

README and Data Documentation

GAMS code for: Reactor network synthesis of enzymatic cascades using superstructure optimization

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1 Project Information

Project Title: GAMS code for: Reactor network synthesis of enzymatic cascades using superstructure optimization

Related Publication:

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2 General Information

Data Set Title: GAMS code for: Reactor network synthesis of enzymatic cascades using superstructure optimization

Short Description:

This repository contains the GAMS optimization scripts and include files used to implement a nonlinear programming (NLP) framework for superstructure-based reactor network synthesis. The framework handles flexible network configurations combining Continuous Stirred-Tank Reactors (CSTR) and tubular Cross-Flow Reactors (CFR) without relying on binary or integer choices. The implementation includes scripts for framework validation via the classical Van de Vusse reaction network and application to a multi-enzyme cascade following the oxidative Weimberg pathway.

Date of Code Creation: 2025-2026

Geographical Coverage: Hamburg, Germany

Keywords: Reactor Network, nonlinear programming, General Algebraic Modeling System, Enzymatic Cascades, Reaction Engineering, Superstructure Optimization, Weimberg Pathway, Van de Vusse Reaction, Radau Collocation

3 Methodological Information

Data Collection and Processing:

Performance results and network configurations are generated computationally using the modeling environment GAMS. The systems of differential equations representing the tubular cross-flow reactors (CFRs) are discretized using a direct transcription technique via orthogonal collocation on finite elements (Radau IIA collocation with a 3-point weight matrix), transforming the differential system into algebraic expressions within a standard NLP formulation.

Software Packages and Solvers Used:

- GAMS (General Algebraic Modeling System)
- NLP Solvers: SNOPT, CONOPT3, BARON, or ANTIGONE (different options can be used)

Experimental Design / Study Context:

The study evaluates the systematic optimization of reactor configurations to outperform standard single-pot configurations. It consists of two benchmark validation and application studies:

1. **Van de Vusse reaction network:** Validating the robustness of the superstructure framework by maximizing the intermediate product yield against established literature targets.
2. **Weimberg pathway cascade:** Maximizing final product concentration and yield given a constrained, distributed total enzyme budget to suppress severe substrate and product inhibition profiles.

Data Validation and Quality Assurance:

- **Numerical convergence checks:** Confirmed across local and global deterministic NLP solver blocks.
- **Degeneracy Prevention:** Explicit bounds and formulations manage fluid distribution nodes (side-feed splits and side-draws) to avoid unphysical internal recycle loops or inactive bypass combinations.

4 Data and File Overview

List of Files and Structure:

The repository is modularly segmented into a core master script, core network configuration modules, and independent case study scripts:

5 Access and Licensing Information

Repository and Persistent Identifier: Published via GitLab / institutional repository.

License for Use: MIT License

Access Restrictions: Open Access

Text for Citation:

Chandra, S., Paschalidis, L., Kinau, S., and Skiborowski, M. (2026). GAMS code for: Reactor network synthesis of enzymatic cascades using superstructure optimization.

File Name	Description	Format
<i>Core Master and Substructure Modules</i>		
<code>RN_optimization_v2.gms</code>	Main optimization master file. Configures option flags, solver specifications, basic constants, global network sets (inlets, outlets, elements), and manages the compilation sequence.	<code>.gms</code>
<code>network.inc</code>	Formulates the structural connectivity equations, splitting/mixing boundaries, feed distributions, and mass balances across the network topology.	<code>.inc</code>
<code>CSTR_model.inc</code>	Implements mass balance equations and residence time constraints specific to Continuous Stirred-Tank Reactor (CSTR) units.	<code>.inc</code>
<code>CFR_model_3.inc</code>	Implements tubular Cross-Flow Reactor (CFR) models utilizing a 3-point Radau IIA orthogonal collocation weight matrix over finite elements.	<code>.inc</code>
<code>constraints_2.inc</code>	Declares definitions for optimization objectives and metric boundaries (conversion, product concentration targets, and operational constraints).	<code>.inc</code>
<code>init.inc</code>	Defines the initialization model (<code>model_init</code>) used to solve a simplified profile first, establishing robust starting parameters for the primary optimization loop.	<code>.inc</code>
<i>Case Study Specific Modules</i>		
<code>VanderVusse_case_1.inc</code>	Contains kinetics data, stoichiometric matrices, boundaries, and test concentrations for the classical Van de Vusse network benchmark.	<code>.inc</code>
<code>Weimberg_case.inc</code>	Contains multi-enzyme Michaelis-Menten kinetics parameters, substrate compositions, and stoichiometry for the 5-step Weimberg pathway cascade.	<code>.inc</code>
<code>weimberg_cfr.inc</code>	Declares variable spaces and balance bounds for total volume and total enzyme budgets specific to the Weimberg cascade CFR units.	<code>.inc</code>

6 Reproducibility and Software Dependencies

Software Required:

- GAMS (General Algebraic Modeling System)
- Valid license for an NLP solver (e.g., CONOPT, SNOPT)

Scripts and Workflow:

To switch between or run the respective case studies:

1. Place all include (`.inc`) modules and the master execution file (`RN_optimization_v2.gms`) in your active GAMS working directory.
2. Open the master file `RN_optimization_v2.gms`. To toggle between case studies, adjust the block includes at the bottom of the file to pull either the Van de Vusse block (`$include VanderVusse_case_1.inc`) or the Weimberg files (`$include Weimberg_case.inc` and `$include weimberg_cfr.inc`).
3. Select the desired active solver by uncommenting its corresponding command (e.g., `option nlp = conopt3 ;`).
4. Execute the master script. The system first triggers `init.inc` to resolve initial structural constraints before executing the complete network optimization model (`model_Optimization`) maximizing the target metric (`Y_Opt` or `M_Opt`).

7 Ethical and Legal Aspects

Data Protection: No personal or sensitive data are contained in this repository.

Consent Statement: Not applicable. No human participants or animals were involved.

8 Versioning and Updates

Version Number: v1.0

Date of Release: [15-06-26]

Change Log:

Version 1.0: Initial public release accompanying the conference proceedings, encompassing the full unified superstructure framework with complete include options for both the Van de Vusse validation and Weimberg case studies.