

Process Simulation of Hydrogen Sulphide-Methane Reforming (H2SMR) for Sustainable Hydrogen Production

Sheeraz Ahmad

Department of Chemical and Petroleum Engineering
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
100062647@ku.ac.ae

Nabeel Sultan

Department of Chemical and Petroleum Engineering
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
100062610@ku.ac.ae

Ismail Alkhatib

Department of Chemical and Petroleum Engineering, Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, United Arab Emirates
Energy Institute, Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
ismail.alkhatib@ku.ac.ae

Lourdes F. Vega

Department of Chemical and Petroleum Engineering
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
Energy Institute, Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
Lourdes.vega@ku.ac.ae

Ali Almansoori

Department of Chemical and Petroleum Engineering
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
Research and Innovation Center on CO₂ and Hydrogen (RICH Center)
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
ali.almansoori@ku.ac.ae

Ali Elkamel

Department of Chemical and Petroleum Engineering
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
Research and Innovation Center on CO₂ and Hydrogen (RICH Center)
Khalifa University of Science and Technology
PO Box 127788, Abu Dhabi, United Arab Emirates
Chemical Engineering Department, University of Waterloo, Ontario N2L 3G1, Canada
ali.elkamel@ku.ac.ae, aekamel@uwaterloo.ca

Abstract

In the current energy transition towards sustainable energy resources, H₂S, a byproduct of the oil and gas industry, is considered a promising alternative source of sustainable H₂ production. H₂ can be produced from H₂S by H₂S-methane reforming (H₂SMR), which serves as an alternative process for the commercial production of H₂ with valuable side products such as carbon disulfide (CS₂) and sulfur. This study focuses on the rigorous process modeling of the H₂S-methane reforming process to determine the thermodynamic feasibility and system performance of the process. A comprehensive sensitivity analysis of various operating conditions, including reaction temperature and H₂S-methane feed ratio, is evaluated to analyze their effect on reactant conversion and hydrogen yield, along with byproduct formation. Preliminary results indicate that the higher temperature significantly enhances methane conversion due to the endothermic nature, and the feed ratio is crucial for managing the side product production. These findings highlight that the optimization of these reactor designs is crucial in improving the economic viability of H₂S-based hydrogen production for commercial applications.

Keywords

Process Simulation, H₂S-methane reforming, hydrogen production, process modeling, thermodynamic feasibility, sensitivity analysis

1. Introduction

Currently, the global energy market is dependent on fossil fuels as energy resources, leading to a surge in atmospheric CO₂ emission levels, further contributing to global warming and associated environmental impacts (Hassanpouryouzband et al., 2021). Transitioning to a hydrogen-based energy economy aids in meeting decarbonization strategies and pledges, while also providing a platform for storing energy derived from renewable sources (Le et al., 2024; Griffiths et al., 2021). This transition projects a six-folds increase in hydrogen demand reaching 530 Mt by 2050 (IEA, 2021). Traditionally, hydrogen is produced from fossil fuels, mainly methane, using steam-methane reforming (SMR), with associated high carbon footprint nearly 10.0 kg CO₂-eq per kg H₂ (Parkinson et al., 2019). The carbon footprint can be reduced to 2.0 kg CO₂-eq per kg H₂ with CO₂ capture (i.e., blue hydrogen), however, the additional investment increases the LCOH to \$1.93 – 2.26 per kg H₂ (Parkinson et al., 2019). Although, hydrogen from water electrolysis with renewable resources (i.e., green hydrogen) is a more environmentally friendly option (0.52 – 2.5 kg CO₂-eq per kg H₂), yet its high LCOH of \$4.61– 14.87 per kg H₂, as well as use of fresh water as a feedstock, is delaying the large-scale deployment of this technology to meet the upcoming boost in hydrogen demand (Parkinson et al., 2019). This requires searching not only for a sustainable resource for producing hydrogen, but also for efficient processes with low production costs, or value-added byproducts that offset production costs with generated revenue. Drawing on concepts of circular economy, waste resources are potential feedstocks for hydrogen production, replacing traditional valuable feedstock (i.e., water, methane) (Rafey et al., 2025; Li and Williams, 2023; Prasertcharoensuk et al., 2021; Wang et al., 2020). Among these, hydrogen sulfide (H₂S), a toxic byproduct from oil and gas operations, is a promising source of hydrogen, with the same number of hydrogen atoms as water (Reverberi et al., 2016; Spatolisano et al., 2024; Chan et al., 2023), and lower standard Gibbs free energy change ($\Delta G^\circ \approx 33 - 36$ kJ·mol⁻¹ H₂) compared to water ($\Delta G^\circ \approx 237$ kJ·mol⁻¹ H₂) (Ali et al., 2025). Currently, H₂S emissions are managed using the Claus process by converting them to elemental sulfur and wastewater, invariably losing the hydrogen atoms from H₂S (Ali et al., 2023). In this context, utilizing H₂S for hydrogen production, where available, might be an effective method for meeting hydrogen economy goals, while also supporting circular economy targets. A variety of processes have been explored over recent years for H₂S-to-H₂ conversion (Reverberi et al., 2016; Spatolisano et al.,

