 0.05%. Despite its structural complexity due to additional recycles, the Satellite column not only showed improved economic performance as demonstrated in the literature but also demonstrated excellent dynamic performance in the face of the imposed disturbances, with fewer deviations from the nominal value and shorter stabilization times.

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Robust Imputation of Soft-Sensor Model Using Recurrent Neural Networks

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Abstract

Soft-sensors have been widely deployed in chemical plants to complement laboratory measurements and online sensors. It has been well documented that soft-sensors lead to improved quality, energy efficiency, and safety in process operations. One important challenge to development and implementation soft-sensor is missing data. In a chemical plant, online sensor data, regressor variables were lost due to communication problems, sensor failure, process shutdown, and multi-rate sampling. Laboratory measurements, i.e., response variables in soft-sensor, are inherently sampled at multi-rate or even randomized intervals.

Methods that make up for the missing data are known as imputation procedures. Many imputations have been proposed in the literature. One notable class is probabilistic methods which rely on the correlation structures between regressor variables, between response variables, and between regressor and response variables. However, it is well known that correlation structures changes as process conditions changes. Constant monitoring and updating of the imputation procedure are required.

In recent years, advances in deep learning resulted in applications many areas, including soft-sensor development. Deep learning has the ability to incorporate different operating scenarios found in the history of the plant so that constant monitoring and updating are not required. Imputation procedures for deep learning methods were also an important field of research.

In this study, a novel soft-sensor model was proposed. The model is a two-input recurrent network with one input being the regular regressor input vector and one input being a one- hot-vector indicating the positions of imputed values. The training data set is augmented with actual data imputed with different values, and different patterns of artificially generated missing data imputed different imputation values.

The concept was implemented on an industrial C_2 stripper. The results showed that if a sufficiently large amount of artificial data were generated, the model predictions are robust to missing data and its imputed values. The model still retains a high predictive ability when multiple physical sensors fail. Furthermore, there is no need to test the correctness of the imputation procedure in the training process. This will substantially reduce the preprocessing effort in the development phase.

A study on the epidemic model with periodic structure

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Abstract

Mathematical models have played an important role in the study of epidemic dynamics and the control of infectious diseases, as the spread of infection can never be experimentally studied in reality. Regarding epidemic spread, periodic recurrence within the same region will lead to a disastrous impact on infectious duration and social economy. Therefore, it is critical to obtain the conditions that causes infectious diseases to develop into periodic repetitions, and to identify whether the current situation is a state point of self-oscillation, so as to assist decision makers to draw correct judgments and to avoid the recurrence of infection.

In this paper, a model based on the propagation principle of Susceptible-Exposed-Infective-Recovered (SEIR) is considered, which can predict the epidemic trend effectively. Through Hopf bifurcation analysis, the parameter range that will generate periodic phenomenon is obtained, and the mathematical conditions for the occurrence of Hopf bifurcation with time lag is also obtained. Besides stability analysis of the lumped system, spatial evolution of epidemic is also studied. Cellular Automata and other intelligent algorithms are introduced to simulate the population movement between communities, which can visualize the evolution of infectious diseases. Based on Cellular Automata, the influences of various parameters on the propagation of infectious diseases are analyzed, the formation conditions of periodic outbreaks of epidemics are obtained, the distribution and evolution of infections are deduced in two-dimensional space, which is important for the prevention of secondary outbreaks of infections and provides a theoretical guidline for adjusting the clinic treatment and control strategy accordingly.

Key words: infectious diseases; Hopf bifurcation; Cellular Automata

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Multi-loop PID Controllers Design Based on Frequency-Domain Direct Synthesis Method for Multivariable Interactive Processes

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Abstract

Chemical and industrial processes are basically multivariable systems with interactions. The multi-loop (decentralized) control structure using multiple single-input-single-output PID controllers remains the standard for controlling multivariable processes because of its simple structure and loop failure tolerance. Due to the interactions between individual loops, the tuning of one loop cannot be done independently. Therefore, multi-loop controllers are usually tuned in a sequential or iterative manner, which complicates the design procedure. This paper presents a novel simultaneous and non-iterative design method of multi-loop PID controllers for multivariable interactive processes with time delays. The proposed design method is based on the direct synthesis (DS) approach in the frequency domain aimed at achieving a desired closed-loop response. The performance of the DS controller strongly depends on the specification of the desired closed-loop transfer function. For a single-loop system, the desired closed-loop transfer function can be easily specified according to a process model and the controller can be obtained straightforwardly by the DS method. However, the application of DS method to a multi-loop system encounters several difficulties. The first one is that a desired closed-loop transfer function matrix has to be carefully specified so that the controller matrix obtained from the DS method is diagonal. Second, calculation of the controller matrix is very complicated because it involves the inverse of the process transfer function matrix and the desired closed-loop transfer function matrix. To solve these problems, we propose a frequency domain based DS method by specifying the frequency response of the desired closed-loop behavior. A method for specifying this desired closed-loop frequency response to achieve better control performance is developed. The frequency response of an ideal multi-loop controller is synthesized numerically point-by-point within a frequency range. Then, each ideal controller is approximated to a PID controller by fitting the frequency response. Simulation studies demonstrate the effectiveness of the proposed design method for multi-loop controllers.

Startup Operation Strategies of Styrene-Acrylonitrile (SAN) Copolymerization Process

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Abstract

Styrene-acrylonitrile resin (SAN) is produced via the copolymerization of styrene (70-80%) and acrylonitrile (20-30%) by the free-radical reaction. In this work, different startup strategies for a SAN process are investigated by using Aspen Plus Dynamics. Due to the highly exothermic nature of this reaction, the startup operation needs carefully monitoring the temperature and pressure to maintain the system safety. In order to have better heat removal, two cooling mechanisms are used for this process. One is cold temperature feed stream; the other is through reactants and solvent vaporization to remove the reaction heat effectively by using a top condenser. This configuration is called auto-refrigerated reactor [Luyben, 1999].

After initiated by slowly heating the monomers to produce free radicals by the reactor jacket, the propagation reaction will take place for this process. However, the reaction rate will suddenly rise while the temperature over 100 ºC. This phenomenon means a lot of heat is released. If the temperature cannot handle well, the system will be out of control and leads to safety issues in the plant. However, if too much reaction heat is removed, the startup will fail to reach the self-accelerating and the reaction finally fades out. Therefore, the feeding time and the switch time for the control mode from manual to automatic are important during the startup period. From the current research, it is found that the time of reactor temperature reaches 140 ºC is the optimal operating point for continuous feeding and pressure controller switching to cascade mode. Compared with 130 ºC, it can increase SAN conversion more 10.2% and avoid excessive monomer to vaporize into the top condenser. Besides, the reactor pressure overshoot phenomenon can also be eliminated because of 18.2% more nitrogen discharging. With this operation, the result shows the overall startup period can be completed within 19.3 hours.

Keywords: Styrene-acrylonitrile resin, Startup, Auto-refrigerator

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Design of a PID controller with valve stiction

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Abstract

In the process industry, control performance may deteriorate due to oscillations generated by control valve stiction. Accordingly, control valve stiction becomes a factor that degrades the performance of the process units. If the stiction is confirmed, the control valve is repaired. This is often done during a scheduled plant shutdown maintenance every few years. Therefore, a suitable compensation method is expected to be used for reducing or eliminating oscillation until the scheduled maintenance.

Various methods to compensate for control valve stiction have already been proposed. The knocker method adds knocker pulse signals to the controller output to prevent process output oscillation. The two-move compensator was proposed by Srinivasan et al. [2008], and moves the valve twice in the opposite direction to maintain the valve at its steady-state position. Recently, Bacci di Capaci et al. [2018] has proposed incorporating the two-move compensator to the standard PID controller. As the controller retuning method does not use a compensator and does not require changing the control loop configuration, the implementation cost is low. Fang et al. [2016] proposed a retuning method using the time domain approach (TDA). The TDA method formulates the analytical relationship between PI control parameters and oscillation amplitude using the stiction model of He et al. [2007], and obtains PI control parameter values that reduce oscillation using robustness constraints on model uncertainty.

The contributions of this paper are as follows. First, we propose a mechanism for executing a simulation with a combination of a stiction model, a process model, and a PID controller, and assessing the control performance using the sampling data obtained as a result. Second, we propose a new quantitative stiction compensation method that uses this assessment mechanism to search for optimal control parameter values.

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Process Control of a Sour Water Stripper Utilizing Feed Condition Estimator and Minimum Heat Duty Model

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Abstract

Sustainable water utilization is an important issue to petroleum refining, which consumes as high as 0.34-0.47 L make-up water/L crude[1]. The realization of reducing water consumption depends on whether the water treatment can meet the stringent water quality requirement for reuse and can be operated with low energy consumption. Every oil refining generates sour water, which originates from delayed cokers, hydrotreaters, hydrocrackers, fluidized catalytic cracker and visbreaker fractionators. The sour water contains NH_3, H_2S, and possibly trace of CO_2. Steam-reboiler heated stripper is commonly employed in refinery plants for sour water treatment. As the sour water feed comes from multiple sources, the stripper operation always faces with frequent and fluctuated disturbances of feed conditions. The NH_3 concentration of stripped sour water is consequently affected, which can further cause the treated water must be diverted to the effluent water treatment plant. Becuse the compositon of both feed and stripped sour water are difficult to measure online, tight control of sour water stripper is a highly challenging task. Many studies have been focused on the alternative designs for energy saving[2,3] or data-driven soft sensor development[4], but the discussion on the control schemes and performance are limited. In this study, an estimator of feed composition and a model for minimum reboiler duty operation are developed. The former is based on easy measurement quantities, i.e. temperature, pH, and density, is developed. The later determines the minimum heat duty requied for given feed conditions. Control schemes utilizing these estimator and model, including feedback, feedforward, and feedforward-feedback, are developed and compared for the responses to the disturbances of feed flowrate, temperature, and composition.

Keywords: process control; sour water; soft sensor; optimization

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Data-based Digital Predictor Design for Processes Comprising Inverse Response

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Abstract

A process is said to exhibit inverse response if its initial response to an input change is in the direction opposite to its final steady state. Inverse response is exhibited by processes that have an odd number of RHP zeros (Vidyasagar, 1986) and is observed in a wide variety of chemical processes (Irshad and Ali, 2017). The presence of inverse response imposes certain inherent limitation on the bandwidth of a conventional feedback control system (Skogestad and Postlethwaite, 2007), which in turn has adverse effects on the achievable control performance. In order to alleviate the aforementioned limitations, methods inspired from the seminal work of Smith (1957) have been devised to compensate the effect of inverse response (Iinoya and Altpeter, 1962; Kashima et al., 2006; Alcántara et al., 2008; Mukherjee and Ghose, 2013). However, all these design methods are model-based and might be cumbersome to apply to complex chemical processes where identifying accurate models is not straightforward. Nonetheless, with the advent of modern technology and data acquisition techniques, we have better access to data and hence data-based controller design methods offer an attractive alternate to the conventional paradigms. Virtual Reference Feedback Tuning (VRFT) is one such data-based controller tuning method wherein tuning is carried out directly from plant data using a desired reference model to formulate an optimization problem (Campi et al., 2002). The VRFT method has been extensively applied to the design of feedback controllers because of its simplicity and hence is an attractive prospect for the data-based design of inverse response compensators. In this work, we extend the VRFT framework to the simultaneous design of a predictor and a feedback controller using a control architecture similar to Alcántara et al. (2008), who proposed a design method under the IMC framework wherein a predictor compensates the effect of the non-minimum phase parts of the plant and the modified plant dynamics is controlled via a PID controller. The design uses a second-order reference model discussed in our recent work (Kumar et al., 2020). To evaluate the performance of the proposed design, it has been first compared to the PID design for the inverse response process studied in Kumar et al. (2020). The simulation result shows that the proposed design can outperform the PID design, which substantiates the addition of the predictor in the control structure. Further, the proposed design has been compared to the design of Alcántara et al. (2008) and shows better performance. Lastly, for a more real application, the problem of concentration control for a desired product around the nominal operating conditions for the Van de Vusse reactor (Doyle et al., 1995) is considered. Simulation results show that the proposed model outperforms the model-based benchmark. Further, in order to test the robustness of the proposed design, it was tested on perturbed models and consistently provided better or comparable performance with respect to the benchmark.

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Yield Conversion Improvement for Continuous Stirred Tank Reactor System using Output Frequency Response Function-based Analysis

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Abstract

The periodic operation of a nonlinear system has a better conversion of the product than the steady-state operation. However, the periodic operation of a nonlinear system is hard to design as there is no analysis done in the chemical process control that can provide the analytical relationship between the output frequency response and the nonlinear parameters. Current analysis in chemical process control only provides a relationship between the input frequency response and the output frequency. In this research, we analyze and design a nonlinear nonisothermal Continuous Stirred Tank Reactor (CSTR) system using the Output Frequency Response Function (OFRF). The OFRF method reveals a significant link between the system output frequency response and the parameters that define the system nonlinearity [Lang, 1998]. An efficient method for determining the Output Frequency Response Function using Associated Linear Equations (ALEs) technique facilitates the OFRF determination [Nik Ibrahim, 2016]. Simulation studies demonstrate the effectiveness of the method. The OFRF-based analysis proves that the periodic operation of a nonlinear system improves the conversion of the product compared to the steady-state operation. Besides, this OFRF-based analysis shows the relationship between the nonlinear parameter and the output of the system. This nonlinear parameter and the output of the system relationship can be used as a basis for a better chemical process design.

Keywords: Nonisothermal CSTR; Mathematical modelling; Periodic Operation; Output Frequency Response Function; Associated Linear Equations.

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New PID Design Method for Under-damped Processes

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Abstract

Although PID controllers are widely implemented in the process industries, only a few PID tuning methods are specifically developed to overcome the oscillatory output response inherent dynamic systems. To design appropriate controllers for such processes, Smith (1957) proposed one design method using the Posicast Input Command Shaping (PICS) mechanism cascaded with the process to attenuate the oscillatory outputs. Vrancic and Oliveira (2012) had combined the PICS and Magnitude Optimum Multiple Integration (MOMI) to develop PID tuning method by removing oscillatory responses in open-loop dynamics tests and subsequently calculate the PID tuning parameters. Besides, several PID tuning methods capable of handling under-damped dynamics were also developed under Internal Model Control (IMC) framework by Revera et al. (1986), Chien and Fruehauf (1990) and Lee et al. (1998). Moreover, Wang et al. (1999) and Shen (2000) had proposed their respective tuning methods for PID controllers for under-damped processes. Although these two design procedures are more sophisticated than their counterparts, they fall short to deliver good control performances in a consistent manner as both methods are prone to give large overshoot and integrated absolute error. Lastly, it is noted that the performances of the aforementioned design method would degrade when they are applied to high-order oscillatory processes due to the modelling error.

To assess the performance of the proposed design method, the design methods by Rivera et al. (1986), Chien and Fruhauf (1990), and Lee et al. (1998) are selected as the benchmarks for most case studies investigated in the comparative study, while the design methods developed by Wang et al. (1999), Shen (2000), Vrancic and Oliveria (2012) are used only at certain examples due to their limitations. Simulation results show that the proposed method can achieve more satisfactory control performances as compared to benchmarks chosen in this study.

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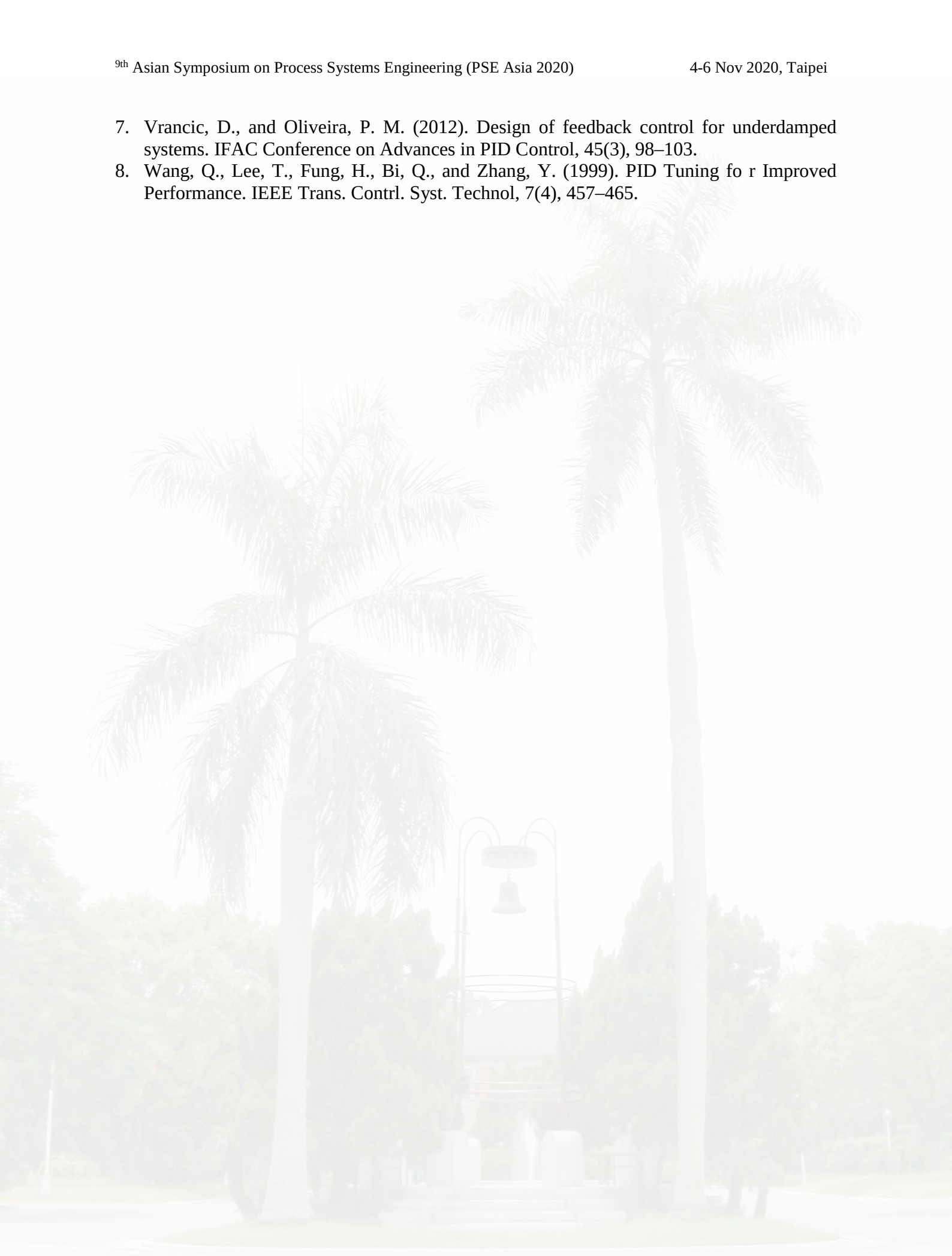

