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Data-Driven Strategies for Green Methanol Process Parameter Optimization Using Machine Learning

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Abstract

Technological advancements in Machine learning, artificial intelligence (AI), and data science are bringing industries to the era of the fourth industrial revolution. The application of machine learning in chemical engineering is in the domains of process modeling, optimization, and predictive analysis. Traditional process modeling relies heavily on first-principal methods, which, while accurate, are computationally demanding and are non-flexible for variable process conditions. Green methanol produced through the power-to-liquid (PtL) process has gained significant popularity due to its various applications in household items, as a raw material for manufacturing valuable chemicals, and as a fuel both in blend or pure form. In today's competitive and uncertain chemical industry market, fast and accurate models are required to predict the plant output. This work aims to develop a surrogate model of the methanol production process based on the data-driven technique and using machine learning to predict energy requirements, final product purity, and methanol production rate. The effect of the sampling size and sampling technique (mainly Latin-Hypercube Sampling - LHS, Monte Carlo, and SOBOL) on the performance of the surrogate model is evaluated. A comparative analysis of different machine learning (e.g., XG-Boost, Random Forest, Decision Tree, Support Vector Regression) and Deep learning models (e.g., Artificial Neural Networks) is conducted using metrics such as coefficient of determination (R^2), mean-squared error (MSE), and mean-absolute-error (MAE). Additionally, this work explores the use of these trained machine learning models in optimizing process conditions to maximize production rate, enhance product purity, and reduce energy requirements.

Keywords
Process Modeling, Surrogate Modeling, Optimization, Machine Learning, Artificial Neural Network

Biographies
Nabeel Sultan is currently pursuing a Master's in Chemical Engineering at Khalifa University. He is engaged in research for his thesis, focusing on machine learning applications in surrogate modeling and optimization of the methanol production process. He earned his B.S. in Chemical Engineering from the University of Engineering and Technology (UET) in Lahore, Pakistan. Nabeel's professional experience includes roles as a Lab Engineer and Teaching Assistant at Lahore University of Management and Sciences (LUMS) and internships at Nestlé Ltd and Shah Taj Sugar Mill Ltd. He is proficient in various technical software and laboratory techniques, underscoring his expertise

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in chemical engineering. His research interests include process simulation and optimization of industrial processes using Machine learning.

Ali Almansoori is Professor of Chemical Engineering and Associate Provost for Education at Khalifa University - Abu Dhabi. He holds a BSc in Chemical Engineering with highest distinction from Florida Institute of Technology, PhD in Chemical Engineering in the area of Process Systems Engineering from Imperial College London, and Executive MBA from London Business School. His specific research interests are in computer-aided modelling, optimization and simulation with applications to energy system design, sustainable operations and supply chain management. He has published over 90 journal articles (of which one appeared in the Science magazine), co-authored 7 book chapters, presented more than 60 conference papers in local and international conferences or workshops, and supervised over 20 graduate students. He was the principal investigators of more than 10 projects, which were sponsored by industry and academia. He is currently a theme lead at KU Research Innovation Center on CO2 and H2 (RICH) on the area of H2 Energy Systems. He has received 10 awards as a result of his research contributions and impact on the scientific community, including the Mohammed Bin Rashid Medal for Scientific Excellence in 2019 and the 2021 Khalifa Award for Education in the field of Higher Education. Along with his academic experience, Prof. Almansoori has 8 years of administrative experience in higher education. He was the Chair of the Department of Chemical Engineering, the Dean of College of Engineering, and the Interim Senior Vice President for Academic Affairs. He also managed the portfolio of policy and performance in higher education at the Executive Council of Abu Dhabi during his secondment in 2013.

Ali Elkamel is a Full Professor of Chemical Engineering. He is also cross appointed in Systems Design Engineering. He holds a BSc in Chemical Engineering and BSc in Mathematics from Colorado School of Mines, MSc in Chemical Engineering from the University of Colorado, and PhD in Chemical Engineering from Purdue University. His specific research interests are in computer-aided modeling, optimization, and simulation with applications to energy planning, sustainable operations, and product design. His activities include teaching graduate and undergraduate courses, supervising post doctorate and research associates, and participation in both university and professional societal activities. He is also engaged in initiating and leading academic and industrial teams, establishing international and regional research collaboration programs with industrial partners, national laboratories, and international research institutes. He supervised over 120 graduate students (of which 47 are PhDs) and more than 45 post-doctoral fellows/research associates. He has been funded for several research projects from government and industry. Among his accomplishments are the Research Excellence Award, the Excellence in Graduate Supervision Award, the Outstanding Faculty Award, and IEOM Awards. He has more than 425 journal articles, 175 proceedings, 50 book chapters, and has been an invited speaker on numerous occasions at academic institutions throughout the world. He is also a co-author of six books.

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