2024; Chan et al., 2023), yet, the closest to market is H₂S-methane reforming (H₂SMR) (Ali et al., 2025; Spatolisano et al., 2022; Cong et al., 2016; El-Melih et al., 2016; Martínez-Salazar et al., 2015). In the H₂SMR reaction (Eq. 1), analogous to SMR, H₂S is reacted with methane to produce hydrogen and carbon disulfide (CS₂), instead of CO₂ in SMR. Other reactions might also occur under elevated temperatures, including H₂S pyrolysis (Eq. 2), resulting in sulfur production, and methane pyrolysis (Eq. 3), resulting in solid carbon production, in addition to hydrogen (Spatolisano et al., 2022; Cong et al., 2016; El-Melih et al., 2016; Martínez-Salazar et al., 2015).



An advantage of H₂SMR is that it does not directly produce CO₂ as with SMR, aside from the indirect emissions resulting from fuel consumption, avoiding the need for dedicated CO₂ capture units. Additionally, the byproducts (CS₂ and S₂) are valuable products which can offset the cost of hydrogen production with their generated sales revenue (De Crisci et al., 2019; Chan et al., 2023). However, the H₂SMR reaction is highly endothermic with $\Delta H^\circ = 232.4 \text{ kJ.mol}^{-1}$ at 298 K (Cong et al., 2016; El-Melih et al., 2016), almost 40% higher than SMR with $\Delta H^\circ = 164.9 \text{ kJ.mol}^{-1}$ at 298 K, which directly impacts the reactor energy consumption. An additional issue is the risk of carbon deposition in the reactor due to methane pyrolysis, requiring careful consideration for H₂S-to-methane ratio and reactor temperature (De Crisci et al., 2019; Chan et al., 2023). This study presents a rigorous process modeling of the H₂SMR process to determine the thermodynamic feasibility and system performance of the process. First, a working model is developed using the Aspen Plus simulator. After that, a comprehensive sensitivity analysis of various operating conditions, including the reaction operating temperature and pressure, along with the input feed ratio, is evaluated to analyze their effect on the hydrogen yield and the byproduct formation. These findings will help in the optimization of the reactor design and improve the overall economics of the process for commercial-scale hydrogen production. The structure of the paper is organized as follows: Section 2 covers the overview of the process model under consideration, along with the different process settings. The results and discussion of the sensitivity analysis conducted for the process are presented in Section 3, and finally, the conclusion drawn from the results is presented in Section 4

2. Process simulation for H₂S-methane reforming

The simulation of the H₂SMR process is done using Aspen HYSYS as shown in the flowsheet Figure 1. The process is divided into three segments, namely, reaction, byproduct sulfur and CS₂ recovery, and H₂ purification, similar to our previous contribution (Ali et al., 2023).