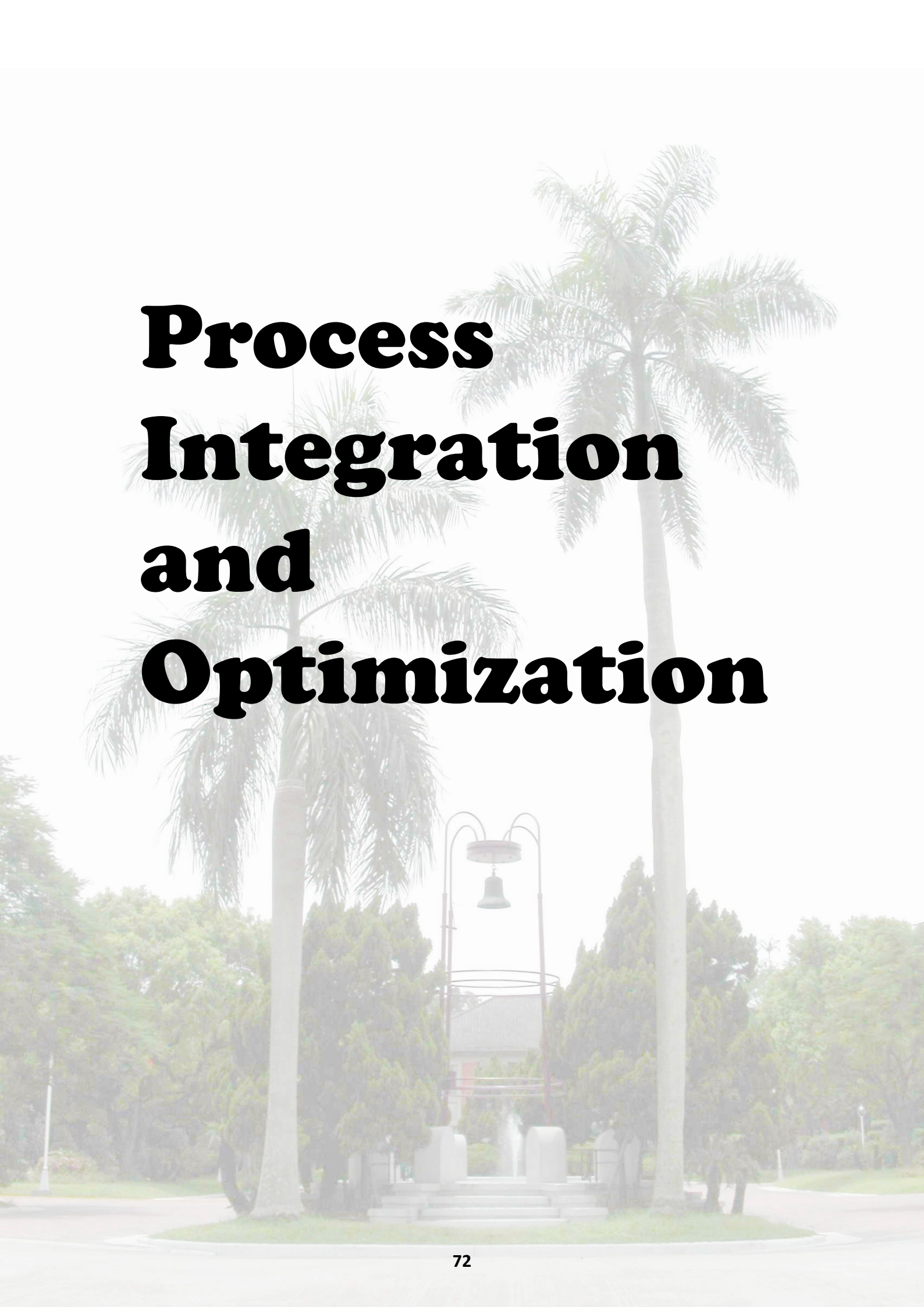

Process Integration and Optimization

Circulating cooling water system optimization under varying parameters

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Abstract

Circulating cooling water systems (CCWSs) are widely used in industries to remove waste heat from process and discharge it to environment. Currently, both design and retrofit problems of this system have attracted much attention due to the intensifying national environmental protection requirement. A general CCWS is composed of cooling towers, pumping systems and cooler networks. Among them, the arrangement and selection of the coolers in a cooler network will affect the amount of cooling water and the size of the pumps. Cooling towers and pump systems consume large amount of power, and their arrangement seriously affect energy consumption. Therefore, it is essential to optimize all the sub-systems to saving energy. The current research on this system mainly focused on the individual optimization design of each sub-system. In addition, most of these methods optimizing CCWSs under the condition that all parameters are deterministic. However, many parameters are constantly changing in authentic environments, which makes the original deterministic system sub-optimal or even unfeasible. Therefore, it is of great significance to consider the influence of changing parameters in CCWSs. The parameters with obvious changes are used to study the changing feature of the system. These parameters include the ambient temperature, air humidity and the electricity price with step changes. There are three problems to be solved on the basis of varying parameters mentioned above. One is to consider the impact of randomly varying uncertain parameters on the optimal system. The probability distribution function is used to describe the different uncertain parameters, the chance constrained programming method is used for modelling the complex system, and the simplified algorithm can be used to obtain the optimal reliable system. The second is to study the optimal design of CCWSs when multiple parameters show different periodic changes. Historical data is used to sum up the changing rules of periodic parameters, and study the different effects of multiple periodic parameters on CCWSs. When these parameters exist simultaneously and the changes are not synchronized, the impact of each parameter and their combined effect are all considered, and the optimal system configuration is also acquired. The third is to explore the methodology of retrofitting existing systems when periodically changing parameters exist. The solution is to find out the optimal start-stop combination of multiple devices in the system or work out the optimal arrangement of the system integrating with frequency converters. In this way, the best operation plan of the system is determined. By considering the optimization of CCWSs with varying parameters, the energy consumption can be significantly reduced and the reliability of the system can be increased.

The coupling integration of ORC and compression-absorption refrigeration system for cooling and power cogeneration

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Abstract

Organic Rankine cycle (ORC) and cascade-absorption cascade refrigeration system (CACRS) are both widely used energy-saving thermal systems as they are able to re-use waste heat to produce either power or low-temperature cooling energy. These systems were usually separately integrated within HENs and processes, however the coupling potential between them are seldom considered. On one hand, the heat source can drive the two systems in different manners (such as series, parrallel or series-parallel hybrid) considering the influence of heat source temperature on energy conversion efficiency. On the other hand, the driven relationship and energy exchange relationship between ORC turbine and CACRS compressor can be explored, so as that between ORC condenser and CACRS generator /evaporator, thus that can constitute a cogeneration system of cooling and power. To this end, a superstructure of the coupling system is proposed, in which different integration sequences between waste heat with CACRS and ORC are considered, and all coupling possibilities between ORC and CACRS are also included. Accordingly, a mixed-integer non-linear programming (MINLP) model aiming at minimum total annual cost (TAC) is formulated to implement the optimization-based design. In order to realize the automatic determination of working fluid and operating parameters, rather than selecting in the finite given operation scenarios, strict thermodynamic models of CACRS and ORC have been established and performed in the model, enabling a more comprehensive optimization. At last, cases are studied to illustrate the superiority of method, and the results have been compared with the basic scenario whose working fluids and integration structure are given before optimization.

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Rigorous Simulation and Techno-Economic Analysis of a Bio-Jet-Fuel Intermediate Production Process with Various Integration Strategies

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Abstract

In this paper, we firstly report on the different scenarios of the process integration to produce jet-fuel intermediates from biomass. Rigorous process simulation, optimization techno-economical evaluation, and carbon emission calculation are performed. We start from the aldol condensation process converting furfural and acetone to the jet-fuel intermediate. COSMO-SAC model and the PR+COSMOSAC equation of state (EOS) are firstly incorporated to estimate the missing physical properties of both pure component and the mixture. In this part, three process schemes (the distillation-only process, the multi-effect evaporation (MEE) assisted process, and the solvent-less process) are investigated, and the total annual cost (TAC) are compared. Comparing with the distillation-only process, the optimization results indicate a more favorable condition in the solvent-less process (89.76% TAC reduction) than the MEE-assisted process (25.54% TAC reduction). Moreover, different strategies of integrating the aldol condensation process with the front-end furfural production process are discussed. They are presented in five Scenarios. YUMC (yearly unit manufacture cost) and ER (emission ratio) are calculated to quantify the economic performance and CO2 emission. Through this work, we suggest that the Scenario 4 (YUMC=0.716 USD/kg, ER= -1.65) would be the most suitable one for CO_2 reduction in the future, and the Scenario 2 (YUMC=0.698 USD/kg, ER=0.28) could be the nearest solution to enhance the economic performance and reducing CO_2 emission based on the current technology.).

A superstructure based approach to work exchange networks synthesis

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Abstract

In the development of energy integration, there are many good developments in the heat exchange networks (HENs). However, there has been relatively little research on work exchange networks (WENs), and it is difficult to implement these achievements in industrial process.

Although the WEN is analogous to the HEN, it is quite different in terms of exchange equipment. We only need to consider heat exchangers, heaters, and coolers for HEN. Instead, pressure manipulating equipment can be classified into direct and indirect devices in the WEN and each of them has its advantages and disadvantages. Therefore, a well-designed WEN needs to pay attention not only to itself, but the choice of equipment is very significant to the performance. Additionally, the most assumption is impractical which may affect the realistic application of WENs [1]. We can address these issues through the superstructure approach.

Therefore, in this study, we propose a superstructure model that aims for avoiding phase change and utilizing rigorous thermodynamics relation to improve the current WEN and take the minimum total annualized cost (TAC) as our objective. For mathematical programming, the superstructure model is formulated into a mixed-integer nonlinear programming (MINLP) problem by utilizing GAMS to solve it. It is expected to get the model close to the actual conditions. Furthermore, we demonstrate the benefits of an optimized network via a case study about the Liquefied Natural Gas (LNG) process. In addition, the efficiency of pressure manipulating equipment as a function of operating conditions will be incorporated. Consequently, the flexibility index of the WEN configuration will also be considered to estimate the tolerance of the optimal design [2].

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Keywords: Mathematical programming, Process optimization, Work exchange network, Energy integration, Process synthesis

Optimal Design, Operation, and Scheduling of Membrane Cleaning for Stand-Alone Hybrid Membrane Osmosis Desalination Systems

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Abstract

Potable water and energy are gradually insufficient for human needs. To exploit sustainable resources, membrane related technologies have been developed to desalinate seawater and produce power using salinity gradient. Reverse osmosis (RO) is one of the major technologies for seawater desalination, while pressure retarded osmosis (PRO) is a promising technology for power generation. The RO desalination plant has the problems of extensive energy consumption and brine discharge, which can be alleviated by hybridizing the RO process with the PRO process as an integrated RO/PRO system. This study is to pursue a higher goal, that is, the power generated by the PRO unit can provide the energy consumption required for the entire hybrid system. Namely, the hybrid membrane osmosis system can achieve stand-alone operation (without external energy supply) for seawater desalination. In this paper, optimization of the design, operation, and scheduling of membrane cleaning/replacement for the stand-alone hybrid membrane osmosis desalination systems is presented.

Two configurations for the hybrid membrane osmosis desalination systems (i.e., RO-PRO and PRO-RO systems) are considered and compared. First, optimal system design for the hybrid systems under stand-alone operation is obtained through minimizing the specific total membrane area requirement. The result shows that PRO-RO system outperforms RO-PRO system. However, operation of the membrane osmosis process is bound to be affected by membrane fouling. This study explores the effect of membrane fouling on system energy and water production efficiency, and proposes a dynamic adjustment strategy of operational variables (applied pressure in RO and PRO) to cope with the fouling effects. The optimal operating strategy is obtained by maximizing the water production while maintaining stand-alone operation of the system in a period of time between membrane cleaning (replacement). It is found that, with a constraint of RO permeate purity, stand-alone operation becomes infeasible for the RO-PRO system under membrane fouling condition. Finally, the optimal scheduling of membrane cleaning and replacement for the PRO-RO system is proposed to maximize the profit of water production during the entire membrane lifetime. Simulation studies are presented to demonstrate the effectiveness of the proposed optimization model and the results of optimization are discussed.

Malaysian palm kernel shell (PKS) for biomass-power generation in Japan considering environmental feasibility of PKS life cycle

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Abstract

Japan has been relied on imported biomass for power generation over the years to reduce CO_2 emissions in power generation sector. Palm kernel shell (PKS) is one of main renewable energy sources that import from Indonesia and Malaysia. PKS is a solid biomass which is a by-product during the crude palm oil extraction from fresh fruit bunches at palm oil mills (POM). Japan is a major PKS importer with 1.27 Mt in 2018 which is 68% of total PKS exports [Strauss and Kusano, 2019]. To identify the sustainability of PKS as the major sustainable energy source for Japan, its life cycle needs to be studied to determine the environmental impacts. The scope of this study covers the life cycle of PKS from the initial land use change (LUC) for oil palm cultivation in Malaysia to the utilization of PKS for biomass-power generation in Japan. Greenhouse gas (GHG) emission, eutrophication and water footprint (WF) analyses were performed to evaluate the degree of environmental impact. The objective of this work is to recognize the environmental viability of the PKS in enhancing the sustainability of power generation industry in Japan. Evaluations were conducted with consideration of four types of LUC, four boiler fuel applications in POM, two palm oil mill effluent (POME) treatment schemes, two PKS transportation distance schemes and two biomass-power generation scales. Information on PKS life cycle stages including LUC, land preparation, cultivation, fertilizer applications, POM operation, waste generation and applications, domestic and international transportation and biomass-power generation process were gathered. Supplementary data were gathered from published databases and articles. From the analysis, it is found that LUC contributed heavily in GHG emission. Meanwhile, POME treatment contributes significantly to GHG emission, eutrophication and WF outcomes. The environmental-related findings in the PKS life cycle stages identified in this study will guide on achieving sustainability in the PKS application as a biomass-power generating resource for Japan and other potential countries.

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Structural Optimization of Reverse Osmosis Desalination Powered by Solar and Pressure Retarded Osmosis

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Abstract

Growing fresh water demands have led to the rapid development of global desalination technologies [Ahmed et al., 2019]. Reverse osmosis (RO) is one of the major membrane technologies for desalination, pressure retarded osmosis (PRO) is a technology genarate power by salt gradients. Therefore, the hybridization of RO and PRO framework enables the build of dual-purpose power and desalination plants. However, desalination usually have high energy comsumption that provided by fossil fuels. The emissions of greenhouse gases which is caused by fossil fuels bring about severe environmental impact. Therefore, it becomes important to find a clean sources of energy for desalination. Renewable sources is a possible way to generate clean energy such as sunlight, wind, hydroelectric energy. Photovoltaic (PV) technology is used to convert solar energy from photons as electricity. PV systems usually require batteries to store energy because of its intermittent nature. There were lots of research about the design and operation of PV/RO integrated system [Kumarasamy and Narasimhan, 2015]. In this study, optimal design of PV/RO/PRO integrated system for seawater desalination without requiring external energy supply is conducted. The optimization problem for synthesizing the integrated system is formulated as a mixed integer nonlinear program (MINLP) to determine the equipment scale and operating conditions. The results shows that the proposed integrated system is effective for stable operation of seawater desalination.

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Near-analytical optimization of seeded batch crystallization processes using optimal control theory

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Abstract

In this work seeded batch crystallization processes are modeled using the standard method of moments and dynamic optimization problems are solved with growth rate as continuous decision variable under constraints on batch time, seed-grown volume, and admissible range of growth rate. Frameworks for applying optimal control theory, developed by Hofmann and coworkers [Hofmann and Raisch, 2010; Bajcinca and Hofmann, 2011], are used to provide nearly-analytical solution to the optimization problems in a computationally efficient way.

Six single objective functions are considered for optimizing crystallization systems with only one internal property coordinate. Pareto-optimal fronts for several sets of two single objective are plotted to analyze trade-offs between objective functions. Results suggest that the trade-off between objective functions based on lower moments (e.g. number mean size) and higher moments (e.g. volume mean size) are more significant. For these cases, a constant growth rate trajectory represents a good compromise between two objectives [Tseng et al., 2019].

For optimization of crystallization systems with two internal property coordinates, aspect ratio, nucleated number, and nucleated volume are considered to be objective functions. Results shows that control strategies for inhibiting nucleated number and volume are similar to those for single-dimensional cases while the batch time constraint might not be active due to an additional constraint on the aspect ratio. Furthermore, the achievable aspect ratio range is narrow if only a single growth stage is applied and another method such as temperature cycling is required to effectively manipulate crystal shape [Eisenschmidt et al., 2016].

The crystallization models considered in this work are relatively simple: Growth and nucletion kinetics are assumed to be temperature and size-independent and crystal aggregation as well as breakage are also neglected. However, the results can still provide insight to optimization of single and multiple dimensional crystallization systems.

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Negative Emissions Technologies for Carbon-constrained Energy Planning

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Abstract

Climate change has been threatening mankind with record-breaking temperatures, intense hurricanes, wildfires, longer draughts, melting of ice caps, etc. Primarily caused by high concentration of greenhouse gases (GHGs) such as carbon dioxide (CO_2), methane (CH_4), etc. within the atmosphere, these impacts would only worsen in the upcoming decade if no mitigation actions are taken immediately. As a result, 195 countries came together to legally adapt a global climate deal or famously known as the Paris Climate Agreement in December 2015. This agreement aimed at limiting the rise of the average global temperature by 2°C relative to the preindustrial levels, while pursuing efforts to limit the rise of temperature by 1.5°C. Present efforts include the integration of renewable energy (e.g. wind, solar) into existing power plants, imposing carbon tax, utilising biofuels from organic waste, re-forestation etc. Unfortunately, despite all these efforts, most countries are still far off from achieving the target set by the Paris Agreement. Therefore, more aggressive actions are required if the impacts of climate change are to be curbed. One such action is to utilise *Negative Emission Technology* (NET).

NET removes historical emissions of GHG, specifically CO_2 from the atmosphere. Additionally, NET could also be used to remove CO_2 from industries where limiting CO_2 emissions is almost impossible such as transport and agricultural sectors. NET is relatively a new technology with limited commercial applications. Some reported NET techniques include direct air capture (DAC), augmented ocean disposal, biochar, bioenergy with carbon capture and storage (BECCS), etc. Among these, BECCS promises great potential due to the present of biomass power plants globally alongside continuous enhancement of *carbon capture and storage* (CCS) techniques [Mcglashan et al., 2012].

This paper addresses the integration of NET for *carbon-constrained energy planning* (CCEP) via *process integration* methods. Graphical and automated targeting methods serve as supplementary role in setting various targets for the CCEP scenarios, and identify trade-off in implementing NET and CCS technologies.

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Synthesis of Heat Integrated Water Regeneration Network with Optimum Process/Regeneration Temperatures

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Abstract

The efficient utilizations of both energy and water are extremely important to achieve sustainability in process industries. In most applications, the consumption of energy and water is intertwined. To conserve energy and water simultaneously, a process integration technique, involving the synthesis of heat integrated water regeneration networks (HIWRNs), can be employed. HIWRNs offer a framework to simultaneously optimize water consumption through reuse, recycle, and regeneration and energy consumption through heat integration between the water streams.

From the recent review on HIWRN synthesis [Kermani et al., 2018], process parameters considered for the optimization are identified as flow rate, contaminant concentration, and temperature. To save more energy, some process and regeneration temperatures can further be optimized. The temperatures can be maintained within a specified range, avoiding any drastic change in the overall operation and production. Kamat et al. [2018] developed a mixed integer non-linear programming model for the synthesis of HIWRNs with variable regeneration temperature, but it was restricted to isothermal mixing of streams. As non-isothermally mixed streams are known to reduce the thermal energy consumption as well as the heat exchanger area, an extended model is proposed to account for the non-isothermal mixing.

This paper proposes an optimization formulation of HIWRNs incorporating non-isothermal mixing and variable process as well as regeneration temperatures. The superstructure based formulation is developed based on the principles of Pinch Analysis. The applicability of the proposed formulation in synthesizing HIWRN is demonstrated through an illustrative example. The proposed formulation reduces a large amount of energy consumption by optimizing the process and regeneration temperatures and thereby reducing the operating costs within the industry. Due to its compactness and capability to handle variable temperatures easily, the proposed heat integration model can be extended towards flexible HIWRNs in the future.

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Pinch Analysis approach for multi-objective segregated targeting problems with common resources

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Abstract

Conservation of different resources is the most important step towards overall sustainable development. Optimization of different source-sink allocation networks can help in resource management. Pinch Analysis has evolved over the years to address resource conservations in various types of resource allocation networks (RANs). Segregated targeting problems are a special kind of structurally different, but mathematically challenging, RANs which consists of multiple sets of demands called zones and a set of common internal sources. Each zone has a dedicated resource associated with it which satisfies the demands present in that zone only. Whereas, internal sources are not zone-specific and can satisfy the demands of all the zones. These problems can be observed in interplant water integration networks, carbon-constrained energy sector planning, and integrated iron and steel mill, etc. Bandyopadhyay et al. (2010) and Chandrayan and Bandyopadhyay (2014) developed algorithms using Pinch Analysis approach to address these problems for resource and cost optimality. However, for a better and informed decision making towards achieving sustainable development, it is important to consider multiple objectives. Therefore, Jain and Bandyopadhyay (2019) applied Pinch Analysis to optimize these problems for multiple objectives. However, in industrial practices, there may exist some common resources with the potential to further optimize segregated targeting problems for different objectives. For example, the introduction of common resources can reduce the cost of otherwise segregated targeting problems. In this work, a mathematically rigorous methodology is developed to optimize the segregated targeting problems with common resources for multiple objectives. The concept of the weighted sum method together with the Pinch Analysis is applied to combine multiple objectives into a single objective function and determining the Pareto-optimal front for the problem. A novel concept of extended multi-objective prioritized cost is introduced to obtain the Pareto-optimal front. The proposed approach is generic in nature and is demonstrated through an illustrative example from the water allocation network.

