Development of a multi-zone, multi-feed adiabatic reactor framework optimization for the exothermic oxidative coupling of methane reaction

Murtaza Ali Khan[1,2], Mamoun Al-Rawashdeh[1]*, Patrick Linke[1]*

1 Chemical Engineering Program, Texas A&M University at Qatar, Doha 23874, Qatar

2 Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, USA

**Corresponding authors: mamoun.al-rawashdeh@qatar.tamu.edu and patrick.linke@qatar.tamu.edu*

Highlights

- Multi-zone reactor network developed for OCM
- Both isothermal and adiabatic operations are tested over multiple reactor zones
- Different heat management strategies in adiabatic operation expected to improve performance

1. Introduction

With the need to improve industrial performance, finding the optimum conditions becomes a significant challenge for an industrial process. Hence, many researchers have explored various optimization approaches on the process level. Some research has been done to examine the optimization principles on a reactor level. Still, those works have been chiefly concerned with productivity indicators such as yield and have not explored the synergies of the chemistries inside the reactor. For example, exothermic reactions release significant energy, so heat management becomes a pressing concern for exothermic reactions. One suggestion to improve the performances of exothermic reactions is to provide side-feeding of reactants to achieve intermediate cooling. This work explores the development of a multi-zone reactor framework with distributed feeds, combining optimization principles with reactor design to explore the synergy of an exothermic reaction. In this work, the oxidative coupling of methane (OCM) is used as an example of an exothermic reaction, and the optimum design conditions will be determined to address the ideal number of reactor zones that maximize the product performance of OCM.

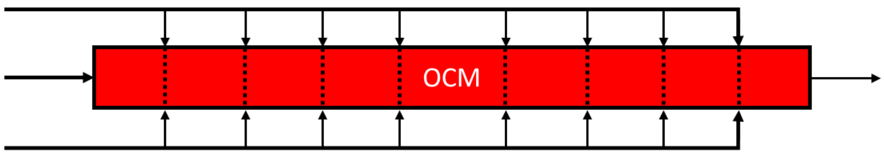

Figure 1. Schematic of multi-zone reactor network for OCM.

2. Methods

A multi-zone reactor network optimization framework was developed in Python. In this methodology, the entire reactor is split into several reactor zones whose configurations are then determined. Each reactor zone is represented by a validated fixed-bed, one-dimensional (1-D), pseudo-homogeneous, and isobaric packed-bed reactor simulation model. Stansch et al. (1997) kinetic model was used to model the OCM kinetics inside each reactor zone. The feeds are also distributed along each reactor zone, where mass and energy balances are performed before and after each reactor zone to simulate the configurations across the reactor network. The optimal settings for design decisions are then identified using simulated annealing (SA). The reactor network and the optimization methodology are first validated by considering the entire reactor as a single zone. Inlet temperature at the reactor zone, O_2:CH_4 ratio, N_2:CH_4 ratio, space-time (amount of catalyst), and split fraction of methane stream at each reactor zone inlet are considered decision variables. The product (C_2) yield is considered as the objective function.

3. Results and discussion

In the base case (single-zone optimization in isothermal operation), 20 different runs were performed with initial guesses based on the bounds for inlet temperature, O_2:CH_4 ratio, and N_2:CH_4 ratio, using the optimization methodology. It was observed that despite the variance in initial guesses, all runs seemingly converged to around the same mark, with the optimum C_2 yield being achieved of about 20.95% at an inlet temperature of 1111.6 K, O_2:CH_4 ratio of 0.5 and N_2:CH_4 ratio of 0.22. Compared with the manual discretization of solution space, this demonstrates that the optimization methodology can successfully determine the optimum configuration in isothermal operation for a single zone optimization.

(a)

(b)

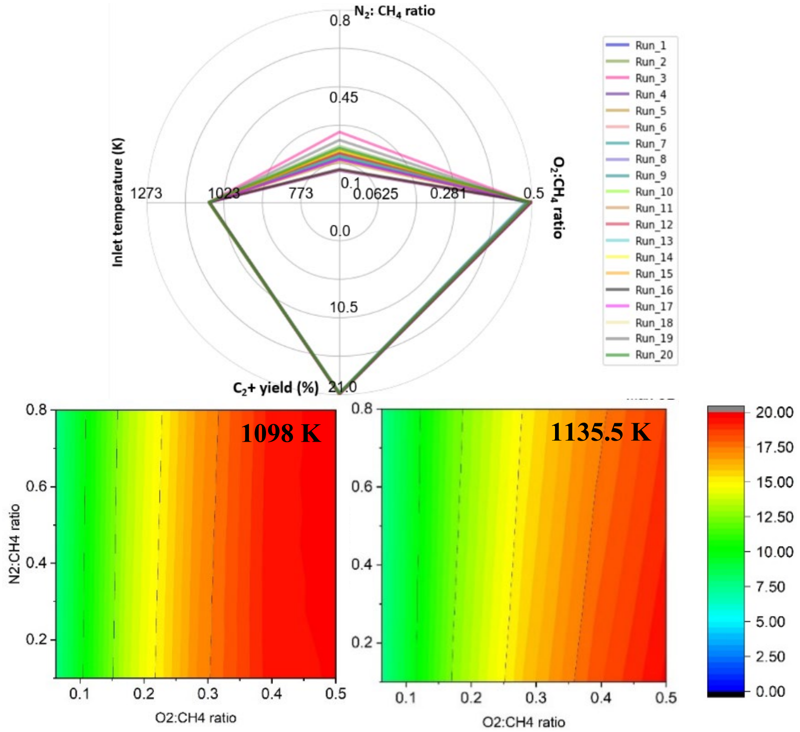

Figure 2. (a) Spider-web showing the results from the optimizer for decision variables and objective function over 20 runs, (b) Solution explored via manual discretization of solution space using the zone simulator

The base case in the adiabatic operation for a single zone is established to determine the efficacy of this optimization methodology. After that, the method is tested by comparing the optimization performance in (1) isothermal and adiabatic operation; (2) single zone to more than two zones; (3) different heat management strategies (e.g., cold shots, external heat exchangers).

4. Conclusions

The multi-zone reactor framework could be a vital tool to model the synergy in an exothermic reaction and explore the heat management of such a reaction. OCM was used in this framework, where the isothermal operation was studied first for a packed-bed reactor. While the results of a single-zone optimization in isothermal operation look promising, heat management in a practical sense would be assessed in adiabatic operation to validate the efficacy of this reactor framework. Single-zone optimization of the adiabatic operation is explored to elucidate the differences in each mode of operation before moving on to multiple zones where various heat management strategies, such as cold shots or external intermediary heat exchangers, are explored.

Keywords

Reactor modeling; optimization; oxidative coupling of methane; simulated annealing

Acknowledgment: This work was made possible by funding from the Qatar National Research Fund (QNRF) project number NPRP13S-0208-200303 and co-funding by TotalEnergies.