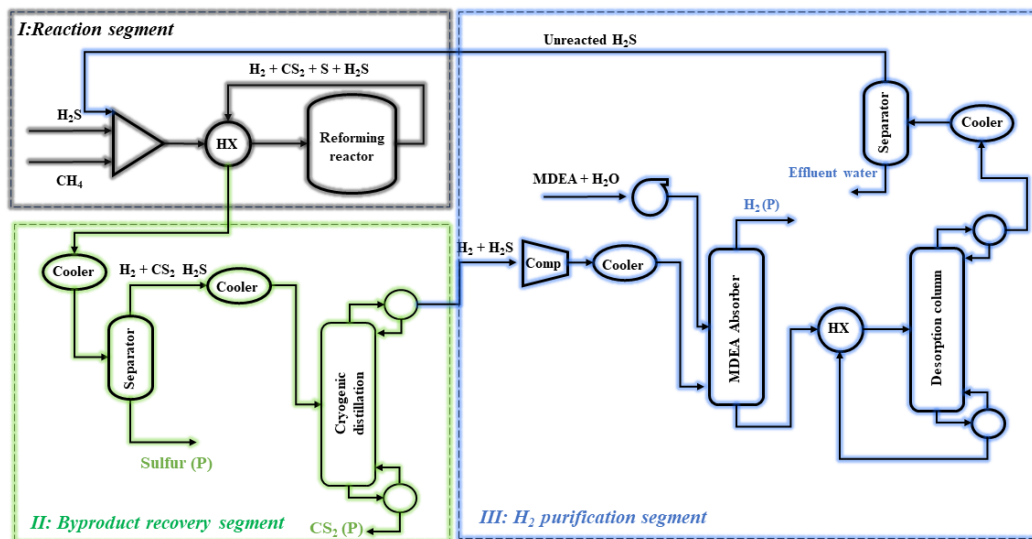


Figure 1: Process flowsheet for H₂SMR, highlighting the three main segments, reaction (black), byproduct recovery (green) and, H₂ purification (blue).

Inlet methane at sales gas quality is received at 313 K and atmospheric pressure, while H₂S is received from natural gas sweetening units at similar conditions, with a 1:15 maximum CO₂:H₂S ratio to limit the effect on H₂ yield (Spatolisano et al., 2022). The feedstock methane and H₂S are mixed at a ratio of 1:3, to prevent carbon deposition by methane pyrolysis in Eq. (3) (Spatolisano et al., 2022), and heated to the reactor temperature (typically 1500 °C). The mixed feedstock enters the reforming reactor, modelled as an ideal Gibbs reactor, as it accurately represents experimental behavior of H₂ yield as a function of temperature (Ali et al., 2023). For the initial simulation of the process, the reactor was modelled under atmospheric pressure and a set temperature of 1500 °C. The reformer reactor was fuelled using imported methane-based fuel gas, with the hot flue gas from the reformer used to preheat the reactor's inlet as well as water for the CS₂ distillation column reboiler. The details of each section and the flow process are shown in Figure 1.

3. Sensitivity Analysis

To perform the sensitivity analysis in order to understand the thermodynamics of the process, the reactor inlet feed ratio and operating temperature are selected as the key variables. The operating range of 800-1600°C is selected for the reactor temperature, and the inlet feed ratio, i.e., H₂S/methane, varies from 1:1 to 1: 9. These conditions are selected to confirm the thermodynamic feasibility of the process and to estimate the effect of these conditions on the output product quality. The main targeted variables in the sensitivity analysis are the H₂S & methane conversion. The input and output of these components are monitored to determine the conversion using the formula shown below:

$$X_{H_2S} = \frac{[H_2S]_{in} - [H_2S]_{out}}{[H_2S]_{in}} \times 100 \text{ --- (eq. 4)}$$

$$X_{CH_4} = \frac{[CH_4]_{in} - [CH_4]_{out}}{[CH_4]_{in}} \times 100 \text{ --- (eq. 5)}$$