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Scheduling for Multipurpose Batch Processes-A Fuzzy Optimization Approach

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Abstract

The aim of this paper is to develop an optimal schedule for multiproduct and multipurpose batch processes using parameter flexibilities, dealt using concepts from fuzzy set theory. The formulation is based on a continuous-time representation and decoupling of the task events from the unit events for multipurpose batch processes. A multiobjective optimization; mixed-integer non-linear programming (MINLP) formulation is proposed to target and satisfy uncertain demand, exceeding from its minimum predetermined value and to trade-off it with maximum profit. This formulation also includes resource minimization constraints calculated on the basis of an optimal schedule. The solution derived from the proposed formulation satisfies the decision maker's desirable achievement level of the profit, excess production in order to satisfy uncertain demand under the desirable possible level of fuzzy demand. It is an effective decision tool since it can reflect the relative importance of each fuzzy component.

Multi-objective optimization of an energy system and its reliability

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Abstract

An energy system is one of the fundamental components in an industrial process. The continuous operation of an industrial process is largely dependent on both the reliability and efficient performance of an energy system to meet the production demands and achieve optimum production targets. Several papers have been presented to discuss emerging mathematical models in the design of an energy system in optimizing the cost and reliability. However, these models consider a specified system reliability and optimize the cost and reliability independently. Hence, this paper presents a multi-objective optimization (MOO) model to concurrently optimize the design and reliability of an energy system based on process unit function, its selection and operating capacity. This model utilizes input-output modelling and linearized parallel system reliability expression to determine the optimal solution. The two objective functions used in the model are the total annualized cost, which accounts for the capital, operating cost as well as the cost of the raw materials required, and the reliability of the system to perform its function. The total annualized cost is minimized while the system reliability is maximized using the linearized parallel system reliability expression. The reliability of individual component process units is assumed to be a function of the ratio of rated capacity to design load. The model determines the required equipment and capacity to satisfy the two objectives. There are two case studies presented to demonstrate the proposed model; both cases involve a polygeneration system where the first case study focuses on its function to produce heat while the second case study focuses on the system's function to produce cooling. These case studies illustrate how the proposed multi-objective optimization model is utilized to design an energy system with minimized cost and maximized reliability.

Keywords: Chemical engineering, Multi-objective optimization, Energy system, Reliability

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Heat integration design of alpha methyl ester sulfonate production process

9th Asian Symposium on Process Systems Engineering

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Abstract

Alpha-methyl ester sulfonate is made from bio-renewable resource, It is the good properties of surfactant when compare to Petroleum-based surfactant such as sodium dodecylbenzenesulfonate, sodium lauryl ether sulfate and sodium dodecyl sulfate. This project studied the simulation of alpha-methyl ester sulfonate process and optimization process condition of heat recovery not effect to properties of the product, because of the production process of alpha-methyl ester sulfonate used high-temperature conditions and very complicated reactions. Therefore, Developed of process for simulation using Aspen Plus to improving efficiency of the heat transfer process and equipment and pre-feasibility study heat exchanger network. In process simulation for investigating the operating condition, area of heat transfer, the efficiency of the heat transfer process and feasibility of investment with various type of cooling, flowrate of sulfur, flow of air dilution. In this simulation can be predicted of properties of alpha methyl ester sulfonate, process condition and heat recovery of each condition, heat transfer process can be used in apply heat exchanger network to minimize energy consumption can reduce the area of heat exchanger 5 % from the normal process, 10% to reduce the cost of alpha-methyl sulfonate production and worth the investment for improvement in the heat transfer process in the alpha-methyl sulfonate process production.

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Microalgae biofuel supply chain optimization under weather uncertainty

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Abstract

Microalgae biofuel is regarded as a promising renewable energy feedstock. Wastewater treatment integrated microalgae cultivation is known as promising strategy for increasing the sustainability of microalgae biofuel production systems. By such a system, municipal, agricultural and industrial wastewater can be used to supply nutrient for the cultivation of microalgae and circulation of the nutrients elements can be possible. A microalgae integrated with wastewater system needs wastewater resources, and the microalgae biofuel products need procurement orders from downstream customers, and a effective supply chain is badly needed, and a challenge is that the supply chain is subject to uncertainty. Uncertainties from the market demand, inventory, and transportation have been addressed extensively in previous work. However, as a bioprocess, the wastewater-based microalgae biofuel supply chain is affected strongly by weather uncertainty. The weather has effect on the transportation and other aspects for a supply chain as well. Nevertheless, previous studies have barely discussed the weather uncertainty in the logistics network, which decreases the reliability of the reported supply chain analysis. To overcome the above-mentioned drawbacks, an analysis approach for optimization of microalgal biofuel supply chain under weather uncertainty is proposed and solved in the present work. The supply chain in this work was composed of three parts: supplier, facility, and customer. We assume that suppliers are located in the regions where cultivation conditions for microalgae growth is satisfied by the probability of the weather condition. Facilities refers to biofuel refineries to produce final microalgal biofuel products and are limited by maximum yield. Costumers purchase final biofuel products from different facilities and, in permission of supplementary procurement, from external market when the demand of customers could not be satisfied. The optimization of the proposed supply chain under weather uncertainty is formulated as a mixed-integer non-linear programming (MINLP) problem to determine strategical decisions variables. The problem of the supply chain optimization with the weather uncertainty is solved by stochastic optimization method. The optimization results showed that the weather uncertainty has the significant influence on the suppliers. Cost of suppliers suffer the mostly from the weather uncertainty and may restrict the performance of the entire supply chain.

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Utilization of Process Network Synthesis and Machine Learning as Decision Making Tools for Municipal Solid Waste Management

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Abstract

This paper introduces the utilization of two different optimization models as a decision-making tool for municipal solid waste management (MSWM). This study aims to provide a framework of decision making in managing municipal solid waste (MSW) in Malaysia and demonstrating the potential of the function model for decision-making tool. Process network synthesis (PNS) used as a first optimization model for the generation of feasible pathway MSW conversion technologies. A standard data mining technique using machine learning (ML) was applied for a simple case study of MSWM. Data were divided with a ratio of 90:10 for training and testing data and further analysis using different model functions. The model functions involved are; linear regression, multilayer perceptron neural network (MLP) and sequential minimal optimization regression (SMO reg). The linear regression function provides a better correlation coefficient compared to other models; 0.5894. The correlation coefficient for testing data slightly increases. The MLP model improved its correlation coefficient when inputting the testing dataset. The MLP model correlation coefficient reached 0.7169 compared to the linear regression function. Therefore, this case study used the MLP model as a basis. Results showed that both integrations of optimization models could be successfully used as a basis in waste management decision-making tools with good performance. The decision-making tool provides a faster and efficient way for the user and stakeholder to manage MSW. The framework of developing a decision-making tool for MSWM can be utilized to achieve better management of MSW.

Keywords: Decision-making tool; municipal solid waste management; process network synthesis; machine learning;

Process Systems Engineering (PSE) Applications In Semiconductor Manufacturing: Contact Pad Structure Design

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Abstract

NAND flash memory is evolving from planer to vertical structure due to the scaling limitation of planar cell. An increase of chip density can be achieved through increasing the number of stacking gate structure instead of the conventional unit cell shrink. Obviously, the more layers can be realized, the lower should be the overall cost. However, the first technology challenge in 3D structures is related to how accessing NAND strings. Specifically, the connection to each layer is the key step that has an impact on the array efficiency. Several architectures have been proposed for a decade in the technical symposiums. The main contributors have been Toshiba [Tanaka et al., 2007], Samsung [Kim et al., 2009] and Macronix [Chen et al., 2012] amongst the memory companies. Developing a new structure is usually a difficult problem due to the complexity. In this paper, a systematic approach based on PSE methodology is proposed. A novel superstructure is developed for the design of contact pad structure, which consists of source, location, and demand. A mixed-integer linear programming (MILP) model is formulated accordingly to minimize the number of lithography steps. Case studies are presented to demonstrate the applicability and significant economic benefits when applied to industrial problems. With the proposed model, the optimal contact pad structure (staircase) can be synthesized and fabricating flow can be determined, as well as a great benefit to evaluating next-generation products can be fulfilled.

Keywords: NAND flash memory, planer, vertical structure, superstructure, MILP

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Process Monitoring and Safety

Gated Recurrent Unit Applied to Fault Diagnosis in Chemical process

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Abstract

Recurrent Neural Networks (RNN) have been widely used in Fault diagnosis. In this study, the Tennessee Eastman process (TEP) was employed as a case study to investigate the performances for the fault diagnosis with RNN, LSTM, and GRU. The gate functions of GRU and LSTM were investigated to show gate function mechanisms and prove why the GRU had the best classification performance. The results showed that the average accuracy of GRU was up to 95.9%. For the hardest classified fault type, GRU can have 76% accuracy which was higher 15% than LSTM.

In the gate investigations, the forget gate of LSTM was always truing on that showed the no functions in the classification. Furthermore, it might affect the accuracy of the classification. While the gates of GRU had significant and frequent actions to filter the fault features. Hence, GRU can obtain the highest accuracy of the classification in this study.

Keywords: Tennessee Eastman process, Gated Recurrent Unit, Recurrent Neuron Network, Fault diagnosis, Gate function

Indoor air quality monitoring in an underground transportation facility using variational convolutional autoencoders-driven anomaly detection and sensor reconciliation

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Abstract

Reliability of the indoor air quality (IAQ) sensors play an important role in the ventilation system control in underground transportation facilities, influencing over crucial factors as ventilation energy consumption and commuters' health since faulty sensors may result in misinterpreting the IAQ conditions and mistreating the air delivery rate [Loy-Benitez et al., 2020]. Given the IAQ data properties of dynamism and non-Gaussianity, linear and fixed models are not sufficient to extract essential features from the multivariate IAQ data [Kim et al., 2014]. The intrinsic properties of the data allow a correct process monitoring; therefore, the present study introduces a novel IAQ monitoring framework based on variational convolutional autoencoders (VAE-CNN). The proposed methodology is divided into three parts. First, the VAE-CNN model is trained by utilizing nine IAQ sensor measurements in normal conditions. Then, the confidence limit for anomaly detection is computed by the Kernel density estimator (KDE), and the model parameters are obtained by the variational lower bound (ELBO) maximization. Second, artificial failures are introduced into a validation dataset for testing the VAE-CNN. Finally, the proposed method is evaluated through its detection capability and reconciliation performance against other methods. The proposed method showed superiority compared to typical statistical methods for anomaly detection and reconciliation assessment.

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Fence line monitoring system optimization for detecting toxic gas considering spatio-temporal risk using gas detectors

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The risk management about hazardous chemicals is getting important with the increment of the number of chemical plants that are close to vulnerable areas such as schools, hospitals, residences. Among accidents, chemical leak accidents are classified as a major industrial accident that can cause damage to areas near the workplace [Kim, 2018]. If the type of leaked gas is a toxic gas, damage of leak accident will increase steeply. To reduce the risk of these plants, fenceline monitoring is proposed. The purpose of fenceline monitoring is to provide air quality information to communities so that it makes them do proper action when an accident occurs in the plant. In the fenceline sampling location(s) and coverage, which is one of the key considerations of the fenceline monitoring system, required 4 factors as followed[South coast AQMD, 2017].

1. Local meteorological condition,
2. Topography,
3. Pollutant hotspot,
4. Spatial coverage of monitors.

In spatial coverage of monitors, It requires the fenceline monitoring system should be designed to ensure adequate coverage of the area along the facility perimeter. In terms of sampling locations, it just suggests a few guidelines and there is no specific guide about detector placement.

In this study, we proposed a fenceline monitoring system which meets 4 factors and focus on minimizing the risk of the residential area through optimal detector placement on the fence line with 3 steps. In the first step, we generate leak accident scenarios data using computational fluid dynamics(CFD) simulator and local meteorological condition, topography, pollutant hotspot data to conduct detector placement optimization. Concentration of each point and leakage area data which are time-variant are extracted from leak accident simulation. In the second step, we define the risk as a function of the damaged population of surroundings from leak scenario and scenario frequency. We calculate the damaged population using population density and leakage area data from the simulations. At the last step, we design mixed-integer linear programming(MILP) to minimize the risk which is precomputed in the previous step. We use W_s term to allocate weight to scenarios that are expected to lead to serious damage.

To test the proposed method, we conduct a case study. The target plant is located in Yeosu industrial complex and surrounded by other facilities. The detector placement is affected by the risk of outside and changed by population density. It is proven that the proposed method would be useful and applicable for chemical plants and highly recommend to use for monitoring plants with high risk

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Data Visualization and Fault Detection of Chemical Process Using UMAP

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Abstract

Visualizing high-dimensional process data into a human-readable dimension can give a better comprehension of the status of the process and bring improvement in product quality and operational safety [Chiang, 2001]. This study introduces uniform manifold approximation and projection (UMAP) to visualize process data and detect process abnormalities. UMAP is a manifold-learning based dimension reduction method that is known to capture primary intrinsic variables to characterize the data variation and preserve both local and global structure of the data [Becht, 2019; Dorrity, 2020; McInnes, 2018]. Comparing the quantitative and qualitative aspects between UMAP and conventional nonlinear dimensionality reduction methods such as kernel principal component analysis (KPCA) [Shao, 2009] and t-distributed stochastic neighbor embedding (t-SNE) [Zhu, 2018], we find that UMAP gives a better representation of the data in two-dimensional space. Benchmark dataset used in this work has been generated through the simulation of Tenneessee Eastman process under three different abnormal scenarios.

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Continuous Wavelet Transform with Neural Network for the Monitoring Chemical Process

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Abstract

Fault detection and diagnosis (FDD) play an inportant role in the monitoring chemical process. Hence, numerous researches of fault detection and diagnosis have been conducted until now. One of main issues of process monitoring is the nonlinearity. Fault detection method which assume that process data is linear will be inaccurate. Another important issue is dynamic behavior of the process.

This work proposes an novel FDD method using continuous wavelet transform (CWT) and convolution neural network (CNN). CWT produces time-frequency domain information from an original time series data2.. CWT is appropriate to handle nonsteady time series data such as chemical process data. We use time-frequency spectra generated by CWT as input data for CNN. The proposed FDD method is applied to a benchmark process and verified the perfomance.

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Verification of ART-based Supervised Data Clustering Using Plant Simulation Data

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Abstract

In order to maintain efficient operation of industrial plants, various methods have been proposed to monitor key performance indicators (KPIs) [Kano, 2004]. We previously proposed a system for evaluating the performance of industrial plants. The system consists of a supervised data-clustering function and a visualization function for clustered results [Hori *et al*., 2019]. The supervised data-clustering technology is based on the ART2 network, one of the adaptive resonance theory (ART) networks, and can correlate plant operational data to the KPI by classifying the operational data. The visualization function uses a 3D graph to illustrate the relation between operational data and the KPI. The z-axis indicates the KPI, and an x-y plane showing the gravity centers of the categories are mapped by multidimensional scaling (MDS). We showed that the system models and visualizes the relation between categories and KPIs on a 3D graph using test data. However, the data was two dimensional, and the system had not been tested using plant operational data.

In the present study, we examined whether the system can be used to analyze plant operational data using the Tennessee Eastman process data. In particular, we chose operational cost as the KPI and selected data sets with a fluctuating KPI caused by disturbances [Downs *et al*., 1993]. The supervised data-clustering function learned the relationship between the KPI and operational data, and the relationship was illustrated using the visualization function.

The operational data were classified into categories with respect to the KPI of the data. The visualization function indicated an area containing high KPI categories, which are categories containing operational data with a high KPI, and an area of low KPI categories. Comparing the patterns of the high and low KPI categories enabled us to extract the factors that affected the KPI. The results described above demonstrate that the proposed system can be used to monitor and maintain the performance of industrial plants.

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CFD-based analysis of the effect on adjacent pipes in the event of pipe accident

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Abstract

Pipeline is an important asset for transportation of fluids, but there are many aged pipes without proper maintenance or replacement. In particular, various accidents occur every year because it is difficult to manage underground pipes that are invisible until an accident occurs or scheduled maintenance is carried out. There are two main quantitative ways to manage these underground pipelines. The first is a statistical approach, which uses historical data to statistically determine the probability of failure. The second is a stochastic approach, which uses probability distribution to stochastically quantify the probability of failure. [C-FER, 2001] [CSA, 2007] However, these methods only indicate the probability that a fault or event, such as corrosion or equipment impact, will lead to a failure of a pipeline, but do not show the effect on the adjacent pipe in the event of a failure. Therefore, in this study, the behavior of the fluid emitted in the event of a pipe rupture was analyzed using CFD, and the amount of impact applied to the adjacent pipe was analyzed. In addition, the case study was conducted depending on the operating pressure, the transport fluid, and the distance between the pipes.

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Optimal Design and Maintenance Strategies of Multi Layer Standby Mechanisms in Continuous Chemical Processes

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Abstract

Each critical unit in steady state processes must always function properly, and a standby mechanism is usually installed to ensure uninterrupted operation. It is also assumed that the load of this standby mechanism does not vary significantly with time, but the critical unit may fail after a long period of operation. The goal of this research is to construct a general mathematical model that can be used to design a multi layer standby structure and the corresponding maintenance policies for any process in order to minimize the total expected lifecycle expenditure. The optimization runs have been carried out with a MATLAB code developed based on genetic algorithm. The effectiveness of the proposed method has been demonstrated by constructing the standby mechanism for pump system in a typical chemical plant, One can obtain the optimal design and maintenance specifications of the multi layer standby mechanism from the optimum solution, which includes (1) the number of layers, (2) the corresponding voting gate logic in each channel, (3) the numbers of both online and spare sensors in each measurement channel, (4) the number of spares for online switch, (5) the inspection interval of online switch, (6) the inspection intervals for warm standbys, and (7) the number of cold standbys.

Nonlinear Dynamic Processes Monitoring using Kernel CVA with Automatic Relevance Determination

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Abstract

The use of kernel methods to address the nonlinear issue in multivariate statistical process monitoring is currently an active area of research [Pilario, 2020a]. Although it is known that kernel design can greatly influence the detection performance, there is still much to be done to improve this aspect. Previous work has shown that mixed kernel designs are promising for incipient fault detection [Pilario, 2019], while deepening the kernel design can improve feature extraction [Deng, 2019]. However, the radial basis function (RBF) kernels used in these works have a single kernel width value, shared in all dimensions of the data set.

In this work, we utilize the concept of automatic relevance determination (ARD) in the RBF kernel design and incorporate them to kernel canonical variate analysis (kernel CVA) to improve fault detection performance. ARD kernels are more commonly used in Gaussian process models but have not been previously applied to nonlinear dynamic process monitoring, to the best of our knowledge. Our most recent work has already shown how ARD can enhance kernel subspace state-space models for system identification [Pilario, 2020b]. The idea is to allow varying kernel widths in each dimension of the RBF kernel during the feature extraction step. These kernel widths are tuned by cross-validation via random search. Hence, smaller kernel widths are given to process variables that are deemed more relevant to the detection model. In this paper, the same concept is applied to statistical process monitoring. To demonstrate the improvements, a continuous stirred-tank reactor (CSTR) and an industrial evaporator system are used as case studies. Results show that kernel CVA with ARD achieves higher detection rates and lower false alarm rates compared to CVA and naïve kernel CVA detection models.

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Infrared Thermography-Based Statistical Process Control for Defect Detection in Vaccum-Assisted Resin Transfer Molding

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Abstract

Vacuum-assisted resin transfer molding (VARTM) is a promising technology of polymer processing, which has been widely used to produce low-cost, lightweight, and high-strength composite parts. Althuogh some nondestructive testing methods have been adopted for the inspection of the VARTM products, research on real-time defect detection during the manufacturing is limited. In this study, an online monitoring strategy based on infrared thermography and statistical process control was proposed. In detail, the VARTM infusion process is recorded by both a visible light camera and a thermal imager. The visible light camera captures the resin flow fronts from the top view, while the thermal imager, i.e. the infrared camera, reflects more information of the subsurface resin flow. If there is no significant subsurface defect occurring during the manufacturing, the flow fronts detected by both cameras are usually coincident. Otherwise, significant mismatches between the images taken by these two cameras are observed. Herein, the difference between the visible and thermal images is quantified by a series of image processing steps, including thermal and visible image registration, image binarization, noise reduction, etc. Then, a statistical process control chart is desighed to monitor such difference. In such a way, the subsurface defects can be detected during the manufacturing, providing opportunities for online quality control by adjusting the inlet pressure, the vent pressure, or the mold temperature. The feasibility of the proposed method was illustrated by experiments.

Improvement of Process Variable Selection Method for Fault Detection System using Negative Selection Algorithm

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Abstract

In chemical plants, early fault detection is demanded. An artificial immune system—especially, negative selection algorithm— has been adopted to fault detection system in our study [Kase, 2019].

