Automatic Optimization of Reaction Engineering Processes

Iliyas Melnikov

Master of Chemical Engineering Technology

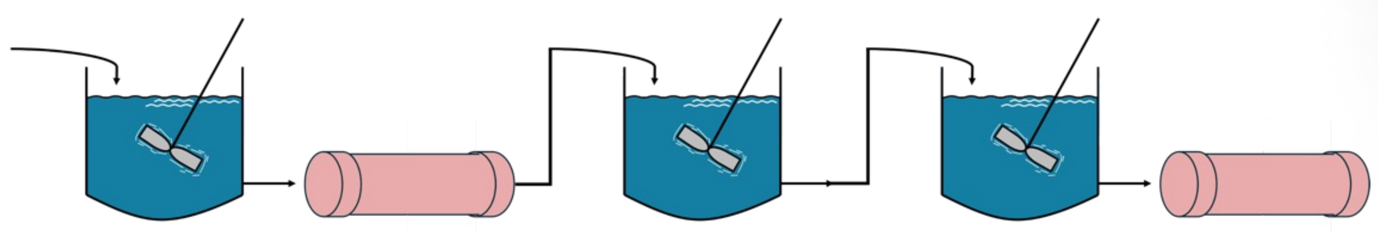
Introduction

This study investigates the application of Genetic Algorithms (GAs) for the optimization of chemical reactor setups. By employing GAs to automate the optimization. The aim is to achieve a working GA that can achieve this for ideal reactors. With a future scope on expanding to non-ideal reactors.

Offering a tool for chemical engineers, as well as non-engineers, to streamline the process of identifying the most effective setup for a specific complex reaction. Serving as a useful starting point for further development, ultimately reducing the time needed for the development process.