The desired and the co-product produced are also monitored to understand the effect of the variation of the system variables. Hydrogen is the desired product, which is produced using a non-catalytic H₂SMR process along with side products like CS₂ And sulfur is also produced. The production rate of these products is monitored under the normalized conditions. The formula for the production rate of products and co-products is as follows:

$$Y_{H_2} = \frac{[H_2]_{out}}{[H_2S]_{in} + 2[CH_4]_{in}} \times 100 \text{ --- (eq. 6)}$$

$$Y_{S_2} = \frac{2[S_2]_{out}}{[H_2S]_{in}} \times 100 \text{ --- (eq. 7)}$$

$$Y_{CS_2} = \frac{2[CS_2]_{out}}{[H_2S]_{in}} \times 100 \text{ --- (eq. 8)}$$

With these defined parameters of conversion, product and co-products production rate, we can carefully analyze the effect of the input variable i.e., operating temperature and the inlet feed ratio, on the overall system performance.

4. Results and Discussion:

The results of the sensitivity analysis, including methane and hydrogen sulphide conversion along with the hydrogen, carbon disulphide, and sulfur production rate, are shown in **Figure 2**. The results reveal that for all feed compositions, the H₂S conversion increases with the increase in the temperature, showing that the reforming reaction is highly endothermic in nature (Figure.2(a)). From the molar ratio of 1:1, it can be observed that the H₂S conversion increases from 38% at 800°C to approximately 98% at 1600°C. The increase of the H₂S-methane molar ratio results in a progressive decrease in the conversion because the system becomes thermodynamically limited due to insufficient availability of methane. The results of methane conversion (Figure.2(b)) reveal that with the increase in temperature, the conversion increases, but with high molar ratio feed (6:1 & 9:1) at temperature ≥ 1200°C the methane conversion approximately reaches 100%. This trend suggests that under high molar ratios, the sulfur-carbon reaction pathway dominates because of the availability of a large amount of sulfur for the carbon conversion. The output production rate of both products and co-products reveals that the hydrogen production increases with the increase in temperature for all the feed molar ratios, which is consistent with the endothermic process (Figure.2(c)). However, the hydrogen production does not increase linearly with the increase in the molar ratio. The highest hydrogen production is observed at the intermediate 3:1 for most of the temperature range, reaching approximately 87% at 1600 °C. This trend suggests that at a lower molar feed ratio (1:1), hydrogen formation is limited due to the low sulfur availability for the reaction, and under very high sulfur

concentration (6:1 & 9:1), a larger fraction of sulfur results in the alternate pathway. Furthermore, the sulfur production rate graph (Figure.2(d)) reveals that it increases with both temperature and molar feed ratio. The sulfur production at low temperature, i.e., 800 °C is negligible for all molar ratios; it increases sharply with the increase in temperature along with the increase in the molar feed ratio. This shows that at high temperatures and under excess sulfur, it promotes the sulfur-sulfur coupling reaction. Conversely, carbon disulfide (CS₂) formation shows the opposite trend (Figure.2(d)). CS₂ production increases under lower molar feed ratio, reaching nearly complete sulfur incorporation, i.e., 98.6% at 1600 °C for the 1:1 ratio, and decreases markedly as molar concentration increases. This inverse relationship between CS₂ and S₂ formation confirms the competitive nature of sulfur reaction pathways. When sulfur availability is moderate, it prefers to react with carbon to form CS₂, and when hydrogen sulfide is in excess, sulfur polymerization becomes dominant.