Negative selection algorithm is one of methods of artificial immune systems which imitate the vital immune systems. Negative selection algorithm is based on the mechanism of T-cell generation and maturity in thymus. Immature T-cells are randomly generated in thymus. Then, if they have high affinity with self-antigen, they are eliminated to avoid response to "self". On the other hand, if T-cells have no affinity with self, they can be matured to react with foreign antigen to protect itself.

We have built up a multiagent based fault detection system using negative selection algorithm. In our system, a set of detectors is generated in each two-dimensional process variable space. In our previous study, we prepare one hundred sets of variable spaces with detectors. To reduce calculation road, we investigated the methods of process variable selection in this study. As a result, the number of process variables are reduced to fourteen sets variable spaces. And also we verified the system has sufficient detection performance with reduced sets of process variables by using several kinds of malfunction—both stepwise and rampwise progress of abnormality cause.

In this study, we will illustrate our fault detection system using negative selection algorithm and how to select adequate sets of process variables to monitor the chemical plants. And we will show the detection results when several kinds of malfunction occurs in a dynamic plant simulator of a boiler plant.

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Verification of firefighters' heuristics through big data analysis

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Abstract

The heuristics accumulated in the field activities of firefighters were reviewed through big data analysis of fire occurrences in Gyeonggi-do and researched to be utilized for proper fire prevention activities according to time, day, and target through quantitative modeling. Empirical rules with high sympathy were collected through direct interviews with firefighters. Among these, three types of high-priority rules were compared and analyzed for big data such as fire occurrence and damage history in Gyeonggi-do in 2018. A big data comparison analysis was conducted, including the number of fires and damages that occurred in Gyeonggi-do in 2018. Furthermore, fire occurrence patterns by region, day of the week, time of day, and building type were derived. Regarding empirical rules that have been validated through research, relatively inexperienced firefighters also can make decisions by relying on refined quantitative predictive modeling and empirical rules including local government and time-based factors that reflect big fire occurrence data.

keywords: firefighters, rule of thumb, fire, fire monitoring, heuristics

Process Modeling and Simulation

Hollow Fiber-based Rapid Temperature Swing Adsorption Process for Carbon Capture from Coal-fired Power Plants

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Abstract

This work proposes a hollow fiber based rapid temperature swing adsorption (RTSA) method for capturing CO_2 from typical coal-fired power plants. The proposed RTSA approach can shorten the operating time and using low-grade heat source for regeneration of adsorption elements. In this study, the tank-in-series model is used to simulate the RTSA process including adsorption and desorption periods. A dual-column operating procedure is used to treat the flue gas continuously from the coal-fired power plants. Main operating variables including inlet gas volume flow rate (0.1 – 0.2 m^3/s), abandon time (0 – 10 s), desorption temperature (80 – 120 °C) on key performance factors such as discharge gas purity, capture ratio of CO_2, and energy consumption per unit mass of CO_2, etc., are investigated for reducing the energy consumption. This study found that the inlet gas volume flow rate will significantly affect the capture ratio, where smaller gas volume flow rate would be beneficial to increase capture ratio. The abandon time obviously affects the purity of the captured CO_2, where the longer abandon time leads to higher purity. Desorption temperature affects both the capture ratio and purity of captured CO_2. The higher the desorption temperature, the greater the purity and capture ratio. For one typical basic unit with dual-column hollow fibers, the study found that when the inlet gas volume flow rate is 0.12 m^3/s, the desorption waiting time is 7 s, and the desorption temperature is 120 °C, both the CO_2 purity and capture ratio can exceed 90 %. With considering the possibility of using steam in a low-pressure turbine as a source of heat required for DC-vRTSA, the impact on the efficiency and stream data of a typical coal-fired power plant are calculated. DC-vRTSA at 120°C, 100°C and 80°C will reduce the efficiency of coal-fired power plants by 8.2%, 6%, and 3.4%, respectively.

Optimal Sustainable Municipal Solid Waste Management to Valuable Products over Long Time Planning Horizon

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Abstract

Municipal solid waste (MSW) generation is increasing globally due to the increase of world's population and changes of lifestyle and consumption patterns. Direct storage of MSW in landfills have negative economic, environmental, and social impacts. Utilization of MSW either through recycling the recyclable material from MSW constituents, or through extracting power and biofuels from the non-recyclable parts has shown promising sustainable path for the MSW management worldwide. In this study, a multi-period capacity expansion planning model is proposed to determine the optimal selection of treatment technologies for the MSW constituents over a long term planning horizon in order to produce valuable products and fuels. This model presents a useful decision-making tool for policymakers to identify the optimal management pathways in the MSW management process. A case study of Abu Dhabi city will be examined during the 2020-2040 time period as an application of the mathematical programming formulation.

Energy-Saving Performance of Advanced Stripper Configurations for CO_2 Capture by Ammonia-Based Solvents

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Abstract

Recently, there has been substantial development in the chemical absorption technology for the post-combustion carbon dioxide capture (PCC) process. Amine- and ammonia-based solvents are two major categories of chemical absorbents being studied. Amine-based solvents exhibit good capacity and fast absorption rate but are expensive, degrade in the presence of oxygen, and cause corrosion of equipment. On the other hand, ammonia-based PCC has received significant attention recently, owing to its technical and economic advantages over the conventional amine-based process. However, the energy penalty of regenerating the CO_2 lean solvent is still a critical challenge. In the previous work [Liu, 2018], the operating parameters, such as NH_3 concentration, CO_2 lean loading and the stripper pressure, were investigated in the energy-saving perspective. In addition, the energy reduction achieved by stripper modifications, which include the cold-split bypass (CSB), interheated (IH) stripper, and the combination of both configurations, was studied. The results indicate that the energy-saving effect of combining the CSB and IH configurations was not as promising as the literature claims [Li et al., 2015]. Recently, Ullah et al. (2019) reported that the advanced stripper configurations, CSB and lean vapor compression (LVC), may reduce 13.6% and 5.5% of energy consumption, respectively. Nevertheless, the energy-saving performance can be enhanced to 19% for the LVC integrating with the CSB configuration. In a standard amine-based system [Liu, 2020], the energy requirement can be reduced 18% and 14% for the CSB and LVC configurations, individually; however, the energy-saving performance was only enhanced 3% for combining the both modifications. In this work, the energy-saving effect of integrating CSB with LVC in the ammonia-based cases will be investigated.

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Parameter Estimation by Bayesian Inference Using Monte Carlo Sampling for Liquid Chromatography Process Model

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Abstract

Liquid chromatography processes are widely utilized in industry to separate chemical products, such as sugars, chiral compounds and petrochemicals. In such industrial applications, it is critical to optimize operating conditions by using a mathematical model to improve purity, recovery ,and throughput of products [Grosfils et al., 2007]. However, parameter estimation for chromatography models is still challenging, and in particular, techniques to evaluate uncertainties of estimated parameters are not established. For this objective, this study estimated model parameters as probability distributions by some methods for Bayesian inference using Monte Carlo sampling.

Liquid chromatography is a separation technique that utilizes the difference of interaction between components and adsorbents. The process model is composed of mass balances and an adsorption isotherm, which leads to a set of partial differential equations (PDEs) [Guiochon et al., 2006]. We obtain experimental data to estimate six parameters: Henry's constants, mass transfer coefficients, and equilibrium constants for two components.

This study estimates parameters by using Bayesian inference, which quantifies uncertainty as probability distributions. Since the probability distributions of the model parameters cannot be obtained analytically, and a numerical solution based on random sampling is employed [Gelman et al., 2004]. The PDE model is implemented and solved within the sampling algorithm in our study.

We carried out parameter estimation by analyzing the experimental and simulated data by two Bayesian inference techniques: Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC). We compare these two approaches by quantified uncertainties and computational time.

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Process Design with ASPEN PLUS when Some or All Experimental Data are not Available

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Abstract

Thermodynamic properties and fluid phase equilibria are crucial for the design and development of a chemical process. However, such data may not always be available, particularly for fine or specialty chemicals. In this work, we present a novel approach combining modern computational chemistry with recently developed predictive thermodynamic models to provide all the required thermodynamic properties in process design. In particular, we developed a web-based platform to automate the whole process such that the user needs only input the chemical names (SMILES) involved in the process. The necessary thermodynamic parameters for the design project will be stored in an ASPEN PLUS readable file. We have examined the platform using nine pure component properties of 972 systems and the binary mixture activity coefficients. Amongst them, the ideal gas heat capacities and properties of formation at standard state are determined from thermochemistry analysis based on the G3 method. PR+COSMOSAC equation of state and COSMO-SAC activity coefficient model are utilized to predict the phase behaviors of pure and mixture fluids. The predictions of most properties are found to be unbiased while the acentric factor, the heat of vaporization, and the vapor pressure exhibit small biases. To test the reliability of using predicted values when some or all experimental data for the constituent chemicals are missing, we compare phase diagrams of four representative systems. Based on that, we found the activity coefficients evaluated by COSMO-SAC are considered sufficiently reliable. Moreover, the vapor pressure is deemed to be the most essential factor for the accurate prediction of phase behaviors amidst all pure properties. According to the statistics, about 94% of the relative magnitude of the predicted boiling points of any two compounds in our test sets are consistent with the experimental data, which confirms the validity and the reliability of our approach in a qualitative sense as applied in process design. This new approach offers a general and reliable means of providing the necessary thermodynamic parameters without input of any experimental data and is suitable for the design and development of processes involving new chemicals.

Modeling and estimating kinetic parameters for CO2 methanation in a fixed bed reactor

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Abstract

CO2 Methanation is one of the promising candidates in developing CO2 utilization technology, which converts CO2 and hydrogen into methane as fuel. One of the reactants in this reaction, hydrogen, is produced by electrolysis of water, which is driven by surplus power generated by renewable energy such as solar or wind; this process is considered as a power-to-gas system. The conversion of CO2 into methane potentially has a substantial cost advantage, since it allows utilization of existing natural gas infrastructure, eliminating the need for new facilities for hydrogen transportation and utilization.

Recently, Hitachi Zosen Corporation has developed a highly active catalyst for methanation [1], and is currently developing a high-performance reactor using this catalyst. However, design of reactor must be carried out carefully, since this reaction is an exothermic reaction with a high heat of reaction, which may cause unexpected damage to the reactor and deterioration of catalysts. For this problem, a mathematical model that can predict the behavior inside the reactor is necessary.

In this research, we model the methanation reaction of CO2 and estimate the kinetic parameters in the reaction rate model from experimental data. In the parameter estimation using literature values [1] and Tikhonov regularization, eight kinetic parameters in the rate equations were identified from the 47 data points with different inlet composition and temperature. We confirm that molar fractions at the reactor exit predicted by this model are in good agreement with the experimental results, and expect the developed model will be a powerful tool for the reactor design.

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Surrogate Model Using Customized Thermodynamics for Online Calculation

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Abstract

Online simulation and optimization of chemical processes are the foundation of real-time optimization and nonlinear model predictive control. However, frequent evaluations of complex thermodynamic models may cause difficulties. On the one hand, they are often highly nonlinear modules with many intermediate variables, being the most complicated part of the entire model. On the other hand, the equation-oriented approach is incapable to cope with if-else statements or sequential iterations inherent in some thermodynamic models. Traditionally, they are approximated by a global surrogate which is still very nonlinear. Fortunately, a flowsheet can be decomposed into unit operations and the state variables for every single thermodynamic system are usually within narrow ranges. In light of this, we propose the customized thermodynamics method in which each thermodynamic system (TS), for instance, each stream or each column stage, uses its own private data-driven surrogate model.

Surrogate models using customized thermodynamics are set up in five steps. First, the range of state variables is determined using a rigorous model. Second, the nonlinearity of the thermodynamic model for each TS is measured by linear regression residuals, deciding the sampling region and the desired type of surrogate (i.e. linear, quadratic, or kriging). Third, the surrogate model is constructed and encapsulated into the dynamic-link library together with its analytic derivatives, which is used by algebraic modeling platforms like AMPL and Pyomo. Fourth, the approximated model is refined to meet the target precision. Otherwise, the rigorous model is adopted. Fifth, the original thermodynamic model is substituted with the surrogate model. An object-oriented modeling approach is recommended for software extendibility.

The effectiveness and performances of the proposed method are demonstrated by the simulation of ethylene slurry polymerization and the optimization of a cryogenic air separation plant. The ethylene slurry polymerization process consists of two flash units and one reactor. Phase equilibrium constant, enthalpy, and entropy are evaluated using PC-SAFT (Perturbed-Chain Statistical Associating Fluid Theory). Sequential modular simulation in Aspen Plus fails to converge using the original model. On the contrary, convergence is reached in 7 equation-oriented iterations using IPOPT after replacing the PC-SAFT model with the customized kriging surrogates. In the second example, a ternary air separation plant producing high purity gases (nitrogen, oxygen, and argon) with three columns and 280 trays are considered. Static state optimization problems under 134 operating conditions of different product demand are investigated using IPOPT. 133 of them converge to the original optimum after substituting the Peng-Robinson and Soave-Redlich-Kwong equation of state with the customized linear polynomial surrogates. Furthermore, the computational time is significantly reduced by 88% on average. To summarize, surrogate modeling using customized thermodynamics facilitates the equation-oriented formulation and speeds up the computation for a large-scale process.

Multi-Task Prediction and Optimization of Hydrochar Properties: Application of Machine Learning on Waste-to-Resource

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Abstract

The increasing population and rapid urbanization has led to tremendous non-renewable energy/resource consumption and serious enviranmental issues, e.g. waste generation and carbon emission. Hydrothermal carbonization (HTC) is a promising technology for carbon and energy recovery from high-moisture wastes with hydrochar production due to its unnecessary prior drying of feedstock, robust and economic operation, energy efficiency. Hydrochar with high HHV and C_char could be as alternative of fossil fuels for heat and electricity generation, and the hydrochar with stable carbon could be used as a fertilizer, conditioner or remediation agent for soil improvement and carbon sequestration. To prepare hydrochar for various applications, the traditional way is to conduct repeated experiments with feedstock condition adjustment, which is tedious, labor-intensive, time-consuming, and quite expensive. Machine learning (ML), as a data-driven approach, can perform prediction tasks after training with HTC dataset and facilitate understanding of the relative importance of input features based on the bridge of inputs and output variables.

In this work, ML method was employed to develop multi-task prediction models for properties prediction of hydrochar with the attendance of feedstock information and operational parameters. Three types of ML models were developed base on the HTC dataset compiled from recent ten-year published literatures. Furthermore, the ML-based feature importance and the multi-objective optimization (MOO) with ML model integration were further explored to prepare the desired hydrochar for different applications. Results showed that the fuel properties (FP) and carbon capture and stability (CCS) of hydrochar could be predicted simultaneously with high accuracy. Deep neural network (DNN) exhibited excellent joint prediction ability with an average R^2 and RMSE of 0.91 and 3.29. In order to make the optimal prediction model widely and easily applicable, a ML-based software with free accessible user interface was developed. Moreover, ML-based feature importance analysis unveiled that both feedstock information (especially elementary composition) and operational parameters (especially temperature) were crucial to FP and CCS. Furthermore, optimal ML model was successfully integrated with MOO to maximize the FP or CCS of hydrochar for the potential application of fuel substitution or carbon sequestration in soil. The insights unveiled from DNN and optimal solutions from MOO benefit for instruction of desired hydrochar preparation with labor, time and cost saving. The combination of ML and MOO models for prediction and optimization of hydrochar properties provides a novel approach for mining the potential of renewable resource recycling from high-moisture wastes.

Quantum chemistry and molecular dynamics simulations on cryoprotective agents for human stem cells

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Abstract

Cryopreservation has become a central technology in many areas of clinical medicine, biotechnology, and species conservation within both plant and animal biology. Cryoprotective agents (CPAs) are essential for the cryopreservation of cells and play a key role in allowing cells to be processed for storage at ultra-low temperature [Hunt, 2019]. In cryopreservation of cells, dimethyl sulfoxide (DMSO) has been widely used as a CPA because DMSO can achieve high cell survival rate in many types of cells [Elliott et al., 2017]. However, several studies reported that DMSO had toxicity to cells and affected the differentiation of many types of cells [Best, 2015; Fahy, 1986]. In particular, the toxicity is very critical for human stem cells because the products are implanted directly into human bodies. Therefore, it is necessary to develop alternative CPAs to DMSO.

This work presents model-based assessment of CPAs for human stem cells. An assessment model was developed that can quantify solvation free energy of a CPA candidate, partition coefficient of a CPA candidate, and root mean square deviation (RMSD) of a cell membrane with a CPA candidate solution. The solvation free energy, the partition coefficient, and the RMSD were defined as the indicators of osmoregulatory ability, affinity with a cell membrane, and ability to spread a cell membrane, respectively. The objective function was defined as the total score which can be calculated by the three indicators. The solvation free energy and the partition coefficient were calculated by quantum chemistry simulations. The RMSD was estimated by molecular dynamics simulations.

Using the developed model, we conducted the assessment of multiple candidates for CPAs. Large difference on the total score was observed depending on the CPA candidate. Classifying the candidates into several chemistry groups, sulfoxide, amide, and amine-related candidates showed relatively high scores. Comparing the high-score candidates with DMSO, we succeeded to identify a couple of compounds to be competitive or even superior than DMSO. Experimental investigations are being planned to validate the performance of the suggested candidates.

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Practical Microkinetic Modeling for Direct DME Synthesis over a CZA/H-FER Bifuncional Catalyst

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Abstract

As global warming is getting worse and fossil fuels are depleted, utilization of carbon dioxide (CO2), which is one of the main components of greenhouse gases, has gained huge interests by many researchers, and CO2 conversion to methanol (MeOH) and dimethyl ether (DME) is one of the promising CO2 utilization methods as they can be used as fuel, solvent, and a precursor to various organic compounds. An effective microkinetic modeling strategy was applied to the reaction kinetics for direct dimethyl ether (DME) synthesis from syngas over a Cu-ZnO-Al2O3/H-ferrierite (CZA/H-FER) catalyst, a core-shell structured bifunctional catalyst for direct synthesis of DME. The plausible reaction networks of CO and CO2 hydrogenation, water-gas shift reaction (WGSR) and methanol dehydration were considered for methanol synthesis from syngas over a CZA catalyst and DME synthesis from methanol over a H-FER catalyst. In our previous studies [Park et al., 2019; Park et al., 2020], the analysis on energetics and structures of the reaction intermediates and transition states included in the reaction mechanisms was conducted on the basis of the computational chemistry such as the density functional theory (DFT) and the second-order Møller–Plesset perturbation theory (MP2), and the microkinetic models were developed respectively for methanol and DME synthesis. In the present study, a comprehensive microkinetic model for direct synthesis of DME is developed, and the reaction kinetics of the comprehensive microkinetic model are compared with those of the respective microkinetic models (i.e. methanol and DME). The pre-exponential factors are estimated by fitting the experimental data, increasing the reliability of our model. Using the developed microkinetic model, the dominant reaction pathways are investigated, and the rate-limiting steps are suggested. Furthermore, the effects of operating conditions on the reaction kinetics are investigated.

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Modelling and Economic Analysis of Methanol Synthesis Process For a Natural Gas Field with High CO2 Concentration

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Abstract

Natural gas fields in Southeastern Asia is known to include vast amount of CO2, which requires large amount of energy for its systematic removal. In addition, the removal of H2S, which is partially contained in the gas field and possesses potential danger of catalytic corrosion in reactors, is essential. In the present study, as one of ways to efficiently utilize CO2-abundant natural gas fields, acid gas removal unit (AGRU) process was considered to remove H2S completely and CO2 partially, and the H2S free gas with methane and CO2 as major components was sent to a reforming reactor, followed by a methanol synthesis reactor. It was shown that the reforming reactor could produce hydrogen which is needed to synthesize methanol, and the recycling loop in the process could enhance the efficiency. Finally, techno-economic analysis was carried out on the entire process to give useful information on the design of commercial processes.

Evaluating the Direct CO_2 to Diethyl Carbonate (DEC) Process: Rigorous Simulation, Techno-Economical and Environmental Evaluation

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Abstract

In this work, the plant-wide process to produce diethyl carbonate (DEC) from the direct reaction with CO_2 and ethanol, which uses 2-cyanopyridine (2-CP) as an in situ dehydrating agent, is proposed for the first time. Rigorous design, optimization, ability in carbon reduction, and techno-economic evaluation are all performed in this work. The process consists of two sections. The first one is the main section, in which DEC is generated, along with the removal of water using 2-CP to form 2-picolinamide (2-PA). The second one is the regeneration section, where 2-CP is converted back from 2-PA and recycled. Using simulated annealing method, the optimized CO2 reduction rate in the main section is 0.230 (Ton CO_2/Ton DEC generated) on an annual basis. We identify that when the regeneration section is operated with a molar ratio of mesitylene to 2-PA being less than 1.95, the overall process can be in net CO_2 reduction. Under the constraint of 90% regeneration of 2-CP as reported in available literature, the produced DEC can match the current market price range under 15% internal rate of return (IRR), if 2-CP can be obtained with a price in lower than 2.028 USD/kg (corresponding to DEC price of 1.1 USD/kg) to 6.738 USD/kg (corresponding to DEC price of 1.9 USD/kg).

