

# An Adaptive Refined Grid Search Strategy for Assessing Operational Flexibility and Application on Refrigerant Selection

Jiayuan Wang<sup>1</sup>, Robin Smith<sup>2</sup>, and Lingyu Zhu<sup>1</sup>

<sup>1</sup>Zhejiang University of Technology

<sup>2</sup>The University of Manchester

September 25, 2021

## Abstract

A novel adaptive refined grid search strategy is developed for representative characterization of process feasible region boundaries and accurate estimation of its hypervolume. In particular, a linked list data structure adopted from the field of computer science is used to maintain the grid connectivity information. A uniform perturbation scheme is used to refine the search only near boundaries. The volumetric flexibility index FLV is calculated directly from a summation of feasible hypercubes in the grid, without the need to apply shape reconstruction techniques. The proposed adaptive grid search strategy can capture complex region shapes with reduced sampling costs and without randomness for better reproducibility. Operational flexibility is optimized traditionally at a process scale. A case study on refrigerant selection is presented to demonstrate that the developed strategy could be combined within a computer-aided molecular design framework for operational flexibility optimization in molecular scale.

## Hosted file

manuscript\_flexibility (0902).docx available at <https://authorea.com/users/437283/articles/539030-an-adaptive-refined-grid-search-strategy-for-assessing-operational-flexibility-and-application-on-refrigerant-selection>