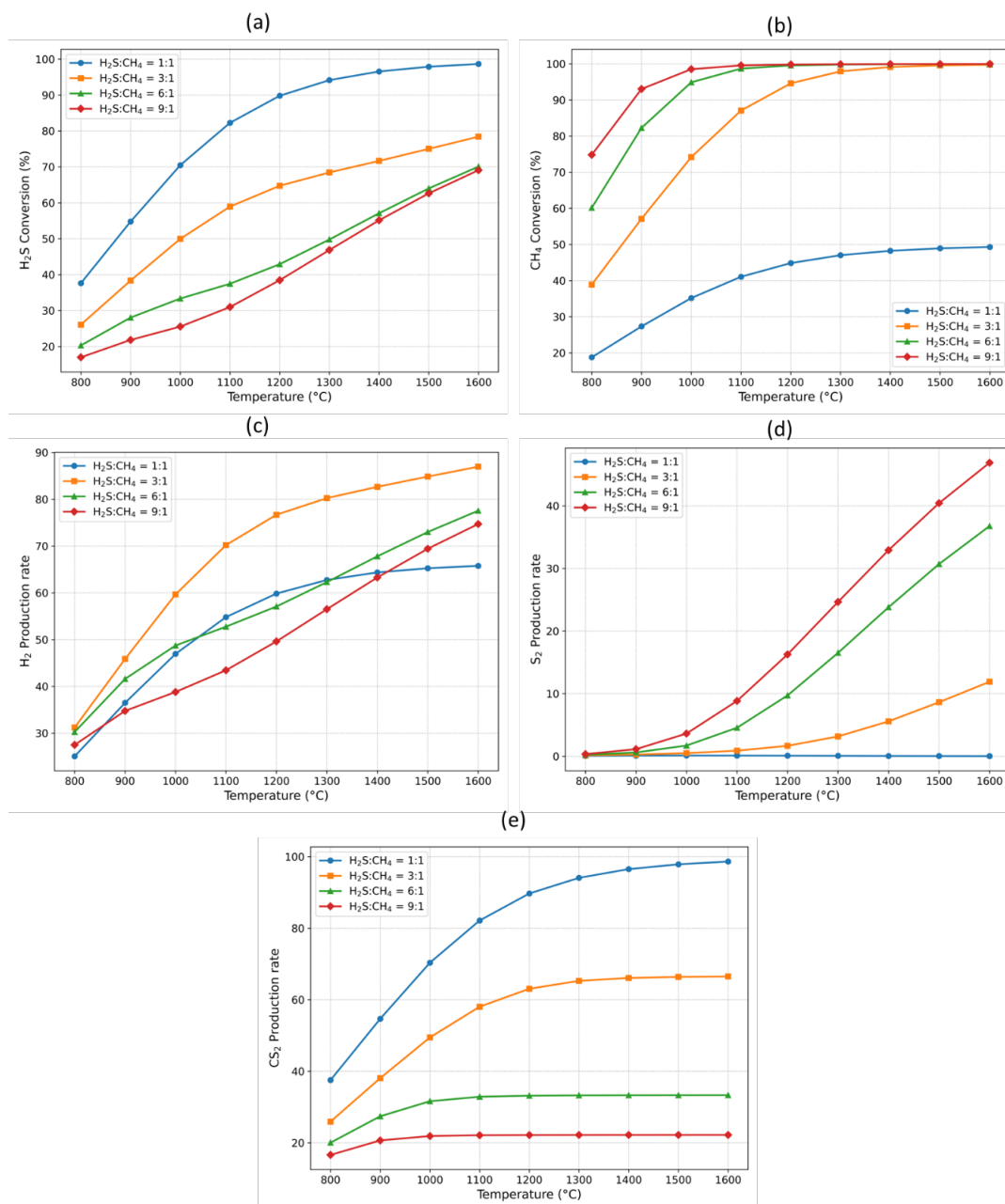


Figure 2: Effect of temperature and feed molar ratio ($H_2S/CH_4 = 1:1, 3:1, 6:1$, and $9:1$) on (a) H_2S conversion, (b) CH_4 conversion, (c) H_2 production rate, (d) S_2 production rate, and (e) CS_2 production rate over the investigated temperature range of 800–1600 °C.