Rigorous Simulation of the Bio-Oil Production Process through Fast Pyrolysis

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Abstract

The bio-oil production techniques have received great interest recently in orderto mitigate the increasing CO_2 emission. In this study, a rigorous plant-wide process producing bio-fuels based on fast pyrolysis of biomass is firstly developed. Through fast pyrolysis,the biomass can be converted into a bio-fuel crude product rich in oxygen atom, which needs to be upgraded through the following hydrodeoxygenation process in order to meet the oil requirement. Three sections are included in the plantwide process. The first one is a the one-dimentional circulated fluidized bed (CFB) pyrolyzer, which is first simulated in Aspen Custom Modeler (ACM), and is later exported to Aspen Plus for process simulation. This 1-dimentional pyrolyzer model rigorously considers the reactions, heat and momentum transfer. Besides, the secondary reaction are also considered. Through this modelling task, deeper results can be obtained in the actual pyrolysis reaction section. The second one is the hydrodeoxygenation seciton containing a reactor and a series of distillation columns for fractionation of the oil products. The third one is the hydrogen production plant based on steam and dry reforming of methane, for the purpose of supplying the required hydrogen for the hydrodeoxygenation process. After the process model is developed, optimization and heat-integration strategies are discussed. Finally, the dynamic simulation of the plantwide process is studied and a suitable control structure is provided. With this work, a better understanding of the overall pyrolysis-based bio-oil process can be obtained.

Batch and flow syntheses of drug substances: a model-based comparison in heterogeneous hydrogenation

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Abstract

For over half a century, the synthesis of drug substances has been conducted using batch synthesis. Recently, flow synthesis is receiving growing attention because of several advantages such as higher yield and better safety. However, the actual impact of introducing flow synthesis is still unclear and should be assessed quantitatively. Most recently, Costandy et al (2019) performed a model-based analysis of batch and flow synthesis, however, the target was limited to a one-phase reaction [Costandy, *et al.*, 2019].

This work aims to conduct a comparative assessment of batch and flow drug syntheses for heterogeneous hydrogenation. This is one of the most used reactions in pharmaceutical synthesis with applying catalysts such as palladium on carbon. Here, a key factor that should be addressed in the reaction system is leaching. Leaching refers to the loss of active species from the solid that are transferred into the liquid medium, causing eventually a deactivation of the catalyst [Sadaba, *et al.*, 2015]. It is crucial to prevent leaching particularly because it can decontaminate products and eventually cause quality problems.

We first modeled batch and flow syntheses of a commercialized antibiotic drug substance. In the developed physical models, the reaction mechanism was assumed to follow Langmuir-Hinshelwood mechanism. Deactivation of catalysts due to poisoning has been incorporated in the model in order to simulate the unsteady-state. Second, experiments using batch and flow syntheses were performed in order to understand the systems performance and to estimate the key parameters such as the reaction rate and the poisoning rate of catalysts. Finally, catalyst leaching was tackled. Experimental results and simulations suggested that the ratio of hydrogen gas concentration in solid phase and hydrogen consumption rate could be critical for leaching. Based on this finding, we defined an indicator for judging the occurrence of leaching, which can serve as a constraint on the operational condition for the syntheses. In the ongoing work, we are comparing both syntheses methods in terms of yield and productivity under different operating conditions such as pressure, flow rate, and stirring rate. We aim to provide a general map that presents the superiority of flow synthesis as a function of the given process setups.

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CO_2 hydrogenation process and reactor simultaneous design using low quality raw material: multi-scale modeling with CFD and ASPEN

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Abstract

The raw material prices(H_2 and CO_2) used in the methanol synthesis process have a great economic impact on the operation of the overall process. Therefore, it is important to find a method that can improve the overall process economy by supplying raw materials at low cost. When using low quality raw materials, the process is complexed and the process design can be difficulty. We conducted multi-scale modeling to applicable reactor and process model. The internal hot spot problem occuring in the existing reactor is reduced by using low quality raw material, and the detailed reactor design applicable in process is modeled with CFD. The process to which the reactor model can be applied is simultaneously designed usign CFD and ASPEN, which can be a mothod to present an economically improved commercial process.

Statistical Modeling of Integrated Continuous Processes in Pharmaceutical Industry

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Abstract

Currently, pharmaceutical manufacturing is making the switch from batch manufacturing towards continuous manufacturing. The implementation of continuous manufacturing brings many advantages such as flexible production on demand, reduction of development costs, and robust process design [Lee, 2015].A lot of research has been conducted on continuous manufacturing, and most of them focus only on a particular process [Vanhoorne, 2020]. However, in order to consistently manufacture high quality products, it is important to focus on integrated processes.

In this research, we focus on the integrated processes, and aim to predict the material attributes (MAs) of the final product from the process parameters (PPs) and the MAs of the intermediate products. Models are constructed using four modeling approaches and three modeling methods. Four modeling approaches are PP & MA-based indirect approach, PP & MA-based direct approach, PP-based direct approach, and MA-based direct approach, and three modeling methods are partial least squares (PLS), random forest (RF), and Gaussian process regression (GPR). In the indirect approach each process is modeled independently, and in the direct approach all the processes are modeled together as an integrated process.

As a result, it was revealed that the direct approach was better than the indirect approach, and that the nonlinear regression method was better than the linear regression method. In addition, the prediction accuracy was high enough for practical use except for one of the MAs of the final product.

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Modeling and Economic Analysis of Alcohol-to-Jet Process: synthesis of Drop-In Aciation Fuel Using Bioethanol

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Abstract

In 2013, global aviation fuel consumption estimated at 18.9 billion barrels and US EIA reported that it will raise doubly by 2031. However, jet fuel is one of the major cause of greenhouse gas emissions and due to the EU emission-control standard, International Air Transport Association (IATA) plans to decrease greenhouse gas emissions by 50% until 2050 by developing sustainable alternative jet fuels (SAJF). In this study, alcohol-to-jet (ATJ) process that converts the fermented bioethanol to drop-in aviation fuel was modeled to evaluate the economic analysis. Reaction kinetic rates of the dehydration process for the conversion of ethanol into ethylene was developed using experimental data and used in the reactor model, and the removal of water, which is contained in the fermented ethanol and produced by the dehydration, was considered because the downstream process is not tolerant to water [Geleynse et. al., 2018]. A yield-shift reactor was used to quantify the catalytic oligomerization reaction that synthesizes C10+ oligomers from ethylene at one-stage; Conventional ATJ processes are based on two-stage oligomerization processes. After the effectiveness of the entire process model was corroborated, an economic analysis was conducted to compare the developed process with conventional processes.

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Process simulation and intensification of auto-thermal co-gasification for syngas production

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Abstract

As the global demand for energy continues to increase, the reliance on fossil fuels to meet these demands have only led to their depletions and serious climate change concerns. Auto-thermal co-gasification (ATCO-GAS) of plastics with waste biomass to produce syngas serves as an effective solution to this cause, as it utilizes biomass residue, plastics and CO_2 in the feed, and simultaneously produces a clean energy source in the form of syngas (Fan et al., 2019). In this study, a steady-state simulation model for ATCO-GAS of plastics with biomass as the feedstock is developed using Aspen Plus. A base case gasification model is developed and validated in terms of syngas composition and fuel parameters with published exerimental work (Shen et al., 2019). The role of parameters such as plastics to biomass ratio (M:B), operating temperatures, equivalence ratio (ER) and steam to feed ratio (SFR) on the resulting syngas composition and its lower heating value (LHV) are then evaluated (Ardolino et al., 2018). The ATCO-GAS with M:B ratio 20:80, SFR 0.3 at 900℃ yielded an optimum H_2:CO ratio of 1:1 in the product syngas with a content (H_2 + CO) of 54.8 mol% and highest LHV at 7.18 MJ/kg on dry basis.

To improve the overall process efficiency, sustainability and energy consumption, the ATCO-GAS is subjected to dual-step process intensification (PI) by coupling the water-gas shift reactor (WGSR) with 4-stage pressure swing adsorber (PSA) unit (Marcantonio et al., 2019). While the WGSR further increases the H_2:CO ratio, the PSA yields a H_2 rich gas as the final product, post CO_2 sequesteration- which is redirected back to the feedstream. The PI is further consolidated by devising an integrated optimum heat exchange network (HEN) to minimize the utility and capital costs of the entire system (Zhang et al., 2013). Techno-economic analysis along with life cycle analysis (LCA) is performed to substantiate the potential economic and ecological benefits of the proposed system compared to standalone gasification systems.

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Simulation and Development of Reactive Rotating Packed Bed for n-Butyl Acetate Process

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Abstract

HiGee (High-Gravity) technology is one of important branches in the process intensification category. This technology uses the centrifugal force generated by rotation to replace gravity to enhance mass-transfer efficiency. Such equipment is also known as a rotating packed bed (RPB). Since the coupling of reactive distillation (RD) and HiGee technology is rarely studied, and the distillation system is the most energy-consuming unit in the chemical process. This improvement can not only greatly reduce equipment volume, but also effectively improve RD limitations. Such as mass-transfer performance between liquid and vapor phase, inefficient catalyst wetting, and flooding limitation.

In this work, the esterification of acetic acid and n-butanol is demonstrated as a target process. The reactant feed streams are set as 50 kmol/hr respectively, and the bottom product purity is set as 99 mol%. Aspen Plus® is used to complete the steady-state simulation for the conventional-gravity field and the design of the reactive RPB (r-RPB). This work is also comparing traditional RD tower with r-RPB about the volume reduction and analyzing the optimal motor power consumption.

Based on the r-RPB design, geometric equivalent conversion of r-RPB is performed to ensure that mass-transfer properties are maintained constant [Gudena, 2012]. This work uses the RADFRAC module to build the basic structure of r-RPB, which including the use of Rate-Based algorithm and FORTRAN subroutines. This work will follow the HiGee and physical geometry concepts [Agarwal, 2010] to adjust the mass-transfer coefficients [Chen, 2011], effective interfacial area, and liquid holdup to replace the system parameters in the conventional-gravity field.

According to the simulation results, the volume of the traditional RD tower and the r-RPB are 25.3 m^3 and 2.67 m^3. The volume of r-RPB has 89.4% reduction. As for the reboiler duty, HiGee and conventional-gravity field processes, 3005 kW and 2781 kW, are almost the same. Under the premise of maintaining production capacity, this work divides r-RPB into several small r-RPBs. Results show that dividing into two small r-RPBs can have a smaller overall motor power consumption, around 21.5% energy saving, from 321.3 kW to 252.2 kW.

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Feasibility analysis on decanter centrifuge design for sludge thickening

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Abstract

Decanter centrifuge exploits high rotational speed for good separation to achieve at least 90%~99% range of solids recovery required by the activated sludge thickening. However, the feed volumetric rate, feed solid fraction, differential speed, liquid discharge radius and median floc size critically affect system operability and feasibility in sludge thickening. In this study, feed volumetric rate and feed solid fraction are considered as uncertain parameters, while differential speed as adjustable control variable, liquid discharge radius and median floc size as design variable. The unit is expected to be operable for 90%~99% solid recovery, specific cake solid fraction 0.06 and centrate solid fraction 0.002 with minimum power requirement.

To determine the operational window for given uncertain parameter ranges, it is necessary to develop understanding on decanter centrifuge and centrifugal sedimentation through NLP mathematical modelling. In this study, GTech 1456 decanter centrifuge model [1] is chosen as it has numerous reference values, while sedimentation model [2] is used for equilibrium solid thickness as it affects the cake solid fraction. Both models are developed on MATLAB platform. The rotational speed will be minimize using fmincon solver under given operational constraints mentioned before. Random line search with bisection method is developed to determine feasible boundaries and compute flexibility index of the corresponding decanter centrifuge unit.

It is worth to mention that the above feasibility analysis can be implemented for different design variables, but the economic impact on operational cost has not been addressed. Therefore, further combination of operational cost and flexibility index will be introduced in the future studies to evaluate the associated costs on realistic working condition.

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Effect of Fluid Flow and Transport on Catalytic Fixed-bed Compact Reactors

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Abstract

Among multiphase reactors in the chemical and pharmaceutical industries, fixed-bed compact reactors with internal diameters on the order of millimeters or micrometers are of interest. However, the design and operation method of fixed-bed compact reactors has not been established because it is difficult to analyze the flow pattern, which greatly influences heat and mass transfer performance, by visualization. In this study, an experimental system consisting of a fixed-bed compact reactor was constructed, and a method of estimating the flow pattern in the reactor was developed through experimental analysis of the measurement results of voltage or differential pressure. The results showed that when gas and liquid were supplied to the reactor, the developed method made it possible to distinguish the flow patterns of trickle flow and pulse flow from the shapes of the measured voltage or differential pressure and to estimate the pulse frequency of pulse flow (i.e., peak frequency of power spectral density), which is useful in grasping the degree of mixing of gas and liquid. Using the developed method, experiments for various operating conditions were evaluated. As a result, it was suggested that the mixer and reactor inlet capable of producing shorter gas and liquid slug should be developed in order to realize the process with higher gas and liquid mixing. In addition, computational fluid dynamics (CFD) simulation was performed to thoroughly understand the flow and its interaction with reaction and transport in the reactor. The different kinds of particles with typical dimensions and their packing methods were evaluated under characteristic reaction conditions. The simulation results showed that devising the packing method so that the fluid velocity in the radial direction of the reactor was generated between particles was effective in realizing a uniform temperature field. As a next step, our CFD simulation results will be utilized in the optimal design and operation of the catalytic fixed-bed reactors.

Generation and Verification of Operating Procedures Based on Timed Automata

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Abstract

For running any chemical plant, the standard operating procedures (SOPs) are needed in performing a wide variety of essential tasks. Despite the fact that the modern chemical plants are becoming more complex than they used to be, these operating procedures are still generated manually in most cases. This approach is clearly laborious, time-consuming and error prone. In order to ensure the efficiency and safety of the operation, it is desirable to develop a feasible approach to systematically generate SOPs for performing various tasks in realistic chemical processes. With the help of dynamic simulation, the impacts of changing each operation step on the process can be investigated without significant costs.

The timed automata are adopted in the study for modeling all components in the chemical processing systems. With software UPPAAL, incorporating and synchronizing these components into a system model results in all viable operation paths. Specifically, the feasible operating procedures can be synthesized according to the following eight steps:

(1) Discretize all state variables in the given process system.

(2) Determine the elapsed times of all possible state transitions for every processing unit with Aspen Plus Dynamics.

(3) Build timed automata for processing units based on step (2) and, also, build untimed automata for other component in P&ID based on generic engineering knowledge.

(4) Stipulate control specifications and build the corresponding automata to ensure that the action sequences are correct.

(5) Integrate and synthesize all automata built in steps (3) and (4) and identify the shortest or quickest trace with UPPAAL.

(6) Summarize the shortest or quickest trace with a sequential function chart (SFC).

(7) Simulate the dynamic process according to the SFC obtained in step (6) with Aspen Plus Dynamics.

(8) If the simulation study in step (7) confirm that the given SFC drives the system to the target state safely and economically, then the procedure can be terminated. If otherwise, return to the step (4) to add/remove/revise the automata and repeat steps (5) – (7) until a satisfactory trace is identified.

Finally, the feasibility of the proposed model building method and procedure synthesis strategy are demonstrated in this work with three realistic examples – the startup processes of a flash drum, a simple distillation column and a reactive distillation column.

Comparison Two Models of Decreasing of the Overall Heat Transfer Coefficient on Heat Exchanger Due to Fouling

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Abstract

Heat exchangers (HE) performance in the heat exchanger network (HEN) of crude oil refinery can decrease due to fouling [Rodriguez and Smith, 2007; Reza et al., 2006]. The fouling can reduce the overall heat transfer coefficient significantly [Huda et al., 2018], and have an impact on operational cost [Ismaili et al., 2019]. The fouling can be used to predict the overall heat transfer coefficient [Biyanto et al., 2016; Licindo et al., 2015]. This research addresses the focus on predicting the overall heat transfer coefficient of eleven HEs in the specific crude oil refinery. There are two models used in this work to predict the overall heat transfer coefficient from clean to foul condition. The models are based on the general equation and exponential equation. The two models then are compared with the overall heat transfer coefficient obtained from the plant. Both models are used to calculate the minimum additional heat duty required for the heat exchanger network. The result shows the exponential equation model simulated for HEN to predict the overall heat transfer coefficient is more accurate than the general equation model except for two HEs in HEN.

Keywords: fouling; heat exchanger network; overall heat transfer coefficient

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Development of the Prediction Model for Microalgae Hydrothermal liquefaction Using Aspen Plus

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Abstract

Microalgae, which are abundant on the Earth, have better energy efficiency than other biomass (aspen wood, soybean, sunflower, etc.). Also, it is easier to build up the cultivation conditions. The extensive research on microalgae converting into biocrude products has been developed in recent decades. In this research, it is focused on the establishment of microalgae hydrothermal liquefaction (HTL) process and further develops a prediction model to assess the distribution of products. However, it is very challenging to identify the constituents of microalgae resulting in predicting toughly the distribution of products. To achieve the purpose mentioned above, the research methods include dividing microalgae into three biochemical compositions (carbohydrate, protein, and lipid), applying the kinetic model developed by Valdez et al.[Valdez, 2014], studying the reasonable mechanism of reactions and developing the appropriate separation method. Therefore, the whole process, which is a rigorous simulation of the HTL reactor, would be discussed.

Key words: microalgae, hydrothermal liquefaction, biocrude, modeling, rigorous simulation

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Kinetic Modeling and Simulation for the Synthesis of Methyl Methacrylate

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Abstract

Methyl methacrylate (MMA) is a high value-added chemical and is mainly produced by the technology of acetone-cyanohydrin (ACH) in the process industry. It is known the synthesis of the methyl ester of methacrylic acid has two important steps. Overall kinetic models used to describe the synthesis of methyl methacrylate are rarely reported in the literature. This work first tests and simulates the kinetic model of the hydrolysis of methacrylamide proposed by Chen et al. (1993). A kinetic model of the second consecutive reversible reaction taking place in esterification of methacrylamide sulfate has been presented by Balák and Polievka (1983). Better kinetic parameters are then found in this study. These kinetic models for the synthesis of methyl methacrylate can be utilized for design and simulation of the pilot-scale and commercial methyl methacrylate plants.

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Design and Simulation of a Methyl Methacrylate Synthesis Process

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Abstract

Methyl methacrylate (MMA) is a chemical with high economic value and is mainly produced by the acetone-cyanohydrin (ACH) technologyi in the industry. This work aims to study the process design and simulation of the synthesis of methyl methacrylate. Effects of the multicomponent behavior for this system can be described by the UNIQUAC thermodynamic model. The kinetic models proposed by Chen et al. (1993) and Balák and Polievka (1983) are then modified to fit the experimental kinetic data. According to the report of Segawa et al. (1991), water and n-Hexane are the solvents for the extraction and azeotropic distillation operations, respectively. Therefore, four major units, an amidation reactor, an esterification reactor, an extractive column, and a distillation column are combined to design and simulate a methyl methacrylate synthesis process.

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A Model for Heat Exchanger Equipped with Thermoelectric Generators

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Abstract

Thermoelectric generators (TEG) are solid-state semiconductor devices that convert a temperature difference and heat flow into electric power (Astrain and Martínez 2012). This generated voltage causes electrical current and produced electric power. Nowadays, industries with high-temperature production processes have heat loss that cannot be avoided. The heat exchangers (HXRS) are widely used (Wang, Luan et al. 2014) for solving the problems of waste heat recovery, caused to reduced energy and production costs. In this research, the effect of temperature and flow rate of hot and cold streams on electric power, Its generated from thermoelectric generators that were investigated by installed Bismuth Telluride (Bi_2Te_3) thermoelectric generators on the heat exchanger. Then create a mathematical model to predict the results of the electric power produced (Lan, Yang et al. 2018). As a result, the model can predict values that accurate and close to the values obtained from the experiment.