$$A + B \longrightarrow 2B + R$$

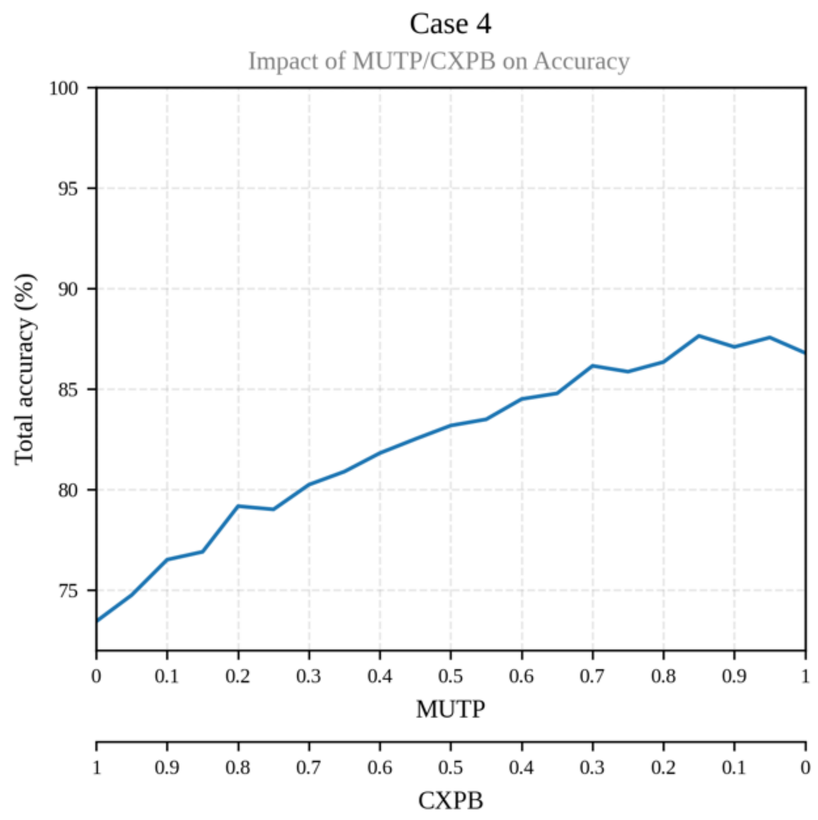
$$3B \rightleftharpoons [B_3]$$



Optimization of Genetic Algorithms

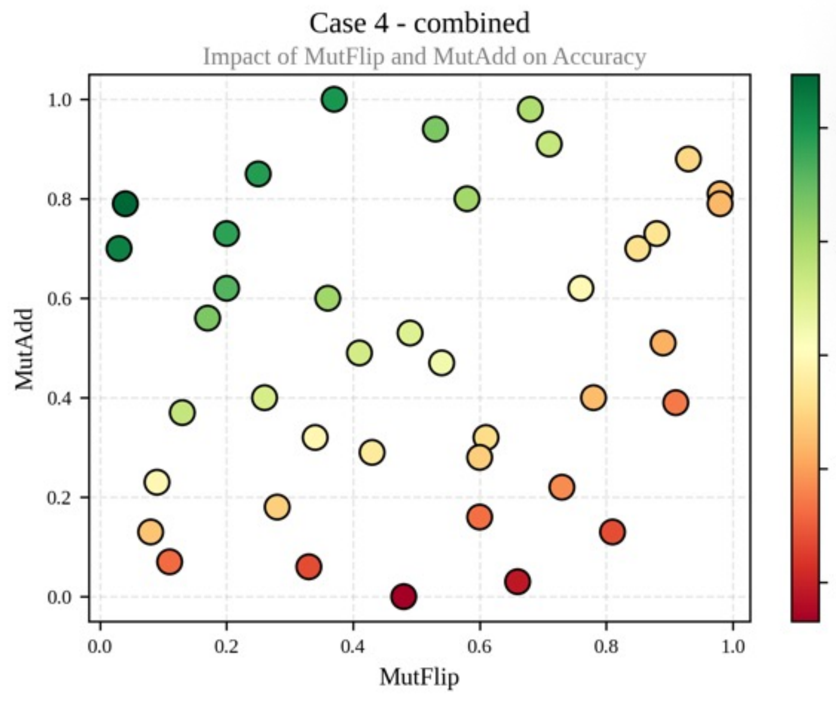
Certain parameters of the GA’s were subjected for optimization, namely:

- Population size
- Breeding balance between mutation and crossover
- Internal mutation probabilities



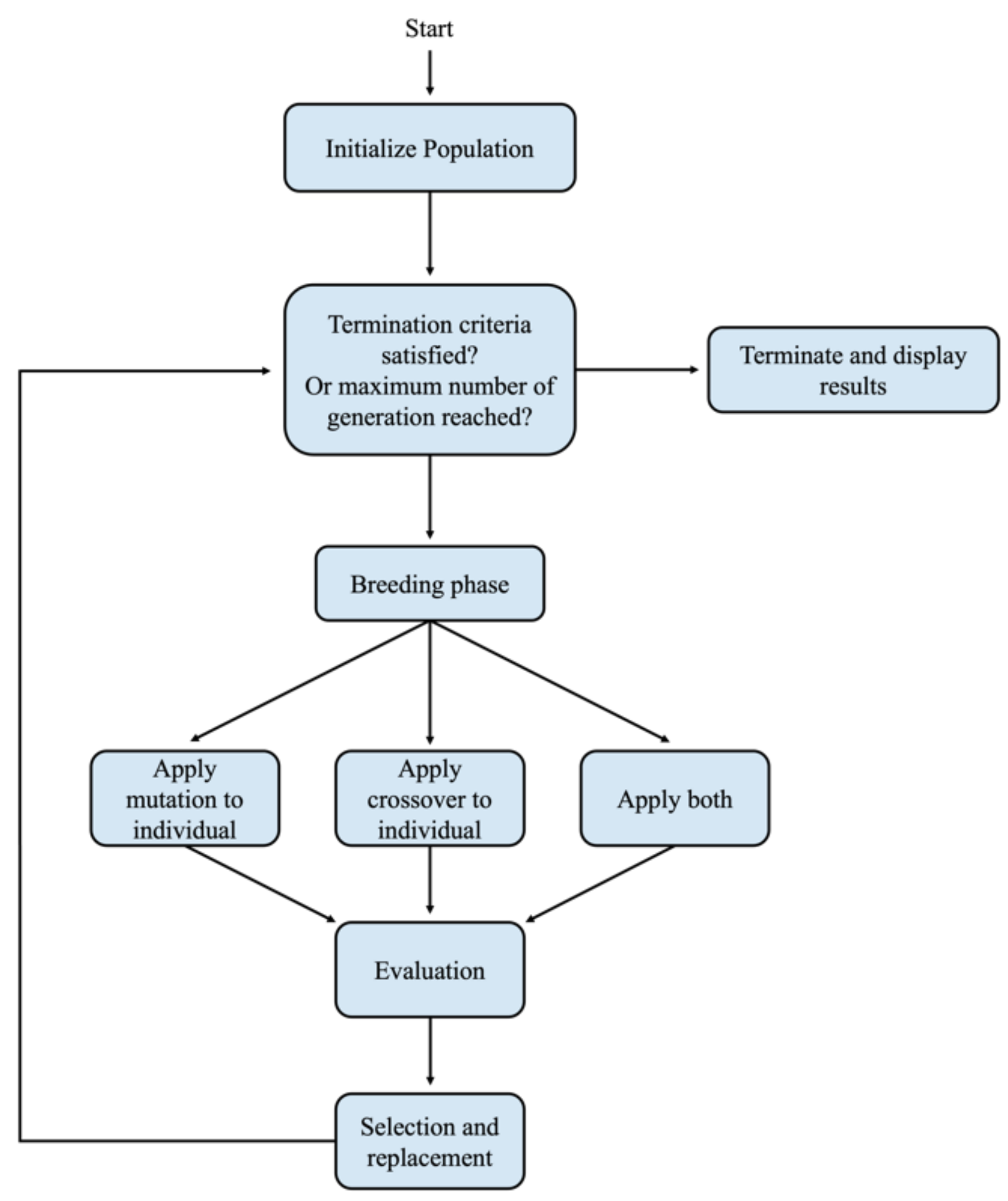
Optimization of the breeding balance revealed that PRGA’s performance increases with higher mutational probabilities.

