Sustainable Hydrogen Production via HSMR: Integrating Machine Learning for Process Optimization and Forecasting

Sheeraz Ahmad

Department of Chemical Engineering, Khalifa University, Abu Dhabi, UAE

Ali Almansoori and Ali Elkamel

Department of Chemical Engineering, Khalifa University, Abu Dhabi, UAE
& Department of Systems Design Engineering and Department of Chemical Engineering,
University of Waterloo, Waterloo, ON, Canada
Ali.almansoori@ku.ac.ae
alielkamel@gmail.com

Abstract

Hydrogen Sulphide Methane Reformation (HSMR) is a viable alternative for simultaneous H_2S valorization and hydrogen production, offering a carbon-neutral alternative. Concurrently, the industrial revolution, driven by emerging technologies like machine learning and artificial intelligence is reshaping chemical industry as well. machine learning offers robust models for accurate process forecasting, overcoming computational demands and inflexibility. This work focuses on developing a surrogate model for the HSMR process, a promising, waste to energy, route for sustainable hydrogen production. Integrating machine learning with design of experiment techniques, the study systematically generates data using Aspen plus v11 simulation and employs established adaptive space filling sampling techniques. Models such as Linear Regression, Support Vector Regression, Random Forest Regression, Extreme Gradient Boosting, and Artificial Neural Networks was trained on the refined data set, an accuracy of up to 97% in predicting the process outputs was achieved. Furthermore, this research extends to the optimization of an artificial neural network (ANN) surrogate model using evolutionary algorithms, specifically genetic algorithms and differential evolution. within the Python environment, this optimization aims to identify optimal process conditions for HSMR. A comparative analysis with the base case provides insights into the effectiveness of these evolutionary algorithms in enhancing the performance of the ANN model. This work contributes to enhancing the efficiency and competitiveness of HSMR, bridging the gap between machine learning capabilities and sustainable energy solutions.

Keywords
Process Optimization, Surrogate Modeling, Design of experiments, Adaptive Sampling Technique, Artificial Neural Network

Biographies
Sheeraz Ahmad is a dedicated M.Sc. student in Chemical Engineering at Khalifa University, his thesis research is focused on the integration of Design of Experiment and Machine Learning for Surrogate Modeling of Hydrogen Sulfide-Methane Reforming Processes. He holds a B.Tech in Petrochemical Engineering from AMU, where he graduated with a silver medal for his outstanding academic performance. Sheeraz has complemented his academic pursuits with practical experience, having served as a trainee engineer at Indian Synthetic Rubber Private Limited (ISRPL), where he was involved in the day-to-day operations of the production reaction area. Additionally, he has gained research experience through an internship at AMU, where he worked on projects such as biomass conversion to biofuels. His research interests also includes simulation and optimization of industrial processes.

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.