Overall, temperature acts as the primary driver of overall conversion, while feed composition governs product selectivity. Increasing the H₂S:CH₄ ratio decreases fractional conversion of H₂S but enhances methane conversion and S₂ formation, while reducing the CS₂ production. Similarly, hydrogen production is maximized at an intermediate molar feed loading along with the high temperature. All this discussion shows that the careful optimization of these process variables is essential for increasing the hydrogen production, along with managing the co-product production to meet the economic standards.

5. Conclusions

In this study, a comprehensive thermodynamic simulation model of the H₂SMR process was developed using an Aspen Plus simulator. The process flowsheet comprises three main sections: (i) a reforming section for reaction modeling, (ii) a byproduct separation section, and (iii) a hydrogen separation section for hydrogen purification and recovery. The sensitivity analysis demonstrated that temperature is the dominant parameter influencing overall system performance, with higher temperatures significantly enhancing H₂S and CH₄ conversion and driving the process toward thermodynamic completion. Feed molar ratio (i.e. H₂S:CH₄) molar ratio found to play a critical role in determining product selectivity. Increasing molar feed ratio H₂S:CH₄ decreased fractional H₂S conversion but enhances the methane conversion and sulfur (S₂) formation, while reducing the carbon disulfide (CS₂) production rate. Hydrogen production exhibited a non-linear relationship with feed composition, with maximum hydrogen production observed at an intermediate H₂S: CH₄ ratio of 3:1. These results highlight the strong correlation between sulfur chemistry and hydrogen formation pathways.

Overall, the developed simulation framework provides valuable insight into the thermodynamic behavior of the H₂SMR system and demonstrates the feasibility of simultaneously producing hydrogen and valuable sulfur-containing co-products. However, in order to achieve the optimal process performance, careful tuning of operating temperature and feed molar composition is a crucial step. Future studies should focus on systematic optimization of these variables to maximize hydrogen yield while controlling byproduct selectivity and minimizing energy demand to meet the economic targets.

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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 include simulation and optimization of industrial processes.

Nabeel Sultan is currently pursuing a PhD in Chemical Engineering at Khalifa University. He is engaged in research for his thesis, focusing on machine learning applications in surrogate and material discovery for hydrogen storage processes. 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 in chemical engineering. His research interests include process simulation and optimization of industrial systems using machine learning, as well as the application of machine learning in materials discovery for hydrogen storage.

Ismail I.I. Alkhatib is a research scientist in chemical engineering at Khalifa University in the UAE. He holds a PhD in Engineering in Chemical Engineering with a specialization in molecular thermodynamics, supervised by Prof. Lourdes F. Vega. His current research centers on applying molecular thermodynamics to multi-scale modelling and machine learning frameworks to address pressing environmental issues. This includes developing new materials for

CO₂ capture, sustainable cooling, and alternative pathways for hydrogen production and transportation. He aims to make a significant contribution to creating cost-effective decarbonization technologies, with a particular focus on hard-to-abate industries and innovative cooling solutions. His research profile can be found with the following link: <https://scholar.google.com/citations?user=KMt1c30AAAAJ&hl=en>

Prof. Lourdes F. Vega is a Full Professor in Chemical Engineering and Senior Director of the Energy Institute at Khalifa University in the UAE; she is also the Founder and was the first Director of the Research and Innovation Center on CO₂ and Hydrogen (RICH) at the same university. She obtained her PhD in Physics from the University of Seville, Spain, in collaboration with the Chemical Engineering Department from the University of Southern California, USA. She has developed her career between academia and industry. Her research revolves around moving fundamental science to industrial applications by combining multiscale modeling with experiments, focused on CO₂ capture and utilization, hydrogen and its derivatives, sustainable fuels, water treatment, and sustainable cooling systems. She has received several awards for her contributions on clean energy and sustainable products. Her research profile on Google Scholar can be found at the following link: <https://scholar.google.pt/citations?user=RUesAz0AAAAJ&hl=en>

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 450 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.