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Assessing the Sensitivity of Disrupted Integrated Biorefineries via Monte Carlo Simulation

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Abstract

Integrated biorefineries (IBR) are facilities that convert biomass into valuable bioenergy products such as power, biofuels, methane, and biochar. However, supply-side disruptions caused by a decrease in available biomass feedstock may result in cascading failures within an IBR due to high degree of interconnectivity. This disruption may cause a decrease in production levels of the process units and in the final output of bioenergy products. The consequence of such risk event is a function of the degree of disruption and the interdependency between equipment. It is therefore important to consider this type of disruption when designing IBRs. Process units are normally designed to consider fluctuations in production levels, but may not anticipate all possible scenarios, making the equipment unreliable. The disruption may cause the equipment to operate below the minimum allowable capacity or beyond the maximum. In this work, the sensitivity of IBRs is assessed using a Monte Carlo simulation approach. The method is able to determine the reliability of the process units amidst capacity disruptions. A case study using an IBR designed from waste of palm oil mills is used to demonstrate the proposed method.

Estimation of Deferasirox synthesis reaction kinetics based on reaction heat flow to upscale in a pilot-plant

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Abstract

Deferasirox or 4-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]benzoic acid marketed as Exjade is an oral iron chelator. It is used to reduce chronic iron overload in patients who are receiving long-term blood transfusions(Jarussophon, Pongwan, and Srikun 2015). Deferasirox was prepared by a batch process through the reaction of 2-(2-hydroxyphenyl) benz[e][1,3] oxazin-4-one (BNZ) and 4-hydrazinobenzoic acid (HYZ) as solid reagents in absolute ethanol. This work is aimed to evaluate the reaction rates and the reaction rate constants through the study of the rates of heat release using a reaction calorimeter (Mettler Toledo, RC1). The kinetic parameters of this reaction were determined at different reaction temperatures (338, 343 and 348 K) and at three mixing speeds of agitator (200, 250 and 300 rpm). Isoperiboric mode (the temperature of the jacket was precisely controlled and held at a specific value) of reaction calorimeter was utilized in order to observe reaction temperatures when the reaction occurs in the reactor. An exothermic was subsequently detected and calculated by the reaction calorimeter as a heat flow of reactions. The kinetics of the dissolution of both reagents ($k_s a$ of BNZ = 0.0433 s^{-1} and $k_s a$ of HYZ = 0.01354 s^{-1}) were simultaneously estimated. The kinetic parameters such as activation energy (317.3 kJ/mol), frequency factors (2.21×10^{46} L/s.mol), and reaction orders were calculated by using MATLAB software and non-linear regression technique. The experiment has been further carried out to demonstrate the ability to model dissolution and reaction. The contribution of this work is to provide useful kinetic data which are critical in the modeling and control as well as useful data to upscale in a pilot-plant.

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Process Modeling and analysis of Alkaline Water Electrolyzer Systems

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Abstract

In order to minimize environmental pollution caused by the use of fossil fuels, hydrogen energy is considered a realistic option and research is being conducted with growing attention. Water electrolysis is one of the sustainable methods for producing hydrogen using non-fossil fuels, which can produce high purity hydrogen without significant costs for environmental pollution.

The most common method of water electrolysis is alkaline electrolysis, which promotes the flow of electricity by using an alkaline solution as an electrolyte and separates the generated gas through a diaphragm. Alkaline electrolysis is thought to be in the commercialization stage due to its high energy efficiency and low installation cost, but there is a difficulty that requires a lot of power to implement water electrolysis. Therefore, a good understanding about the process characteristics is required to develop systematic design guidelines to improve energy efficiency. In this study, a mathematical modeling of an alkaline electrolyzer system is designed and the key design variables affecting the performance of electrolyzer are investigated. Through this developed electrolyzer model, the operating characteristics of alkaline electrolyzer systems can be analyzed and the hydrogen production capacity for operating conditions can be predicted.

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Systematic Approach for Prioritizing Critical Sectors for Post-Pandemic Recovery Measures

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Abstract

The recent COVID-19 pandemic has pushed policymakers around the world to impose drastic lockdown guidelines. However, the shocks caused by the pandemic has led to disruptions across economic sectors worldwide. Policymakers have dedicated efforts to contain the effects of the pandemic. But at some point, the containment phase of the pandemic will end, and the economic recovery phase will soon follow to sustaint the national economic. In this phase, it is essential to develop optimal economic measures for post-pandemic recovery. Such economic recovery measures are imperative to allow maximum economic gain from minimal inputs. As such, this work presents a systematic approach to prioritize critical economic sectors for post-pandemic recovery measures based on the developed mathematical optimization model. The developed approach firstly ranks economic sectors based on sector criticality index (SCI) (Yu et al., 2014). SCI is a measurement of five underlying components: (1) economic impact, (2) connectivity, (3) sector size, (4) income multiplier, and (5) employment. Following this, optimization is performed to determine the optimal allocation of economic stimulus among critical economic sectors. To demonstrate the developed, Malaysian palm oil industry is solved. Further analysis of the optimum results with the available government initiatives are also performed.

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Optimal start-up and shutdown operational scheduling of ironmaking

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Abstract

Ironmaking is an essential industry for the manufacturing of steel and other metals used widely on various applications. The production flow of an iron plant is observed in this study, auxiliary units are introduced when the main equipment is shutdown for maintenance. A mathematical framework is proposed for the optimal use of the main and auxiliary units considering the maximum operability of the equipment and minimizing the costs for startup and shutdown while satisfying the iron demand. An operating time of 80 hours is observed in this analysis where it is divided into 8 time periods of 10 hours each. The concept of penalty costs is introduced for instances that the iron production is less than the demand. Several case studies of inoperability in some equipment for certain time periods are solved. The study aims to provide a prospect of having better maintenance for the main equipment in ironmaking.

Process Modeling for Artificial Photosynthetic in Capsules

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Abstract

With breakthroughs in the field of artificial photosynthesis in recent years [Liu *et al*., 2016; Guo *et al*., 2018; Litman *et al*., 2018], photosynthetic is regarded as a promising solution to convert CO2 in the atmosphere into fuel or useful organic compounds. Effective approach to the modeling of the process is of great importance especially for industrialization of the artificial photosynthesis process. The capsules immobilization protocol has been selected to build artificial photosynthesis systems [Cai *et al*., 2018; Ji *et al*., 2016]. However, as demonstrated in many investigations, dynamic properties of the microcapsule immobilization can be hardly described by the traditional microcapsule immobilized enzyme theory, and reliable model to represent or predict behaviors of the photocatalysts and enzymes in the experiments are not available.

This is the motivation of the present work. A mathematical model based on ordinary differential equations is established in this paper to interpret the immobilized artificial photosynthetic process in capsules. We validated our model using experimental data published in the literature. The results show that, regarding the concentration of coenzyme NADH, the prediction by the model is quite consistent with the experimental data. We then extend the model to cover either the steady-state solution and transient solution of the process. The steady-state solution enables us to explain the contradiction between microcapsule immobilization experiment data and the classic theory. The influence of the mass transfer resistance of the microcapsule on the dynamic behaviors of the process is analyzed through transient solution. We analyze the influence of the geometry of the microcapsules on the experimental results as well. We found that the activity of enzyme catalysts and the mass transfer resistance of the microcapsule walls have profound influence on the profitability of the process.

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Modelling and simulation of toxic gas dispersion

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Abstract

Gas chlorine is a toxic and corrosive gas with yellowish-green gas apperance but difficult to visualise. This gas is denser than the air and persists to human breath at ground level. There are emergency responses has been planned by local authorities in order to minimise casualties and damage to the surroundings. An effective system is important to response to any incidents related to toxic gas so more life can be saved during the golden period. However, it is very much dependent on limited human resources, which have slower responses. The objective of thie work are to simulate Jack Rabbit Field Experiment Trial 2 and analyse the effects of adsorption of gas chlorine using a computational fluid dynamics (CFD) simulation called ANSYS FLUENT 14.0. The detailed steps includes the time dependence of the emission release, selection of most applicable source term model for the situation, gathering of specific input data and physical properties necessary for the source term model and finally calculate the source emission rate. The standard k-ε model was used to stimulate turbulence flow of the gas chlorine dispersion. In addition, a continuity equation, a momentum balance equation, a turbulent kinetic energy and dissipitation equation, a species transport equation, a diffusion flux of species equation, a naveir-stokes equation were used as governing equations. Case 1: Modelling and simulation of the Jack Rabbit chlorine release experiment (Trial 2) The JR experiment Trial 2 using the computationa fluid dynamics (CFD) and Case 2: Simulation of chlorine adsorption in a system. Referring to the simulation results, it was found that the vapour cloud formation near the source after 1.1 s and the chlorine gas released from the 2 meter above the ground tends to persists so low to the ground and formation of low level gas cloud. The decrease in cloud height of a flowing dense gas due to the effects of gravity, which is called negative buoyancy. The second part of the reseach focused on the effects of adsorption of chlorine gas by comparing the simulation with and whithout adsorption. The concentration measured at distance 110 m to determine whether adsorption affects the concentration of chlorine gas in an open area. At distance 0 m, the mass fraction of chlorine is 1 coming out from the source and 0.1 mass fraction at distance of 120 m. There are some gaps around the position of 100 m. Similar findings obtained for similation without absorption. It can be conlcluded that the gas chlorine disperse at the lower parts of the domain. Moving to different level can help in escaping.

Keywords: Gas Chlorine, CFD, dispersion, safety

Oleic Acid Molecular Recognition Study as Wax Chemical Inhibitor utilizing Molecular Dynamics Simulation of Material Studio 8.0 Software Package

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Abstract

Among the various flow assurance problems that the petroleum industry is facing, dealing with deposition of paraffin wax onto the wall of pipeline and wellbore is the most challenging. The challenge arises when there is a temperature gradient between the crude oil and wall surfaces which leads to the wax molecular crystal in the crude oil to crystallize. An efficient method in remedying paraffin wax deposition is by utilizing chemical inhibitors. However, currently used chemical inhibitors are costly and environmentally harmful if a leakage/spillage occurs. Therefore, the use of biodegradable or environmental friendly inhibitors as potential chemical inhibitors are being studied by various researchers. This study investigated oleic acid, poly (ethylene-co-vinyl acetate) (EVA) and triethanolamine (TEA) as inhibitors that perform based on the van der Waals intermolecular interaction between the main wax component molecule eicosane $C_{20}H_{42}$ using Molecular Dynamics simulation (MD) procedure via Material Studio 8.0 software package. In order to analyse the desired structural property which is the Radial Distribution Function (RDF), COMPASS force field was used. The RDF and g(r) function portrayed the functional atoms which aid in inhibiting the agglomeration and crystallization of the wax crystal formation. This means that the higher the RDF value, the higher the space between the H59 and H60 molecules, hence the lower the ability of the wax molecules to agglomerate between each other. In this simulation study, we found that at 0.5 wt% and 1 wt% concentration, oleic acid is able to increase the RDF of wax molecules similar to commercial inhibitor, ie: EVA and TEA. Whilst, at 5 wt% and 10 wt% concentration, oleic acid and TEA perfomed better than EVA. It is concluded that the presence of a carbonyl/carboxylic group in oleic acid plays a vital role to inhibit the wax formation through the Van der Waals repulsion force between eicosane wax molecules.

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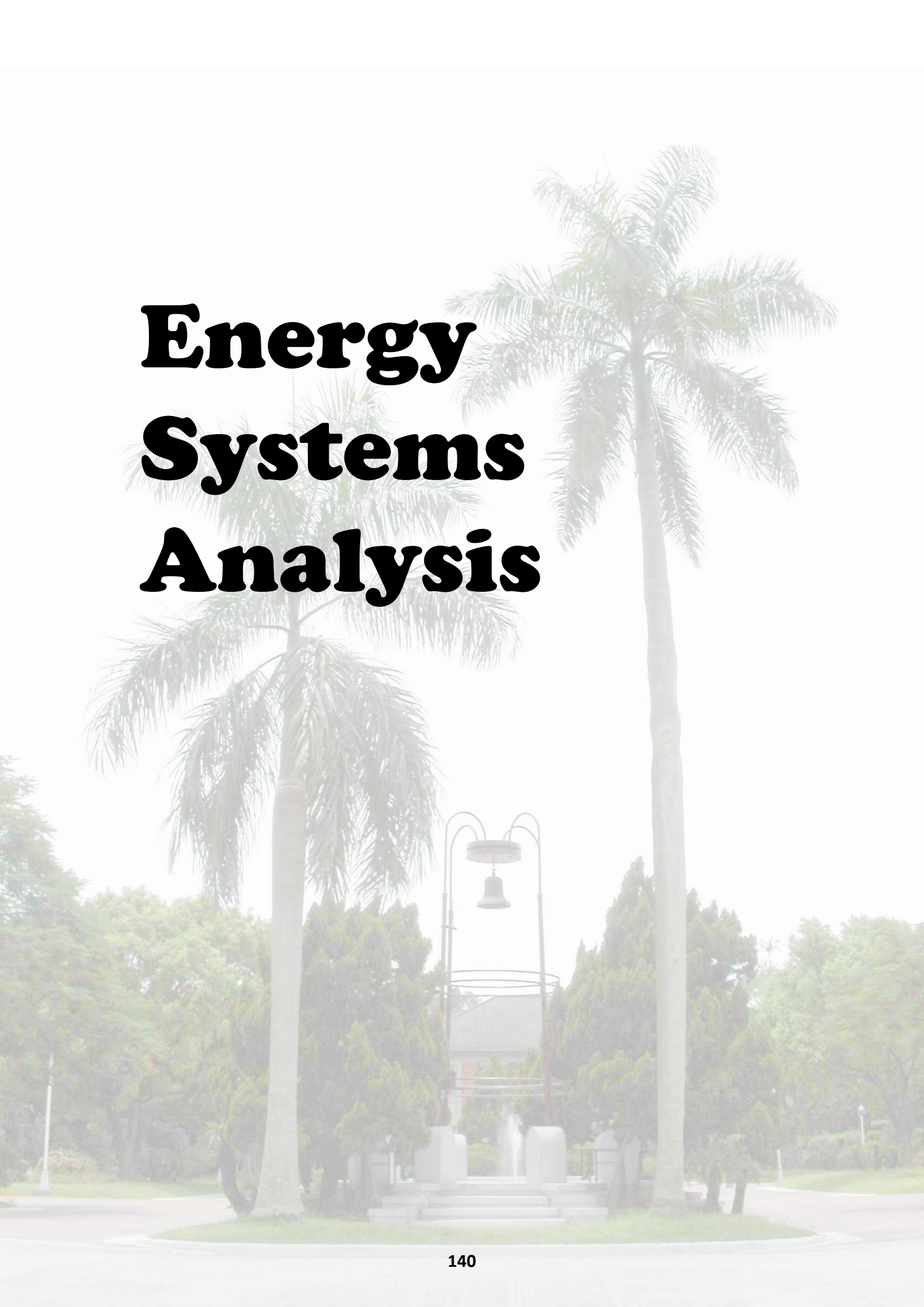

Energy Systems Analysis

Modular design of a new methanol reformed fuel cell vehicle

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Abstract

The feasibility of a proton exchange membrane fuel cell (PEMFC) vehicle coupled with a lightweight methanol reformer [1] is validated by the modular design and simulation analysis. The design procedures include (i) the exergy assessment for major units embedded into the fuel cell vehicle and (ii) the creative 3D modular layout of methanol reformer installed into the automobile chassis. Through the exergy-based modular design procedures, a new configuration of methanol reformed compared to the previous design [1] can reduce 0.18 m^3 of installation space and increase the overall exergy efficiency by 7.26% due to using the low energy duty of heaters and increasing the waste heat recovery of exhaust gas.

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Expert guidelines in power plants for energy optimization

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Abstract

Operators should adjust operating conditions to minimize energy costs, but such frequent adjustment is a challenge for operators. Expert system can provide immediate operational strategies to minimize operating costs. Technically, firstprinciple models and data-driven models can be the kernels of the expert system. However, the first principle models have an offset with the process when the process drifted and have convergence problems; while the data-driven models might limit the prediction ability of the model due to the narrow range of history-data variation. The purpose of the study was to present a hybrid method that combines a process-like first principle model with the data-driven model of deep neuron network (DNN) to establish a robust model as the kernel of the expert system. A large variety of data was generated as a training set of the DNN model by the first principle model to improve the range of DNN predictions. The offset between the DNN model and the real process was eliminated by the transfer learning. The results showed that the hybrid method can predict the data of the first principle model. With transfer learning combined with process data, the DNN model can accurately predicted quality values of power plants.

Keywords: operational strategies, first principle model, deep neuron network

Causal Analysis of NOx Generation of Coal-Fired Power Plant with LiNGAM

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Abstract

Coal has been an important energy source worldwide, and over 30% of electricity in Japan is covered by coal-fired power plants. However, its NOx generation is higher than other fossil fuels, hence precise control of NOx generation is required in coal-fired power plant operation. Although the trend of NOx generation can be theoretically estimated, it is difficult to predict the value of real power plants because there are complicated factors in NOx generation such as boiler design, coal properties, and operating conditions. Therefore, for more effective control NOx generation, precise factors of NOx generation should be identified.

Linear Non-Gaussian Acyclic Model (LiNGAM) is an exploratory causal analysis method, which identifies causal order of variables and their connection strengths without any prior knowledge on the causal relationship among variables. In this study, real operation data of a coal-fired power plant which consists of 53 variables and 10,763 records were collected and used. The operation data include the coal fuel properties such as carbon, nitrogen, and oxygen contents, and the operating conditions such as the flow rate of fuel and air supplied into the boiler. The causal relationships between these process variables and generating NOx values, and their connection strengths on NOx generation were estimated by LiNGAM. In this study, DirectLiNGAM was used for calculation [S. Shimizu, 2011].

Our analysis results indicated that the combustion air temperature was one of the important factors of NOx generation. This is reasonable because higher air temperature causes higher combustion temperature in the boiler, which increases thermal-NOx generation. This result is supported by the previous research that thermal-NOx is generated by the oxidation of nitrogen in the combustion air and its generation strongly depends on the combustion temperature [H. Niko, 2014]. Our results also showed that the steam temperature on a specific side of the furnace wall was another factor of the NOx generation. In our data, the more NOx generation increases, the more the steam temperature on this side of the furnace wall decreases in comparison with the opposite side. It may indicate this NOx increase was caused by the uneven combustion in the furnace.

This research showed that LiNGAM would be a persuasive method since our results agreed with previous reports about NOx generation factors in coal-fired power plants. LiNGAM also suggested the factor about the association of the NOx generation and combustion balance, we need to confirm this point in the future.

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Design and Performance Analysis of a Solid Oxide Cell Integrated System Applied to High-Efficiency Hydrogen Production

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Abstract

The operation of solid oxide cells (SOC) can be divided into two types, namely, solid oxide fuel cells (SOFC) and solid oxide electrolysis cells (SOEC). In the past, researchers have proposed to combine SOEC with SOFC in order to achieve the integrated system energy balance of each other. Although the integrated system can achieve this target, the current density is low which means that it produces little hydrogen [Iora et al., 2010]. In recent years, a new form of SOC has been derived from technological innovation, called fuel-assisted solid oxide electrolysis cells (SOFEC) which requires lower power than the conventional SOEC [Patcharavorachot et al., 2016]. With the advancement of technology, people have begun to pay attention to environmental issues. Hydrogen is considered to be a new generation of clean energy carriers in recent years. Therefore, this study proposes a new integrated system combining fuel-assisted solid oxide electrolysis cells (SOFEC) and solid oxide fuel cells (SOFC) for hydrogen production. In the integrated system configuration, the SOFEC anode outlet stream which still has hydrogen-rich fuel can be used as a fuel for power generation in the SOFC included in the integrated system. The electrical energy and thermal energy generated from the SOFC can also be supplied to the SOFEC as an energy integration. In addition to the fuel required for SOFC, integrated system can also operate independently without power input under specific operating conditions, and generate hydrogen, electric energy and heat energy. Under this operating condition, the system can become combined hydrogen, heat and power (CHHP) integrated system, the main operational variables considered in the study include operating temperature, cathode recycirculation, fuel utilization of SOFC, fuel inlet to the system and electrolysis utilization of SOFEC. The overall performance of the CHHP integrated system will be evaluated through system simulation. Simulation results show that the integrated system can achieve independent operation by adjusting the operation parameters at high electrolysis utilization.

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Simulation of energy flows at a paper mill with thermal energy storage for reducing greenhouse gas emissions by wind energy

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Abstract

Power generation by variable renewable energy (VRE) is increased for decarbonization, although it is difficult to ensure stabilization of the energy demand due to fluctuations in the power output from VRE. To accelerate VRE implementation, the combination of wind-thermal energy converters and thermal energy storage (TES), called wind-powered thermal energy systems, has been proposed [Okazaki, 2015]. In this study, we examined thermal energy storage system at a paper mill (TESP) and simulated energy flows of paper mills with/without TES. Paper mills use large amounts of energy generated from in-house boilers and turbines fueled by fossils, wastes or by-products from paper milling processes.

