Doctoral (Ph.D.) Thesis

MODELING AND SIMULATION OF NOVEL CATALYTIC REACTORS FOR CO_2 HYDROGENATION TO HYDROCARBON AT DIFFERENT MODES AND OPERATING CONDITIONS

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1. Introduction and aim

The depletion of fossil fuels, the issue of global warming, climate change, and the sharp increase in fuel costs are motivating scientists to explore alternatives in the form of commercially viable and eco-friendly fuels. The process of converting CO_2 into hydrocarbons is being examined as a potential solution to meet these demands, but has the issues listed below:

1. Integration of reaction heat: due to the existence of both endothermic (RWGS) and exothermic (FTS) reactions in the single reactor.
2. Low CO_2 conversion: the formation of huge amounts of water along the single reactor causes catalyst deactivation due to the inhibition effect of water on the active sites of the catalyst, thereby shortening the catalyst's lifetime.
3. Low production capacity: due to the loss of hydrogen in the sweep part of the membrane reactor as H_2O, which means that hydrogen dosage might be required to adjust the H_2/CO_2 in the reactor.
4. Pressure drop across the reactor: due to the existence of an intrinsic limitation on the diffusion along the fixed-bed reactor.

The main goal of this research is to compare fixed-bed, annular, and spherical reactors with and without a membrane based on modeling and optimization. The comparison between the simulated data and the experimental ones will be made in order to validate the models for the production rate of the entire investigated reactors. Consequently, this case will demonstrate the viability of a new reactor alternative using theoretical investigations. The advantages of the new alternative over the conventional ones will be discussed based on the temperature and concentration profiles and the catalyst activity profiles along the reactors.

2. Modeling and simulation

In this study, the governing equations were derived and solved using the Rung-Kutta method (ode15s) in MATLAB based on mass and energy balance for the solid and bulk phases. The study utilized modeling and simulation to investigate the impact of reactor configurations and operating conditions on hydrocarbon distribution. Kinetic parameter estimation was controversial due to reaction complexities and species varieties, hence, the study proposed using ABC, DE, and DA optimization algorithms to estimate the parameters based on the LHHW mechanism. The theoretical reactor's performance was compared with experimental data, and the effects of in-situ water removal on annular membrane reactor performance were analyzed. The concentration of each component and temperature profiles were compared in various reactor configurations like fixed-bed, annular and membrane, and cylindrical and spherical reactors. The details of modeling and simulation can be found stepwise as follows:

2.1 Using the ABS and DE optimization algorithms

The optimization of the kinetic parameters for the assumed reactions was performed using Artificial Bee Colony (ABC) and Differential Evolution (DE) optimization algorithms based on the LHHW mechanism. To this end, a one-dimensional heterogeneous plug flow model comprising detailed reaction rates of RWGS, FT reactions, and direct hydrogenation (DH) of CO_2 is developed. Parameter identification is a crucial step in establishing kinetic models. Thus, it can be transformed into an optimization problem by constructing an objective function (O.F) that minimizes simulation errors.

2.1.1 Artificial Bee Colony (ABC)

The Artificial Bee Colony (ABC) optimization algorithm is a population-based metaheuristic optimization algorithm inspired by the behavior of honeybees. The algorithm is developed based on the concept of food source exploitation by honeybees. In this algorithm, the population of artificial bees is divided into three groups: employed bees, onlooker bees, and scout bees. Employed bees explore the food

sources and communicate their findings to the onlooker bees. Onlooker bees evaluate the information provided by the employed bees and choose a food source to exploit. The scout bees explore new food sources to replace the exhausted ones. The algorithm starts by randomly initializing the population of food sources (initial guess), where each food source represents a potential solution to the optimization problem. The employed bees exploit the food sources and update the solutions based on the quality of the food sources (based on their guess). The onlooker bees choose the best food sources and exploit them further. The scout bees explore new solutions in the search space (using the new data as the initial guess for the next evaluation). This process continues until a stopping criterion is met (minimization of errors via O.F.), such as reaching a predefined number of iterations or a target fitness value.

2.1.2 Differential Evolution (DE)

Differential Evolution (DE) is a population-based metaheuristic optimization algorithm that is widely used for solving optimization problems that involve continuous variables. In this algorithm, a population of candidate solutions, known as individuals or agents, is evolved over a number of generations to find the optimal solution. At each generation, each individual is evaluated based on its fitness value, which represents how well the individual solves the problem. The DE algorithm operates by creating new candidate solutions by combining existing solutions through mutation and recombination operations. Specifically, the DE algorithm selects three distinct individuals from the population and uses their differences to create a mutant vector. This mutant vector is then combined with the target individual to produce a trial vector. The trial vector is then evaluated, and if it has a better fitness than the target individual, it replaces the target individual in the population.