A more detailed examination of the internal mutation probabilities has revealed that specific components of the mutation operation are more effective than others.



Development of Genetic Algorithms

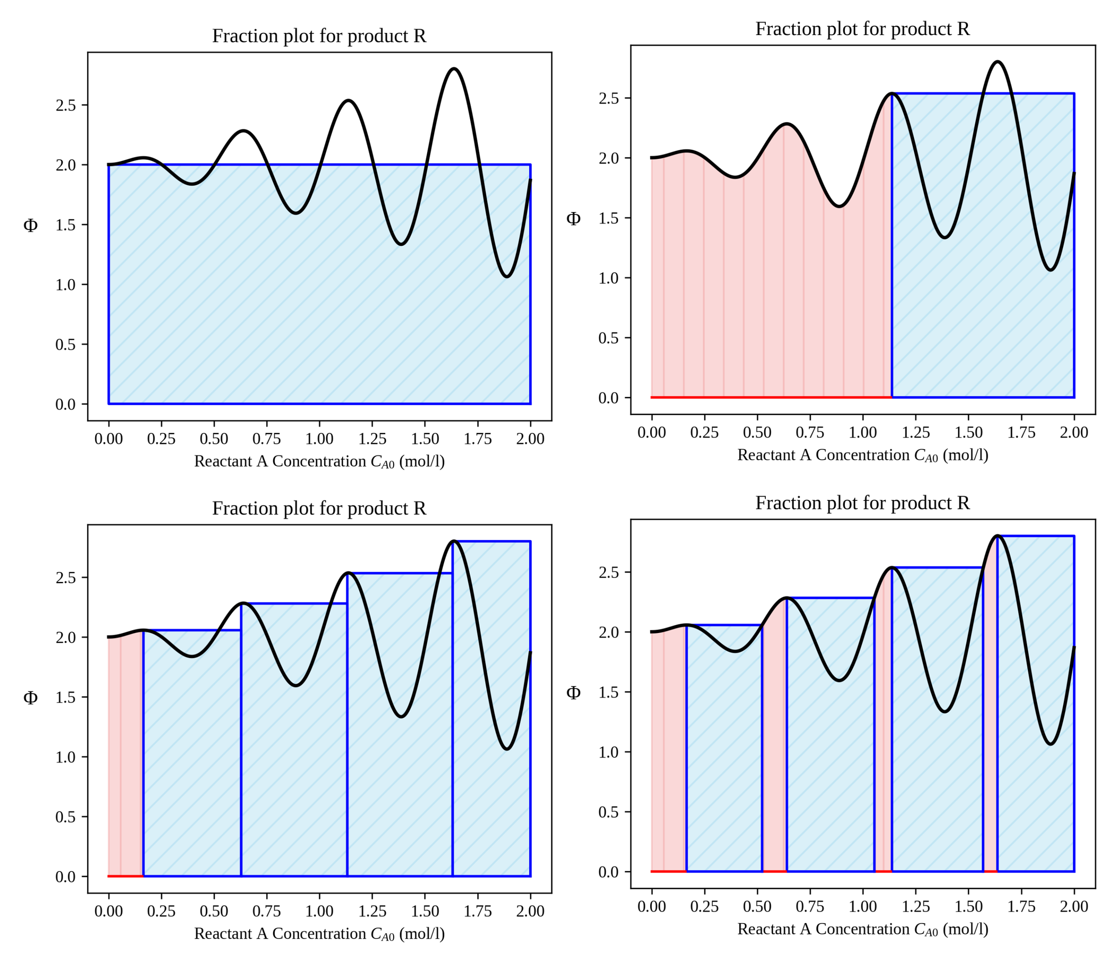
Two GAs were developed to specifically address the optimization of reactor sequences for chemical processes, dubbed SRGA and PRGA. By utilizing modified genetic operations such as selection, crossover, and mutation, these algorithms can evolve setups and discover optimal configurations. They are tested with hypothetical kinetic models, enhancing their efficiency and ability to deliver solutions beyond the reach of traditional heuristic or deterministic models.



Result

After optimizing and comparing the two developed GAs, PRGA has proven to have a superior framework. It delivers optimal solutions for complex parallel reactions in a significantly shorter time frame than SRGA when addressing a problem of similar complexity.

The GA provides optimal solutions for various reactor configurations. Depending on process needs and financial constraints, informed decisions can be made more quickly.



Supervisors / Co-supervisors / Advisors: dr. Di Caprio Ulderico, prof. Leblebici Mumin Enis