A concept of TESP is that thermal energy from many kinds of fuels and VRE is stored in TES and converted into steam or electricity [Yamaki, 2019]. Excess heat stored in TES can be applied into generating transmittable power to the power grid to reduce other dispatched power sources, assumed as coal-fired one for baseload power. Life cycle assessment was used to assess the environmental impacts of TESP, e.g., greenhouse gas (GHG) emissions.

With the installation of TES and wind energy, transmittable power could be increased with GHG emissions reduction. However, their excess installation or unbalanced combination resulted in an increase in GHG emissions and a decrease in transmittable power by the lowering of the average temperature of TES due to the shortage of thermal energy input filling the capacity of TES. Appropriate capacity of TES can efficiently convert thermal energy stored in TES into steam or electricity. The possibility of operating the paper mill without fossil fuels was investigated.

We conducted simulations to design appropriate specification of TES depending on paper milling process and operation. Stored energy in TES can be applied for providing transmittable power derived from wind energy. Paper mills with TES can be regional suppliers of power and thermal energy derived from distributed VRE.

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Integration of Hydrogen Production and Greenhouse Treatment by Utilizing Nitrous Oxide as Sweep Gas for Solid Oxide Electrolysis Cell

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Abstract

Solid oxide electrolysis cell (SOEC) for hydrogen production is generally operated at thermoneutral voltage, at which the cell does not generate or require additional heat. When SOEC is operated above the thermoneutral voltage, it consumes more electricity energy. However, operating below the thermoneutral voltage will cool the cell and result in a temperature gradient within the electrode due to the endothermic cell reaction. In order to avoid the circumstances, SOEC requires more heat input to maintain a constant temperature. Apart from this, the use of a thinner electrolyte can reduce ohmic polarization that dominates the total polarization to decrease the cell voltage (power consumption) but increasing the heat consumption. There is an experiment using nitrous oxide as the oxidant entering the solid oxide fuel cell (SOFC), and it not only indicates that the N_2O is an operable oxidant but also shows nitrous oxide can improve cell performance, successfully integrating the electrical generation and greenhouse treatment [Li et al., 2016]. Recently, nitrous oxide, namely laughing gas, has become a global concern for its high global warming potential which is 298 times greater than that of carbon dioxide and it can be produced from many industrial and agricultural activities. Conventional removal of N_2O requires high temperature and catalyst to which SOEC can conform. Because the SOEC is operated at high temperature and its electrode is a catalyst of N_2O, nitrous oxide can decompose into nitrogen and oxygen, which can be used as a N_2O treatment. In this paper, we propose to use nitrous oxide instead of air or pure oxygen as the sweep gas for SOEC. Simulation study for the SOEC system is carried out. With the heat released from the decomposition of N_2O, SOEC can be operated below the thermoneutral voltage so as to expand the operable range, be suitable for thinner electrolyte, and improve the hydrogen production efficiency of the system.

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Global potential for carbon reduction via renewable energy and negative emission technologies: a systematic approach

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Abstract

Due to the delayed action in climate change mitigation, we need to multiply our efforts in the next decade to avoid the growing threat of abrupt and irreversible climate change. Learning from the COVID-19 experience, an effective and sustainable greenhouse gas mitigation strategy is urgent with immediate actions needed in a short response time. The practical implementation requires us to know where the resources locate and how to plan the utilization of the resources. Renewable energies (RE) are critical alternatives to fossil fuels for emission mitigation and negative emission technologies (NET) are promising candidates to mitigate emissions by removing CO_2 from the atmosphere. As the intersection of both, bioenergy with carbon capture and storage (BECCS) and biochar (BC) are two key NETs based on the thermal conversion of biomass. However, the amount of renewable resources is usually constrained by the geographical boundaries. There is a lack of geographical survey on the carbon mitigation and reduction potential that could be synthetically achieved by RE, BECCS, and BC in different regions around the world. This study sheds light on the carbon mitigation and reduction potential achievable by such combination of technologies globally and provides an overview of the best options for technology implementation to meet the Paris Agreement from a global perspective.

A snapshot of the current waste, emission, and policy information in different countries around the world was first obtained according to real-world data sources. The GP_assess (Global Potential assessment) tool, containing the conversion models for the RE technologies and NETs as well as the economic and emission assessment models, was then applied to estimate the economic and emission reduction potential for the deployment of different technologies in different regions. The marginal profit and the consequential life cycle greenhouse gas emission caused by technology deployment were used as the economic and environmental evaluation metrics. Uncertainty analysis was carried out following the IPCC good practice guidance. The data-driven GP_project tool was further developed to estimate future profiles of global temperature rise for the scenarios of technology deployment in any region at a given time point. The GP_optimize, a mixed-integer linear programming (MILP) optimization model, was finally used to recommend the most suitable technologies and regions for technology deployment based on the economic and climate-change-mitigation objectives from a global view.

The result shows a globally net-zero emission is achievable when the BECCS and BC are used together with solar and wind technologies, although not all the countries could realize negative emissions. The ranking of the conversion technologies based on economic, environmental, and technical readiness levels for each region was also demonstrated.

Oxy-Fuel Power Generation with CO_2 Capture using Liquefied Natural Gas Cold Energy

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Abstract

As the annual importation of liquefied natural gas (LNG) increases gradually, LNG cold energy recuperation and reutilization during regasification process is attached great importance in order to enhance energy efficiency of imported fuel and decrease the enviromental impact. Zhang et al. (2010) proposed a novel CO_2-capturing oxy-fuel power system with LNG coldness energy utilization (COOLCEP) that has integrated both power generation cycle and LNG regasification cycle to form a high energy efficiency system. Like a Rankine cycle, COOLCEP system uses CO_2 as working fluid driving turbines to generate electricity and LNG acts as refrigerant to liquefy CO_2 before CO_2 is being pressurized by pump. In addition, low temperature pressurized CO_2 stream (about -50^{o}C) can acts as a cold energy source for other systems during evaporation. The evaporated CO_2 is then mixed with O_2 stream and sent to the combustor before driving the turbine. The CO_2 that produced from the combustion is captured after condensing. However, there are still some drawbacks existing in the system. The CO_2 capture section in the system that compresses and condenses the mixed gas stream is recognized as an energy-intensive strategy. Secondly, it is not realistic as what Zhang et al.(2010) assumed that the H_2O in the CO_2 stream can be perfectly removed before sending to the condensation unit. Furthermore, the power generation efficiency can be improved by increasing the CO_2 pump pressure and the combustor temperature. Hence, system modification, sensitivity analysis, heat integration and economic evaluation is carried out to enhance the performance of system. Moreover, reheated system is also considered to obtain an optimized system. The Optimized Reheated System shows its superiority to annual revenue and CO_2 recovery which are 15.8 MUSD and 57.32% respectively on the basis of recirculating CO_2 flow rate at 60.45 kg/s and LNG flow rate at 58.30 kg/s. The concentration of captured CO_2 stream is 99.75 mol%. In this case, the application criteria is the instrument materials should be improved and allowed the turbine inlet temperature (TIT) and heat exchanger inlet temperature (TBT) reach 1700^{o}C and 994^{o}C respectively. With the same basis, Optimized HI Modified System-S has the greatest thermal efficiency (69.03%), it reflect the system require lesser fuel to produce electricity. The highest thermal efficiency does not mean a significant revenue because the total amount of generated electricity is relatively low compare to other optimized system but the capital and operating cost is still high.

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Life Cycle Assessment of Phenol Production via Cumene Process

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Abstract

Phenol is an essential industrial intermediate in the commercial production of bisphenol-A (BPA), nylon, epoxy resin, and polycarbonate; furthermore, they are commonly used as a raw material in the manufacturing of drugs and household products. The main route for producing phenol is cumene peroxidation process (Hock Process), which produces acetone as a co-product (Hock and Lang 1944). Life Cycle Assessment (LCA) is used for analyzing and assessing environmental impacts (EPA 2006). In this study, the phenol production via cumene peroxidation process was investigated by considering a part of the production process (Gate-to-Gate). The process was simulated by using Aspen Hysys program. The environmental impact assessment were evaluated through the Eco-Indicator 99 method (Frischknecht, Jungbluth et al. 2007), which covers the assessment of human health, ecosystem, and resource depletion, and the carbon footprint technique (Wiedmann and Minx 2008). The study showed that the environmental impact based on single point of the phenol production was 190 Pt and the carbon footprint of the process was 13 kgCO_2e.

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Reformulation of Heat Exchanger Network Synthesis for Better Industrial Implementation

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Abstract

There are a large number of highly sophisticated mathematical-programming-based approaches for synthesizing heat exchanger networks (HENs), these approaches usually generate the optimal or quasi-optimal solution of the mathematical model. This solution is not necessarily acceptable for industrial implementation. For implementing a HEN, in addition to cost minimization, further practical requirements must also be satisfied. For instance, complicated piping arrangements, controllability concerns, or safety issues may exclude the proposed solution. Therefore, the single "optimal" solution is not necessarily a good base for the final design.

Instead of reducing the search space of HEN synthesis to a single solution, another possible philosophy is to generate all HENs that satisfy the general requirements of the designer for later selection of the most preferred network. For example, the generation of all HENs that consume minimum amount of utilities can be the base of the selection of the designer.

Enumeration type HEN synthesis method has been developed on the basis of the formerly available P-graph framework. The proposed method is capable of generating all HENs that have minimum (or at most a prespecified) utility consumption and satisfy additional structural constraints. The generation is exhaustive, still the number of the generated networks is surprisingly small. For example, 368 HENs were generated in a case study for the extensively examined synthesis problem of Papoulias and Grossmann [1983].

Though it was not the purpose of the current work to improve the single solutions generated by other approaches, still there is an improvement in the cost. There are several networks better in terms of cost than the best found solutions (see e.g., Escobar and Trierweiler, 2013; Bao et al., 2018; and Kayange et al., 2020).

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Design and Analysis of Energy Systems for Electrified Chemical Processes

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Abstract

Conventional utility system in chemical processes is highly dependent on fossil fuel, in which steam is in the highest demand. Steam is usually generated with boiler, where combustion heat of fossil fuel is transferred to water. It can bring issues such as enormous emission of greenhouse gases, leading to high ambient temperature. To solve the current situations, Paris Agreement was effectuated in 2016, urging aggressive actions to go sustainable.

In response to the enhanced awareness, measures taken by the industry came to shape of decarbonization. Proven technology among the various decarbonization methods is electrification, which is also referred as power-to-heat technology. Electrification has a long history, especially, when it comes to microwave heating. However, attention is paid recently, due to the surplus electricity from grid and prevalent production of electricity based on the renewable resources. It is believed that the development of electrification technology and increased generation of electricity based on renewable resources can bring synergistic effect to enhance sustainability.

The goal of this study is to investigate the feasibility of electrified chemical processes when it is compared to the conventional energy system. It is demonstrated with a case study of oil refinery. One of the widely accepted technology, namely, heat pump, is considered and its process model is developed. Analysis of the energy system is based on Heat Integration. Specifically, maximum energy recovery is achieved with Composite Curve, while Grand Composite Curve directs efficient use of utility. The utility system is assessed under different source of energy including fossil fuel. The results implies that further reduction in the electricity cost is required to break the economics of fossil fuel system.

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Artificial Intelligence and Big Data in Chemical Engineering

Using Big Data Analytics to Reduce the size of High-Dimensional Attributes for Multiscale Decision-Making: Applications to Energy Hub Demand Data

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Abstract

It is trustworthy proven that supply chain management and optimization has superior performance in driving the profits while sustaining customer satisfaction. Different decision levels with different time scale are usually involved in managing supply chain enterprise-wide operations. Integration across a supply chain decision levels is crucial on improving investment returns. However, integration of different time scales level leads to large scale problems usually computationally intractable. In addition to that, modelling modern Supply chain facilities become more complex. Therefore, it is necessary to develop new tools to overcome the new challenges and reduce its complexity. In this work, the goal is to develop novel clustering methods with multiple attributes to tackle the integrated problem. As a result, a clustering structure for shape-based time series data with multiple attributes is proposed. The clustering structure is formulated as Mixed Integer Nonlinear Program (MINLP) with a multi-objective optimization approach (since different attributes have different scales or units). The MINLP then converted into a Mixed Integer Linear Program (MILP) using linearization techniques. The developed clustering algorithms can work with real-time and Multiple-dimensional data patterns. The proposed clustering approach can be applied in long-term scheduling and integrated scheduling and planning problems.

Keywords: Multiscale, Clustering, High-Dimensional Attributes, Modeling and Computational performance.

An Expansion strategy for optimization of ethylene cracking furnace based on ANN combined with RSM

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Keywords: Ethylene cracking furnace, expansion, ANN, RSM

Abstract

As a basic product in petrochemical industry, ethylene plays a pivotal role in economy and living standard. Cracking furnace is one of the key equipment of large ethylene production plant. The quality and yield of the main products in the ethylene cracking furnace is determined by the operation level and optimization situations.

In recent years, many studies have been carried out on optimizing the operational conditions of cracking furnace and scheduling the cracking system. Geng et al. designed an adaptive multi-objective particle swarm optimization (AMOPSO) algorithm based on dynamic analytic hierarchy process(AHP), which adopts fuzzy consistent matrix to select the global best solution. Yu et al. developed a self-adaptive multi-objective teaching-learning-based optimization algorithm to solve the multi-objective optimization problem. To summarize, the optimization of ethylene cracking furnace has been handled properly by AMOPSO and teaching-learning-based method. However, these methods are based on a wide variety of data to ensure the accuracy of the algorithm. For those plants with urgent demands for the operation optimization but without enough data, or even sometimes the range of the operation conditions is unknown, these methods might be unfeasible to be implemented.

In this paper, we design an expansion strategy based on artificial neural network (ANN) combined with response surface method (RSM). For the first step, initial data are available or designed by D-optimal design. Then, we determine the effect of independent variables on dependent variables by RSM to obtain the expansion direction and length. After that we use ANN to predict dependent variables in expansion space, select the top data and add these new data into initial data. The iteration would not be stopped until the new operation is no longer better than previous operation. This method is used in a specific ethylene cracking furnace whose batch length is constant to maintain the stability of cyclic production. The simplified three-parameters coil outlet temperature (COT) curves are utilized to optimize product value with restriction of defined cracking severity range. The strategy is helpful to quickly find the optimal solution with less data in this case. In addition, it is applicable in other ethylene cracking furnace with less data and unknown variable range.

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Uncertainty Quantification for Estimating Molecular Weight Distribution by Gel Permeation Chromatography

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Abstract

Estimation of molecular weight plays an important role in development of polymer materials. Unlike the molecular weight of a single molecule, the molecular weight of a polymer material is quantified as a molecular weight distribution. Molecular weight distribution is one of the important factors that determine the physical properties such as strength and fluidity of polymer materials. Gel permeation chromatography1) (GPC), a technique to obtain molecular weight distributions, is widely used for polymer compounds. In gel permeation chromatography, separation is achieved by the difference in the molecular size. The relationship between the molecular size and the molecular weight can be approximated by a polynomial, which is called a calibration curve.

The calibration curve is used for molecular weight measurement, but there is a problem that a calibration curve is required for each molecular species, and a method capable of measuring the molecular weights of various molecules with one calibration curve is required. For this problem, the universal calibration curve approach2) can handle multiple polimers. The relationship between the molecular size and the molecular weight differs depending on the type of molecule. Therefore, a calibration curve that considers the size of the molecule, that is, a universal calibration curve, is necessary. In this approach, the intrinsic viscosity, which is one of the indexes that express the size of the molecule, must be obtained for each polymer.

The purpose of this study is to quantify uncertainty of molecular weight distributions using Bayesian estimation. Although the universal calibration curve approach has been studied since the 1960s, the uncertainty of the obtained molecular weight distribution has not been addressed. The slope and intercept of the universal calibration curve and two constants in Mark-Houwink's formula representing the intrinsic viscosity are estimated as parameters. We also estimated the credible intervals of the parameters, and examined the uncertainty as probability distributions using Bayesian estimation from obtained data. Since the integration that appear in the Bayes' theorem cannot be calculated analytically, the Markov chain Monte Carlo method was used as an approximation method.

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Hybrid intelligent IAQ management framework for environment-energy-risk improvement in subway station using ensembled deep learning and fuzzy TOPSIS technique

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Abstract

Mechanical ventilation systems have been widely employed to alleviate low indoor air quality (IAQ) since passengers are directly or indirectly exposed to fine dust in indoor air of subway stations [Heo *et al.*, 2019]. However, due to time-varing and highly-flucutating trends of IAQ that are influenced by several outdoor and indoor environemnts, real-time control trading off bewteen energy saving and IAQ improving has limitation on a conventional ventilation system [Nam *et al.*, 2020]. Therefore, to deal with the various IAQ circumstance, this study proposes a data-driven and intelligent IAQ management framework for ventilation system, based on the hybrid deep learning(DL)-based outdoor air quality (OAQ) prediction and fuzzy TOPSIS-based control system. The proposed method for the hybrid IAQ management is divided into four main parts. First, the IAQ process and its relationships with OAQ, passing subways, and passengers were identified. Second, DL-based prediction model was employed to predict the nonstationary and nonlinear dynamics of OAQ, which is major disturbance variable on the IAQ process. Third, fuzzy TOPSIS algorithm was implemented to logically discriminate the IAQ process by analyzing the conflict objectives of environment, economics, and risk. Finally, DL-based tree search algorithm was employed to suggest optimal control policy for discriminated the IAQ processes by the fuzzy TOPSIS, so as to minimize the energy and risk while improving the IAQ. The proposed hybrid prediction and control system was compared with the manual ventilation systems on subway stations in terms of total environemtal, economical, and risk evlauations. The hybrid system showed high prediction performance on OAQ and improved IAQ and operating efficiency since the system reflected uncertainties and simultaneous consideration of the positive and the negative slutions.

Acknowledgement

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Automated Synthetic Pathway Design Support System Based on Public Data in Terms of Safety

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Abstract

As the Industry 4.0 has recently emerged, computer technologies such as artificial intelligence technology and data analysis have attracted attention, and many of the data underlying this technology are made up of private data as well as data that can be accessed through the Internet. Among them, data related to chemical engineering such as chemicals, reactions, safety, and risks are essential for researchers to search before starting projects like experiments and process design. However, this information is widely spread on the Internet and formats are also different, so searching is not easy. Difficulties in selecting an appropriate synthetic pathway also exist because reactants used for each pathway are different. Despite the efforts of researchers to prevent safety accidents, various safety accidents such as laboratory safety accidents and reactor operation accidents are still occurring due to the difficulty in retrieving information. In this study, we proposed a smart pathway search and generation system via open source and open data to help solve these problems. System DB construction was conducted through automatic Web Crawling with Python and is based on open data collection.

In general, operation time of search algorithms increases in proportion to the number of data. In order to improve operation time, we made chemical reaction data into digraph network data. The algorithm was set up in a way that prunes data that is not related to the target chemical. The weight of the algorithm is determined with the degree of risk of the reaction, the hazards of the reactants and products. A change of reaction energy was calculated for the risk of reaction. The hazards of chemicals were classified with relevant public data. Based on the data like reaction, hazard, risk and energy, results are generated by searching within a specified step. Synthetic pathways generated through algorithm appear with a knowledge graph, which shows pathways from the target chemical node to substrate nodes, and represented in a tree format, which shows what information each pathway has. Each node of a knowledge graph is displayed in a different color according to the degree of risk, and a result shows the reaction information, the chemicals used, risks, and hazards for each node. The DB can be continuously updated through automatic Web Crawling. A system test was performed using small random data from the DB. Compared to another S/W that shows proper results under certain expert conditions or designs direct synthetic pathways by a human, the proposed system has the advantage of automatic generation of synthetic pathways that can be applied over a wide range based on huge open data.

Big Data Analysis of Plant Operation Data for Identification of Repeating Sequential Alarms

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Abstract

Plant alarm system notifies an operator of plant state deviations. The advance of distributed control systems (DCS) in the chemical industry has made it possible to inexpensively and easily install numerous alarms in DCS. A poorly designed alarm system might cause sequential alarms. Sequential alarms reduce the capacity of operators to cope with plant abnormalities because critical alarms are buried under many unnecessary ones.

