Master's Thesis Engineering Technology

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Automated compartmental modelling of chemical reactors

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Master of Chemical Engineering Technology

1 Introduction

Optimal design of adiabatic reactor configurations for exothermic reactions (Figure 1) is challenging due to **multiple, conflicting objectives**. This thesis presents a **two-stage genetic algorithm** to optimize reactor configurations by maximizing the efficiency of the reactor configuration, while minimizing the total reactor volume, the amount of intercooling, and the number of adiabatic steps, ensuring a total conversion of 0.95.

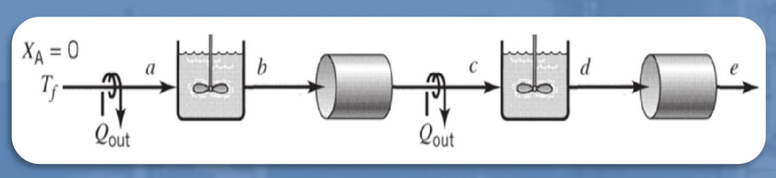


Figure 1: Adiabatic reactor configuration [1]

2 Materials & Methods

A two-stage genetic algorithm was developed using Python 3.10, with Google Colab as the primary environment and DEAP 1.4.2 which provides tools for implementing evolutionary algorithms. In the **first stage**, a **multi-objective NSGA-II** optimized adiabatic step sequences by minimizing total reactor volume, intercooling, and number of steps (Figure 2) [2]. In the **second stage**, each segment was assigned the most suitable reactor type (PFR, CSTR, hybrid, or PFR with recycle) to further reduce total reactor volume (Figure 3) [3]. The algorithm's sensitivity to design priorities was tested by **varying objective weights** (equal, and multiplied by 5, 10, 25, or 50 per objective). Four case studies were used for validation.

Multi-objective Algorithm

Reactor volume
Intercooling
Number of steps

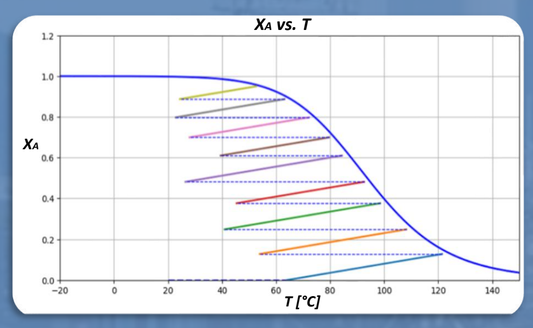


Figure 2: Adiabatic step configuration

Single-objective Algorithm

Reactor volume

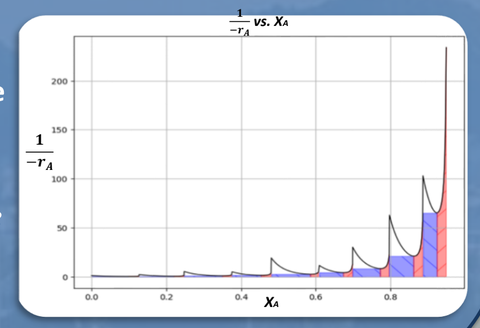
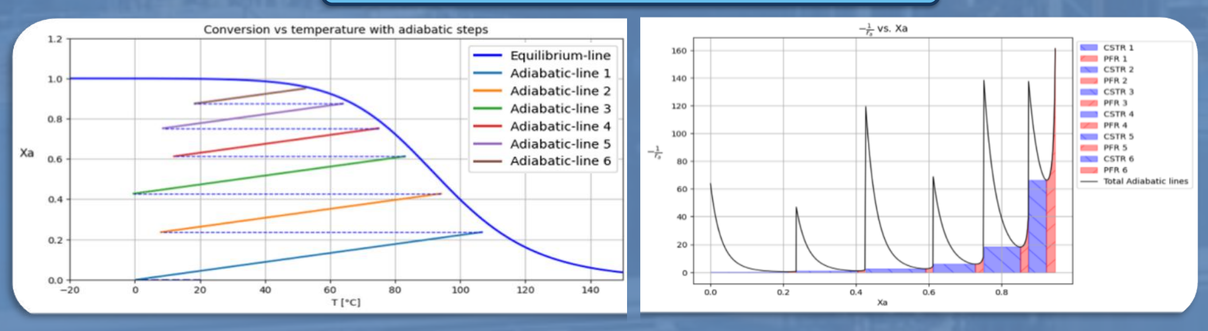