2.2 The overall solution of the governing equations:

First, the initial guess for each unknown kinetic parameter is introduced to the code as an input, also, the reactor's operating conditions and dimensions are inserted as inputs. Using either the ABC or DE algorithms, the mass and heat balances are solved using the ode15s command in MATLAB. The initial guesses result in the outlet

concentration of hydrocarbons, which is compared via the O.F. with the experimental data, and if they don't match, the optimization algorithms produce a set of next initial guesses for the kinetic parameters based on the obtained results and continue solving the governing heat and mass balance to finally set the O.F. to minimum error. When the error is minimized, the kinetic parameters are estimated, and the codes can be used further with the estimated parameters for the prediction of reactor performance at different operating conditions and configurations.

2.3 Effect of operating conditions:

Then, using the estimated kinetic parameters, we use the heat and mass transfer governing equations to assess the effect of changes in input variables such as T, P and GHSV on the product distribution.

2.4 Effect of in-situ water removal:

In the next step, we changed the configuration of the fixed-bed reactor to an annular reactor consisting of an H_2O-permeable wall on its inner wall and introduced a sweep inert gas (N_2) in the outer tube to sweep the permeated water and avoid its accumulation in the outer tube. It is noteworthy that the in-situ water removal could shift the equilibrium of the RWGS reaction towards the production of more CO and provide more feed for the FT reaction while hampering the inhibition effect of H_2O on hydrocarbon formation and catalyst deactivation.

2.5 Effect of reactor configuration:

After evaluating the model in both fixed-bed and annular membrane reactor modes, we decided to change the configuration to spherical reactors both in axial (AFSR) and radial (RFSR) modes to investigate the influence of reactor configuration with different heating locations (inside and outside) on the hydrocarbon distribution and pressure drop.

2.6 Three-sided membrane reactor

In this configuration, we changed the configuration in a way to simultaneously have a reaction in the middle tub, remove H_2O from the inner membrane tube, while injecting H_2 from the H_2 permeable outside membrane tube to adjust the H_2/CO_2 ratio and compensate for the removed H_2 as H_2O during the reaction to study the impact of H_2 dosage on the product distribution. Moreover, we used a new optimization algorithm (Dragon Fly) to improve the CO_2 conversion estimation. In addition, exploiting the statistical analysis, the influential factors and the effects of their interactions on the reactor's performance were also investigated.

The study concluded that rigorous mathematical modeling is a powerful tool to investigate and predict reactor performance and provide insights into influential parameters for designing advanced reactor configurations in the CO_2 hydrogenation process. However, further studies are needed to determine optimal reactor conditions and investigate the contribution of significant factors to reaction rates and product distribution.

3. Summary of New Scientific Results

T1. As the best kinetic model, carbide and enolic mechanisms have been exploited to obtain the microkinetic rate equation to reach into LHHW for the CO_2 reduction process.

The Langmuir-Hinshelwood-Hougen-Watson (LHHW) model is considered as one of the most suitable models for describing the kinetics of CO_2 hydrogenation to hydrocarbon via RWGS and FT routes, but it is not necessarily the "best" model for every process. It is a surface reaction model, which assumes that the reaction occurs on the surface of a catalytic material and that the rate-determining step is the collision of the reactant with the surface. I derived back the microkinetic of CO_2 hydrogenation to hydrocarbon based on the carbide and enolic mechanisms to obtain the microkinetic rate equation to reach LHHW. The details of reaction steps and RDS can be found in our recently published research.

T2. Reactor configuration has been proposed as an efficient parameter for CO_2 hydrogenation to hydrocarbons, among other effective parameters.

The reactor configuration is a crucial factor in the performance of the CO_2 reduction reaction, as it determines the transport and distribution of reactants, products, and catalysts within the reactor. Compared to operating conditions and catalyst type, the reactor configuration can significantly impact the reaction kinetics, selectivity, and overall efficiency of the CO_2 reduction process. It should be emphasized that all the effects of the debated factors (catalyst type, operating conditions, and reactor type) have been investigated on the production efficiency of hydrocarbons through the hydrogenation of CO_2. It was discovered that in addition to catalyst promoter selection, the increase in reaction temperature and pressure as well as the increase in space velocity all improve CO_2 conversion with enhanced hydrocarbon yield; higher yields usually result from changing the reactor configuration. In other words, a simultaneous increase in the hydrocarbon/olefin/paraffin ratio would be obtained only if the reactor configuration was changed to limit thermodynamic equilibrium, enhance kinetic-limited reactions, and control the stoichiometric feeds. Therefore, this achievement persuades us to propose a novel reactor configuration in order to cover the above-mentioned limitation. The proposed novel reactor configuration consists of a water perm-selective membrane and an H_2 perm-selective membrane, with detailed configurations and elemental volumes.