Nishiguchi and Takai (2010) proposed a mining method of sequential alarms in plant operation data using event correlation analysis. The method can identify sequential alarms from the operation data of chemical plant, but it occasionally failed to detect similarities between two physically related sequential alarms when deletions, substitutions, and/or transpositions occurred in the alarm sequence. Wang and Noda (2017) proposed a mining method of sequential alarms in plant operation data using dot matrix method. The method can identify sequential alarms from the operation data of chemical plant, but it occasionally failed to detect sequential alarms between two related sequential alarms when two types sequential alarm occurred at the same time.

In this research, we propose a new identification method of sequential alarms by analyzing plant operation data. In the method, plant operation data is converted into alarm subsequences using windows. All combinations of alarm subsequences are compared, and repeating similar subsequences are identified according to the similarities between them. The alarms in each repeating subsequence comprise a sequential alarm. Proposed method was applied to the simulation data of an azeotropic distillation column. Simulation results showed that the method can extract sequential alarm in plant operation data.

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Identifier Information based Variable Extraction from Scientific Papers for Automatic Physical Model Building

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Abstract

Physical models are crucial for process design, construction, and control. When building a physical model, we look for a model that meets our demand, and if such a model exists, we implement and use it. Although many researchers have proposed many types of models, it is not easy to find the desired model in the literature, such as articles, books, and web pages.

We aim to develop an automatic physical model building system that extracts information about models of a target process from papers and books and builds a physical model. One of the essential pieces of information in building a model is the information about the variables included in the model. For example, when we want to build the model which contains variable *A*, any model that does not contain variable *A* is useless. Many of the previous studies, such as [Pagel and Schubotz, 2014] and [Schubotz *et al.*, 2016], aim to extract the meaning of the equation and the equation itself. Those methods, however, cannot extract all of the variables and the meaning of variables. Also, many of the conventional variable extraction methods are based on supervised learning and require labeled data. Since physical models have been proposed for various processes, it is impossible to create labeled data covering those models.

As a first step towards the realization of an automatic physical model building system, we focus on a method for correctly extracting variable identifiers and their definitions from scientific papers. In this research, we propose a method of variable extraction using information about which identifier is used in the variable. For example, temperature and pressure usually expressed as "*T*" and "*P*," respectively [Seborg 2011]. The subscripts also have useful information, e.g., the steam temperature is represented by "T_S." Tests with simple documents showed that the proposed method could extract the meanings in good agreement with the actual meanings.

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Safe Reinforcement Learning for Process Control

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Abstract

With the development of parallelization and deep learning, reinforcement learning, which has been successful in various fields such as video games and board games, is also attracting attention in the process industry. Advanced process control generally requires a high level of expertise in the design of controllers and the construction of process models. And even those with such knowledge have devoted a lot of time and effort to it. By contrast, reinforcement learning can only learn the optimal policy from data obtained by interacting with the process. From this property, reinforcement learning can theoretically learn optimal control in real-time while adapting to the environment.

Several recent studies, such as [Spielberg, 2019] and [Wang, 2018], have discussed the possibility of applying reinforcement learning, especially model-free deep reinforcement learning, to process plants. Reinforcement learning agent generally treats learning as a failure and initializes states when process-derived constraints or state-space limitations for efficient search are violated during learning. Because the reinforcement learning agent learns the optimal policy through such failures, a certain number of failures will inevitably occur during learning. However, previous studies have not mentioned these failures. Therefore, this study aimed to reduce failures during learning to expand the application potential of reinforcement learning.

We applied an idea similar to the one proposed in [Dalal, 2018], modified it to make learning suitable for process control applications, and succeeded in reducing the number of constraint violations during learning. First, before reinforcement learning, we constructed a neural network that uses the current state and action as input to predict the next state. Then, during reinforcement learning, we used a pre-learned neural network to modify the action so that the change of action would be minimal if the next state violated the constraint. We found a decrease in the number of constraint violations during learning for simple blending processes when using Deep Deterministic Policy Gradient as a baseline reinforcement learning method.

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Stage Selection with Group-Lasso for Prediction of the Yield Rates Depending on Machine Combinations in Multi-Process Production System

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Abstract

In a multi-process production system such as a semiconductor manufacturing process, products are manufactured through multiple stages, and each stage has parallel machines. In such a production system, the machine combinations may affect the yield rate of final products. For example, if machine A in stage 1 and machine B in stage 3 have a strong interaction with each other, the yield rate of the final products will increase or decrease by using the two machines together. Hence, the use of appropriate machine combinations can improve the yield rate of the final products.

In a large scale production system that has many stages and machines, it is difficult to examine the yield rates of all machine combinations because the number of machine combinations is enormous. Therefore, to get the yield rates of all machine combinations, we have to predict the yield rates of the unused machine combinations from the yield rates of the used machine combinations. Suzuki et al. constructed prediction models of the yield rate using various regression methods and compared them [Suzuki, 2019]. They showed that field-aware factorization machines (FFM) [Juan, 2016] can predict the yield rates and identify important machine pairs with high accuracy.

In the yield rate prediction method proposed by Suzuki et al., the prediction accuracy decreases when the ratio of used machine combinations to all combinations is insufficient. To solve this problem, we attempt to remove stages that have little effect on the yield rate of final products from the prediction model. By reducing the stages, we can decrease the number of machine combinations required to construct the prediction model that achieves certain prediction accuracy. In our presentation, we propose the stage selection methods with group lasso [Yuan, 2006], which is one of the variable selection methods, to select the important stages efficiently. Also, we compare the method with the forward stage selection method and the backward stage selection method in terms of prediction accuracy and computation time.

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Equipment Monitoring and Fault Diagnosis to an LDPE Autoclave Reactor by Machine Learning

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Abstract

Autoclave reactor works at a particularly harsh condition where the operation pressure and temperature is about 1800 atm and 200℃. To ensure the well mixing of reagents, a unique stirrer which can withstand such ultimate condition is utilized. These conditions are challenge the bearing lifetime of stirrer. This study presents two machine learning methods to identify the potential failure to reduce risk.

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Boosting Monitoring Performance for Nonlinear Processes with Limited Samples Using Gaussian Mixture Latent Distribution in Variational Autoencoders

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Abstract

In the chemical industry, manufacturers produce various types of products with different grades to fit customer needs and market demands. Multi-grade products are produced via the same production line with different operating conditions of raw materials. If 50 grades of products are made per year, each of the grades is produced for no more than a week and then it will be changed to another one. The limited samples collected in a week are insufficient to build individual models for each grade. Transfer learning has attracted attention from researchers because it relaxes the hypothesis that the training data must be independent and identically distributed with the testing data. However, most of the transfer learning algorithms with the two-step procedure would cause information loss. As only the general information of the target and source domains is obtained, it is not really helpful for the target model.

In the past decade, multivariate statistical process monitoring methods with either the projection or probability approaches were developed. Principle component analysis (PCA) and probability PCA (PPCA) are the most popular process monitoring methods. However, because of the process nonlinearity in chemical plants, the performances of PCA and PPCA are limited as they are linear methods. Then the kernel PCA (KPCA) with a shallow structure and the stacked denoising autoencoder with a deep model structure were developed to solve nonlinear problems. The variational autoencoder (VAE) was also developed by adding latent variable constraints to the deep model structure. Nevertheless, these process monitoring methods were developed under the assumption that the collected process data are evenly distributed in a wide region and they are sufficient to build a reliable model.

In this research, a model called Gaussian mixture variational autoencoder (GMVAE) is developed to share and transfer information from one grade to another. Since the information obtained from the insufficient samples of each individual grade is limited, the information from another grade may provide similar and helpful information for the enhancement of the monitoring performance of the target grade. The objective of constructing the GMVAE model is twofold: With the unique characteristic of the target grade, the common direction of both the target and the source grades is defined using the complementary encoder and decoder networks to extract the common information among the target and the source grades. Also, with a simultaneous one-step procedure, the extracted features from the source grade can be used for the target grade in the modeling process. Based on the constructed GMVAE, the probability densities of latent variables and residuals rather than point estimates are then given so that distribution-based monitoring indices of the target grade can be designed and the fault detection decisions can be made opportunely. An industrial ammonia synthesis process will be presented to show the effectiveness of the proposed method.

Developing Dynamic Soft Sensor Based Variational Autoencoders

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Abstract

A common obstacle in the implementation of soft sensors onto the on-line prediction of the quality variable is attributed to the dynamic and nonlinear characteristics of the chemical plant. The soft sensor is typically trained under the assumption of a steady-state condition. However, chemical plants generally have dynamic properties and complex correlations among a large number of process variables and disturbances,. Those properties and correlations ultimately affect the underlying quality data of interest. This causes most of the predictions to be inaccurate in representing the system as the model does not learn the underlying dynamic characteristic of the process. Thus, the dynamic data-driven model is proposed to learn the dynamic properties of the system using a huge number of historical data.

A common method of extending data-driven models to learning the dynamic properties of the system is using moving window. The moving window mimicks the concept of autoregressive moving average exogenous time series model, which simply extends the data to the matrix form to include the data at each specific time point within the specified past time range. Thus, DPCA (dynamic principal component analysis) and DPLS (dynamic partial least squares) are proposed to solve the dynamic properties of the data. However, like the original PCA (principal component analysis) and PLS (partial least squares), DPCA and DPLS are still limited to linear processes. Then, by applying kernel tricks to DPCA and DPLS, DKPCA (dynamic kernel PCA) and DKPLS (dynamic kernel PLS) were respectively proposed to solve nonlinear dynamic processes. However, with a huge number of data available in chemical plants, kernel tricks have limited usage as the computational load of training models with huge data would be too large. The shallow nonlinear structure in DKPCA and DKPLS also means that the model cannot solve a complex nonlinear system. Recently, data-driven soft sensor models were proposed based on deep neural networks, such as stacked autoencoders and VAE (variational autoencoders). Nevertheless, these deep soft-sensor models were still assumed to be developed in the static condition; it is necessary to develop a model for dynamic systems.

In this paper, a latent dynamic variational autoencoder is proposed. According to the principle of Kalman filters, the proposed method models the dynamic properties using the bi-directional RNN (bi-RNN) framework. The dynamic changes are learned in a non-linear fashion without the constraint of the LGSSM model. The input data are projected to a lower dimension to remove noises and disturbances while the computational load can be significantly reduced during learning of the dynamic properties in the latent space. The bi-RNN is also a robust learning method. It move the data in a cyclical loop, in which the forward RNN models the dynamic relation in the data while the backward RNN adjusts the parameters accordingly to prevent the over-fitting issue. A CSTR study is conducted to show the effectiveness of the proposed method.

Small Data Integration for Process Modeling by Feature Learning via Deep Convolutional Autoencoder

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Abstract

In recent years, "big data" has become a popular concept in research and industry. However, in high value-added manufacturing industry, it is common that only a small amount of data is collected especially at the design stage, which poses a serious challenge to data-driven process modeling. Therefore, there is great necessity to integrate the "small data" measured in different tasks and build the process model by sharing the information. The problem investigated in this study is the modeling of a twin screw extrusion process. In the design stage of this process, a small amount of process measurements are collected under different combinations of screw elements. It is desired to integrate all these process data by incorporating the qualitative variables, i.e. the schematic diagrams of screw elements, into the modeling of this process. Herein, a deep neural network is designed to solve this problem, where a convolutional autoencoder is used to extract the geometric features of each screw element which are combined with the quantitative process conditions as the inputs of a feed-forward neural network to produce the final predictions. The case studies illustrate the feasibility of the proposed network, showing that the model has good prediction accuracy and interpretability.

Investigating Factors Affecting Future Circularity with Machine Learning

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Abstract

Recent academic works, industry initiatives, and government interventions align itself with Circular Economy as sustainability paradigm. Circular Economy promotes recirculation, prolonged utilization, and resource efficiency as attractive economic tools. It aims to integrate economic sectors to the end-of-life component of physical products. Attaining a state of circularity decouples a system from material dependency, promotes economic growth, and reduces total emissions. Shifting current practices towards circularity, however, requires a guiding performance indicator for assessment. On a country-wide performance, aggregated material flow provides crucial information on circularity. Domestic material consumption (DMC) is among the integral measurement [Mayer et al., 2019]. The indicator, however, provides a concurrent assessment of circularity describing assessment on snippets of time frames. Understanding the factors that enable the reduction of DMCs will help in planning strategic interventions. This work, therefore, investigates the factors that reduce future DMCs through a machine learning approach. This work employs machine learning techniques, artificial neural networks and decision trees, due to the high complexity in recognizing patterns between the factors and future DMC. Predictors considered in this work are the factors outlined in the Global Innovation Index (GII) due to its broad scope of indices. The following GII factors institutions, human capital and research, infrastructure, market sophistication, business sophistication, knowledge and technology outputs, and creative outputs of the countries, were considered as the predictors. The results revealed that the decision trees performed better than artificial neural network with an accuracy of 66.90%. Comparison with other machine learning algorithms may improve the prediction accuracy in future studies. Future works can utilize the findings of this work in assessing the enablers of the Circular Economy.

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Real-time Intelligent Knowledge Service as Symptom-based Expert for Advanced Response to Chemical Hazards (SEARCH)

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Abstract

The risk of chemical accidents is increasing as the volume of chemicals in circulation increases, and chemical exposure accidents have the risk of expanding the casualties if the initial response is inadequate. However, existing chemical detection technologies are focused on developing technologies to respond to leaks, and research based on symptoms of chemical exposure is insufficient. Research is needed to quickly detect exposed chemicals when unexpected symptoms are found on the site and to cope with dangerous situations. To analyze and data the symptoms in chemical exposure accident or chemical contact, we intend to build domestic and international symptom knowledge as a knowledge base. Based on the knowledge base established, we would like to develop a symptom-based chemical estimation algorithm that can detect dangerous situations based on mechanical learning and take immediate action on site.

Keywords : knowledge -base, chemical contact information, machine learning

Artificial Neural Network for Predicting Discharge Conditions in Solution Plasma Using Optical Emission Spectroscopy

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Abstract

We study optical emission spectroscopy (OES) of solution plasma under various pH conditions and train an artificial neural network (ANN) with acquired spectra. OES is composed of multiple emission lines from active species in the solutions. By monitoring OES, non-invasive and real-time diagnosis of solution plasma can be achieved without interrupting the ignition process. Due to the non-linear and unstable relationship between emission lines and pH conditions, it is impracticable to determine the characteristics of solution plasma by a single emission line in OES. Thus, an analysis method considering multiple emission lines and handling nonlinear and nonuniform relationship of solution plasma is needed. ANN can capture features, such as edges, height, and width from high dimensional spectra, and addresses the non-linear relationship with the rectified linear unit (ReLU). A total number of 72k OES with pH ranging from 2.23-5.67 are collected and preprocessed by feature selection and normalization. We investigate the effect of using different labels on the accuracy of predicted pH values from OES. To test the robustness of the ANN model, we also compare the generalization capability of ANN on unseen testing data with or without using dropout as regularization methods.

Development of an Efficient Spectra Collection Platform for Machine Learning Optical Emission Spectroscopy of Plasma Ignited in Water

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Abstract

This work presents development of a spectra acquisition platform for machine learning optical emission spectroscopy (OES) of plasma in solutions. A specially designed platform allowing for efficiently acquiring spectra is developed, and several machine learning algorithms are used. This platform enables acquiring up to 10k spectra in solutions with various pH values under constant solution conductivity, or vice versa, within 15 min. This rapid acquisition scheme provides a sufficient dataset for machine learning. We test the OES of plasmas ignited in solutions with designated conductivities and pH of 2.2-5.2. A total 40k spectra are collected and tested with principal component analysis (PCA) and artificial neural network (ANN) to predict the conductivity of solution. In PCA, the results show that most data points are overlapped in the score plot, implying that PCA cannot discriminate the conductivity. In ANN, several network structures are constructed. The results show that deep ANN significantly improves the accuracy of conductivity prediction in mean square error by three orders of magnitude compared with the method of using single emission line. Dropout and early stopping show promise for mitigating overfitting. Such improvements suggest that ANN considers the nonlinear behaviors of plasma. In addition, the application of ANN with a large number of parameters makes using this platform for efficient spectra acquisition highly desirable.

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Physics-Informed Neural Networks for Solving Polymer Self-Consistent Field Equations

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Abstract

In this presentation, we employ a neural network (NN)-based architecture, physics-informed neural networks (PINNs) [Raissi et al., 2019], to solve the self-consistent field theory equations for polymeric systems. Traditionally, SCFT problems are solved numerically using a finite-difference or pseudo-spectral method combined with an iteration algorithm to obtain the microstructure of polymeric fluids. Such a method often suffers from a substantial memory cost for high-dimensional problems. Here, the PINN architecture utilizes a loss function to couple the governing partial differential equations (PDEs) for the polymer segmental partition functions and self-consistent fields with their own network outputs subjected to relevant physical constraints/conditions. Within each epoch, partition functions and self-consistent fields are solved simultaneously. With appropriate initialization of the field parameters the correct polymer microstructure is predicted, and vice versa. We demonstrate the effectiveness of the PINNs using two polymer systems: homogeneous homopolymers and AB-block copolymers. The potential applications of the proposed PINNs for SCFT equations will also be discussed.

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A Machine Learning Method for Identifying Rules for Synthesis of Ternary-distillation Systems Based on Decision Tree

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Abstract

Ternary distillation is widely used in industries for the separations of various mixtures, and its optimal synthesis has been extensively investigated. However, with the emergence of various energy-saving configurations, e.g. dividing wall column, partial thermal coupled distillation etc., the search space become much more extended, and development of a model imbedding all the possible configurations and evaluation and comparison among different configurations become much more difficult. Quick recognition of the optimal configuration of ternary- distillation becomes a challenge.

Decision tree (DT) (Gordon et al., 1984), as a machine learning method, has been proven effective in identifying decision rule set for handling complex problems. In a decision tree, data are partitioned along a binary tree structure into subsets at nodes with values of the dependent variable, and the selection of the orientation to the left or right at a node is determined by an information entropy gain estimated based on the dada. With repeated passing of data through the nodes, the orientations are trained and become rules for the decision making. Such a trained decision tree can be used to make decisions from new input data.

In the present paper, a method based on decision tree is proposed for identifying a set of rules for making decisions in ternary distillation synthesis. To generate the data for training the decision tree, we use FUG-based shortcut method to estimate quickly the minimum total annual costs (TACs) of all the candidate configurations with various values of the input variables. We select 7 ternary distillation configurations as candidates for the optimal selection, including direct sequence (D), indirect sequence (I), direct sequence with backward integration (DI), indirect sequence with forward integration (II), side rectifier (DS), side stripper (IS), and dividing wall column (DWC). Five hydrocarbon ternary mixtures alone with their relative volatilities, various compositions of the mixtures, and the operating pressures for the utility selection are used as the input variables to generate the minimum TACs for the candidate configurations. BARON/GAMS is used parallelly through Python as the optimizer to obtain the minimum TACs.

By using the data generated, a data-driven decision tree is trained for identifying decision rules. Mixtures with their relative volatilities and the compositions of the mixtures are used as the main features and the information entropy gains are estimated based on the TACs data at every node of the tree. By data set classification, the most important features and the optimal split point of the features are identified to ensure a high accuracy classification. Finally, a set of rules, involving the rules for the application orders of the rest rules, is obtained in a form of the decision tree.

To validate the proposed method, we apply it to a case of three different ternary mixtures and check the identified DT by comparing the results with the those from our previous work for ternary-distillation synthesis. The results show that the rate for giving a right answer by the DT is more than 90%, and the rules identified in the DT are not only consistent with industrial experiences and heuristic rules in the literature, but also able to identify new rules for ternary distillation synthesis.

References

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Big data analysis of chemical plant data

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Abstract

In chemical process, the important key units are reactor and separation devices. Due to the complexity of the reactor internal structure and the reaction mechanism, it is difficult to develop a rigorous mathematical model for industrial application. There are lots of DCS historical data which are kept “sleeping” and “untouched”.

The principle component analysis (PCA) is one of the most popular statistical methods for data mining and analysis. PCA can help to reduce the dimensionality of the variable space by representing it with a few orthogonal (uncorrelated) variables that capture maost of its variability. So PCA retains those characteristics of the data set that contribute most to its variance, by keeping lower-order principal components (the ones that explain a large part of the variance present in the data) and ignoring higher-order ones (that do not explain much of the variance present in the data).

In this work, these plant data of reactor was selected from the DCS device, and PCA technology was used to dig the relationship between these reactor parameters. The rigorous model of distillation column was used to prepare plenty of process data which was analyzed by PCA to give detailed relationship analysis.

Finally, the results showed that these outliers can be effectively detected as abnormal or normal data point and the former data would be removed from the data before next analysis. These conclusions from this PCA analysis could be used as useful guide for chemical process operation and optimization.

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