Figure 3: Reactor combination

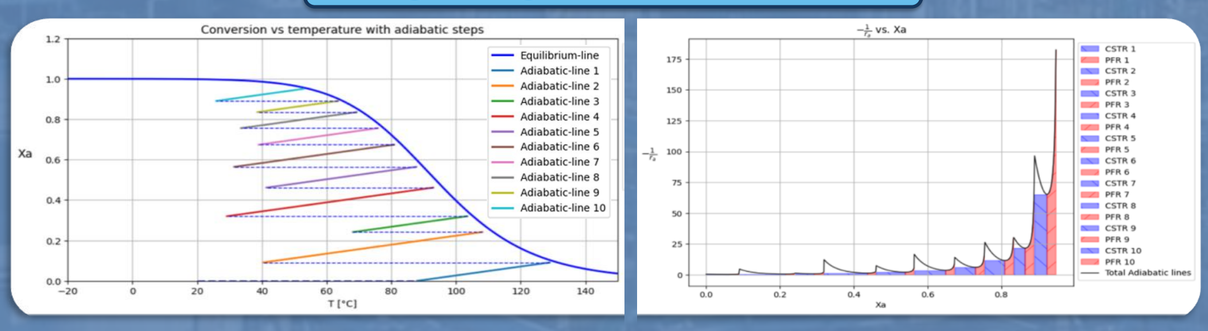
3 Results

Results Case 1

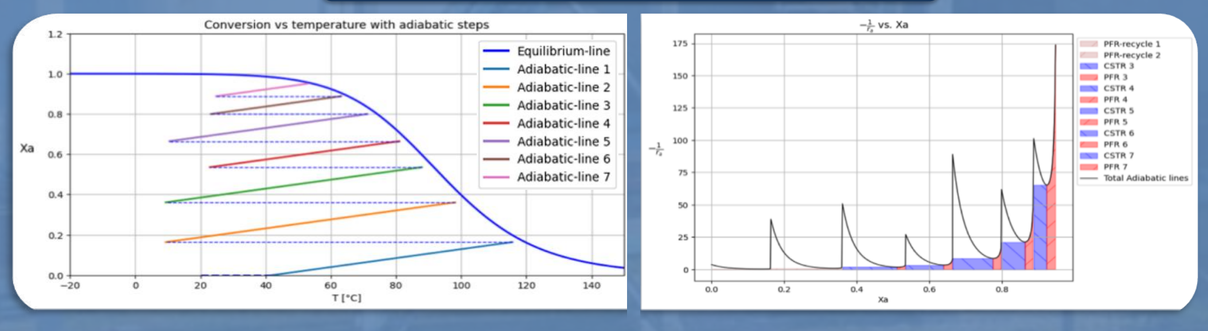
Equal weights



High weight for surface area



High weight for intercooling



High weight for number of steps

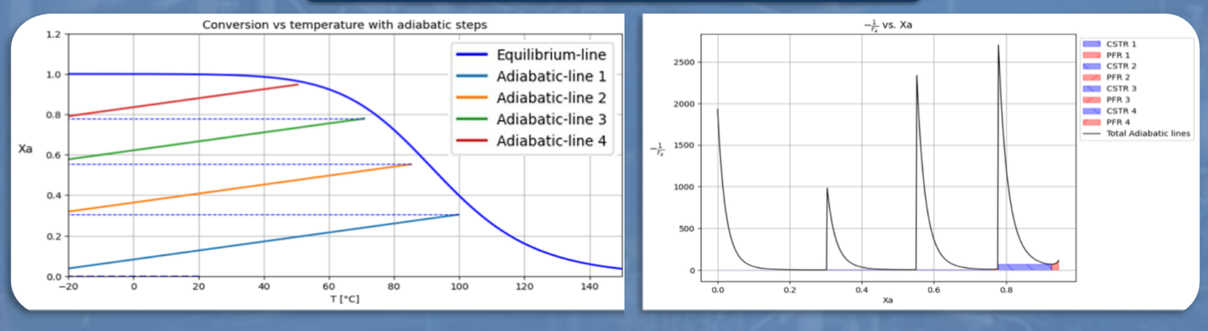


Figure 4: Optimal results for different objective weights (top left: equal weights, top right: reactor volume, bottom left: intercooling, bottom right: number of adiabatic steps)

The results confirmed that the **algorithm successfully adapts** its configuration strategy in response to changes in objective priority. Increasing the weight of the **surface area** objective (Top right) led to reactor designs with a greater number of adiabatic steps, as the algorithm favored smaller conversion increments to reduce total reactor volume. Conversely, emphasizing the **intercooling** objective (bottom left) caused the algorithm to focus more on optimizing the starting temperature of the first step rather than increasing the number of steps, due to the near-constant total heat release at a fixed conversion. Lastly, assigning high weight to the **number of adiabatic steps** (bottom right) resulted in more compact configurations, as the algorithm prioritized structural simplicity over volume minimization.

4 Conclusion

These findings demonstrate that the developed optimization framework can generate **logical and balanced optimal adiabatic reactor configurations** based on user-defined priorities. The algorithm efficiently calculates configurations in about **10 minutes** per weight combination, which is much faster than manual methods that can take a **full day** and may still miss the optimum, making it a valuable tool for automated modelling and decision-making in chemical engineering. It lays the groundwork for future extensions toward more complex reactor systems, endothermic reactions, non-adiabatic conditions, or integration with economic criteria.

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[1] O. Levenspiel and Department of Chemical Engineering, "Chemical Reaction Engineering", John Wiley & Sons, 1999, New York, USA.

[2] A. D. Nandasana, A. K. Ray, and S. K. Gupta, "Applications of the Non-Dominated Sorting Genetic Algorithm (NSGA) in chemical reaction engineering," International Journal of Chemical Reactor Engineering, vol. 1, no. 1, Apr. 2003, doi: 10.2202/1542-6580.1018.

[3] "Non-Isothermal Reactors," in Elsevier eBooks, 2001, pp. 424–551. doi: 10.1016/b978-088415481-5/50008-5

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