T3. On the basis of modeling and simulation of the membrane reactor, the effect of in-situ water removal on the enhancement of hydrogenation of CO_2 to hydrocarbons has been scrutinized.

In-situ water removal refers to the removal of water during the reaction process, without the need for a separate water-removal step. Specifically, in the hydrogenation of CO_2 to hydrocarbon process, water removal can have a significant effect on the reaction kinetics and product distribution. Hydrogenation of CO_2 to hydrocarbons in fixed-bed and annular reactors (AR) can be limited by problems associated with high water production as the main by-product. Selective in-situ water removal using a hydrophilic membrane can be a promising solution for enhancing reactor performance. To this end, a one-dimensional heterogeneous model comprising mass and heat transfers in the shell and tube of a membrane reactor (MR) is proposed. Firstly, the

performances of different reactor configurations exhibiting similar cross-sectional areas and volumes are compared. Afterward, influential factors affecting the MR performance, such as shell/tube temperature, sweep ratio (θ), and pressure ratio (φ) are thoroughly investigated. Results show that increasing the initial tube/shell temperature has a positive effect on total hydrocarbon yield. However, sharp and sudden temperature elevation (hot spot) due to the large extent of water removal may have detrimental effects on catalyst performance. Moreover, it is observed that increasing θ and φ alter product distribution due to equilibrium displacement and result in a lack of H_2 for further FT reactions. In addition, kinetic parameters corresponding to the inhibiting effect of water are indicated to have significant roles in hydrocarbon distribution. Therefore, water removal imposes various changes, that cannot be considered independently in analyzing the MR performance.

T4. The effect of operating conditions and the effectiveness factor have been investigated on the hydrogenation of CO_2 to hydrocarbons.

The development of an efficient reactor for hydrocarbon (C_2–C_4) production through the hydrogenation of CO_2 requires a deep understanding of the operating conditions effects. Subsequently, a model is proposed to analyze the reaction rates and investigate the sensitivity of hydrocarbon yield and product distribution to variations in temperature, pressure, and space velocity (SV). Besides, the Thiele modulus and effectiveness factor are calculated for all the reactions considered in the model. Results reveal that the simultaneous occurrence of both endothermic RWGS and exothermic FT reactions may be the main reason for temperature and rate fluctuations at the fixed-bed reactor inlet. In addition, increasing temperature and pressure and decreasing space velocity (SV) can shift the process to produce more light olefins. Finally, sensitivity analysis demonstrates that reactor behavior is independent of changes in pressure and SV at high temperatures, which is an indication of the high-temperature dependency of this process. These findings can be effectively employed to achieve a better insight into appropriate operating conditions for hydrocarbon production via hydrogenation of CO_2.

T5. Kinetic parameters have been estimated based on new heuristic optimization algorithms like Artificial Bee Colony (ABC) and Differential Evolution (DE) for the hydrogenation of CO_2 to hydrocarbons.

In fact, the complexity of the reactions and the variety of species produced, as well as the process mechanism and subsequent estimation of the kinetic parameters, have all been controversial. Therefore, estimating the kinetic parameters using Artificial Bee Colony (ABC) and Differential Evolution (DE) optimization algorithms based on the LHHW mechanism is proposed as a possible remedy to fulfill the requirements. To this end, a one-dimensional heterogeneous model comprising detailed reaction rates of RWGS, FT reactions, and direct hydrogenation (DH) of CO_2 is developed. It is observed that ABC, exhibiting a 6.3% error in predicting total hydrocarbon selectivity, is superior to the DE algorithm, with a 32.9% error. Therefore, the model employs the estimated kinetic parameters obtained via the ABC algorithm for product distribution analysis. Results reveal that maximum 73.21% hydrocarbon (C_1-C_4) selectivity can be achieved at 573 K and 1 MPa with a 0.85% error compared to the experimental value of 72.59%. Accordingly, the proposed model can be exploited as a powerful tool for evaluating and predicting the performance of the CO_2 hydrogenation-to-hydrocarbons process.

T6. The performances of cylindrical and spherical reactors have been compared for CO_2 hydrogenation to hydrocarbons, and the kinetic parameter has been estimated based on the Dragonfly algorithm.

Indeed, finding an in-depth understanding of the CO_2 hydrogenation reactors and simulating reactor responses to different operating conditions are of paramount importance. However, the reaction mechanisms for CO_2 hydrogenation and their corresponding kinetic parameters have remained disputable. In this regard, considering the previously proposed LHHW mechanism, which considered CO_2 hydrogenation as a combination of RWGS and FT reactions, and using a one-dimensional pseudo-homogeneous non-isothermal model, the kinetic parameters of the rate expressions are estimated via relevant experimental and modeling data through a novel swarm intelligence optimization technique called Dragonfly. The predicted reactant conversion using the Dragonfly is closer to the experimental data (with about 4% error) compared to those obtained by the ABC algorithm and is in significant agreement with available literature data. The proposed model is used to assess the effect of reactor configuration on performance and temperature fluctuations. Results show that the axial flow spherical reactor (AFSR) and radial flow spherical reactor (RFSR), which exhibit

the same surface area as the cylindrical reactor (CR), i.e., AFSR-2 and RFSR-2-i, are the most efficient, exhibiting hydrocarbon selectivity of 40.330% and 40.286% at CO_2 conversions of 53.763% and 53.891%, respectively. In addition, it is revealed that the location of the jacket has an essential role in controlling the reactor temperature.

T7. Modeling and statistical analysis of the three-sided membrane reactor have been scrutinized for the optimization of hydrocarbon production from CO_2 hydrogenation.

In fact, reactor design and performance have remained challenging because of low olefin efficiency and high water production as a by-product. Accordingly, a one-dimensional non-isothermal mathematical model is proposed to predict the membrane reactor performance, and statistical analysis is used to assess the effects of important variables such as temperatures of the reactor (Tr: A), shell (Ts: B) and tube (Tt: C) as well as sweep ratio (θ: D) and pressure ratio (φ: E) and their interactions, on the products yields. In addition, optimized operating conditions are also obtained to achieve maximum olefin yields. Results reveal that interacting effects comprising AB (TrTs), AC (TrTt), AE (Trφ), BC (TsTt), CE (Ttφ), CD (Ttθ), and DE (θφ) play important roles in the product yields. It is concluded that higher temperatures at low sweep and pressure ratios can maximize the yields of olefins while simultaneously minimizing the yields of paraffin. The optimized values for Tr, Ts, Tt, θ, and φ are determined to be 325 °C, 306.96 °C, 325 °C, 1, and 1, respectively.

List of Publications – Samrand Saeidi

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A. Related to the dissertation

1. ***S. Saeidi***, NAS. Amin, MR. Rahimpour "**Hydrogenation of CO_2 to Value-added Products–A Review and Potential Future Developments**", *CO_2 utilization journal (IF=8.321)*, 5 (2014), 66–81 (**Most cited**).
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2. ***S. Saeidi*,*** Sara Najari, Farhad Fazlollahi, Maryam Khoshtinat Nikoo, Fatemeh Sefidkon, Jiří Jaromír Klemeš, Larry L. Baxter **"Mechanisms and kinetics of CO_2 hydrogenation to value-added products: A detailed review on current status and future trends"** *Renewable and Sustainable Energy Reviews (IF=16.799),* 80 (2017), 1292–1311. DOI: https://doi.org/10.1016/j.rser.2017.05.204

3. ***S. Saeidi****, S. Najari, V. Hessel, K. Wilson, Frerich J. Keil, P Concepcion, S.L. Suib, Alírio E. Rodrigues "**Recent advances in CO_2 hydrogenation to value-added products — Current challenges and future directions"** *Progress in Energy and Combustion Science (IF=35.339)*, 85 (2021), 100905. (**Most cited**).
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4. *Sara Najari, Gyula Gróf,* ***S. Saeidi****, Fausto Gallucci* **"Modeling and optimization of hydrogenation of CO_2: Estimation of kinetic parameters via Artificial Bee Colony (ABC) and Differential Evolution (DE) algorithms"** *International Journal of Hydrogen Energy (IF=7.139)*, 44 (2019), 4630-4649.
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7. S. Najari, G. Gróf, ***S. Saeidi****, P. Bihari, W-H. Chen, **"Modeling and statistical analysis of the three-side membrane reactor for the optimization of hydrocarbon production from CO_2 hydrogenation"**, *Energy Conversion and Management (IF=11.533)*, 207 (2020) 112481.
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B. Related to the dissertation

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