REACTION TEMPLATES AS A CONSTRAINT IN PROGRAM SYNTHESIS OF CHEMICAL REACTION NETWORKS

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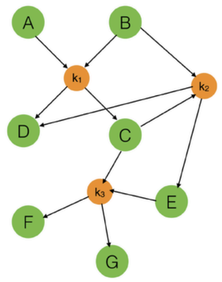
01 BACKGROUND

- Chemical Reaction Networks (CRNs): mathematical models that describe the behavior of chemical reactions in a system, and are widely used as fundamental tools in many domains such as chemistry and biology.

Reaction mechanism

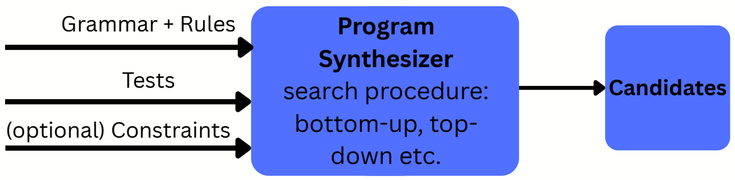
$$A + B \xrightarrow{k_1} C + D$$
$$C + B \xrightarrow{k_2} E + D$$
$$C + E \xrightarrow{k_3} F + G$$

Reaction network

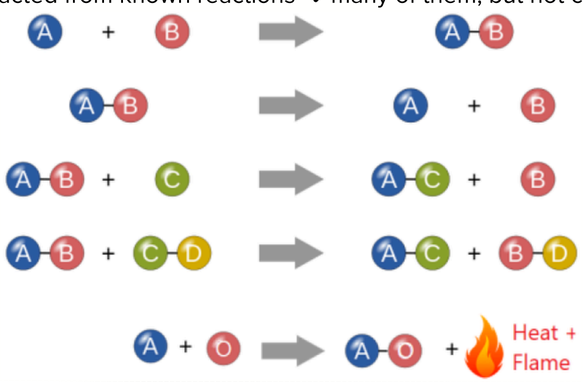


- Inverse problem: given the evolution of species concentration over time and a partial CRN, reconstruct the whole network.

- Program synthesis: subfield of AI that can automatically find a program given a language and some specification. ⟶ Herb.jl [1]



- Reaction templates: encode common patterns of chemical reactions abstracted from known reactions ➜ many of them, but not complete!



02 RESEARCH QUESTION

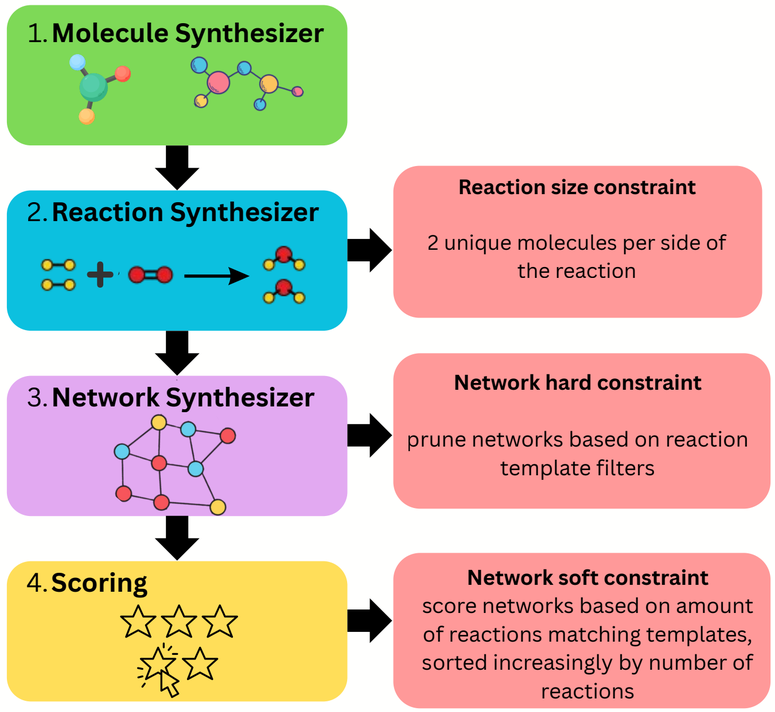
How do we implement reaction templates into the program synthesis of CRNs, such that we avoid exploration of chemically implausible reactions?

(Experimental) Sub questions ⟶ Target Rank, Search Space, Runtime

03 METHODOLOGY

This project builds on top of R. Wijers Thesis and code-base. [2]

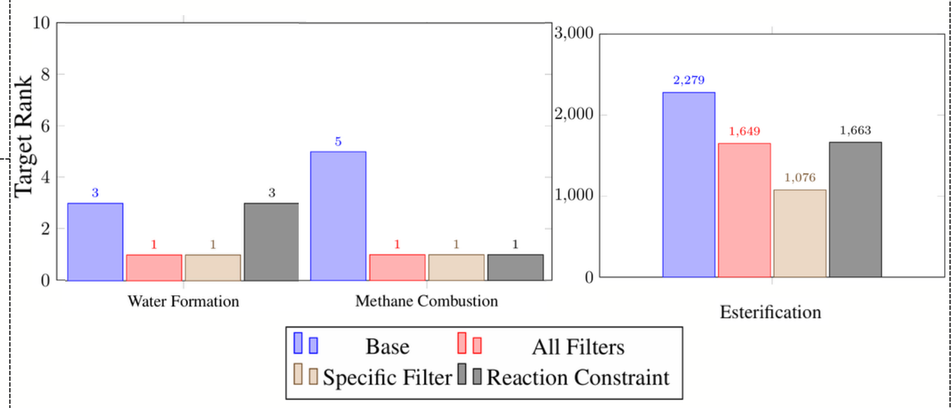
Pipeline and Constraints

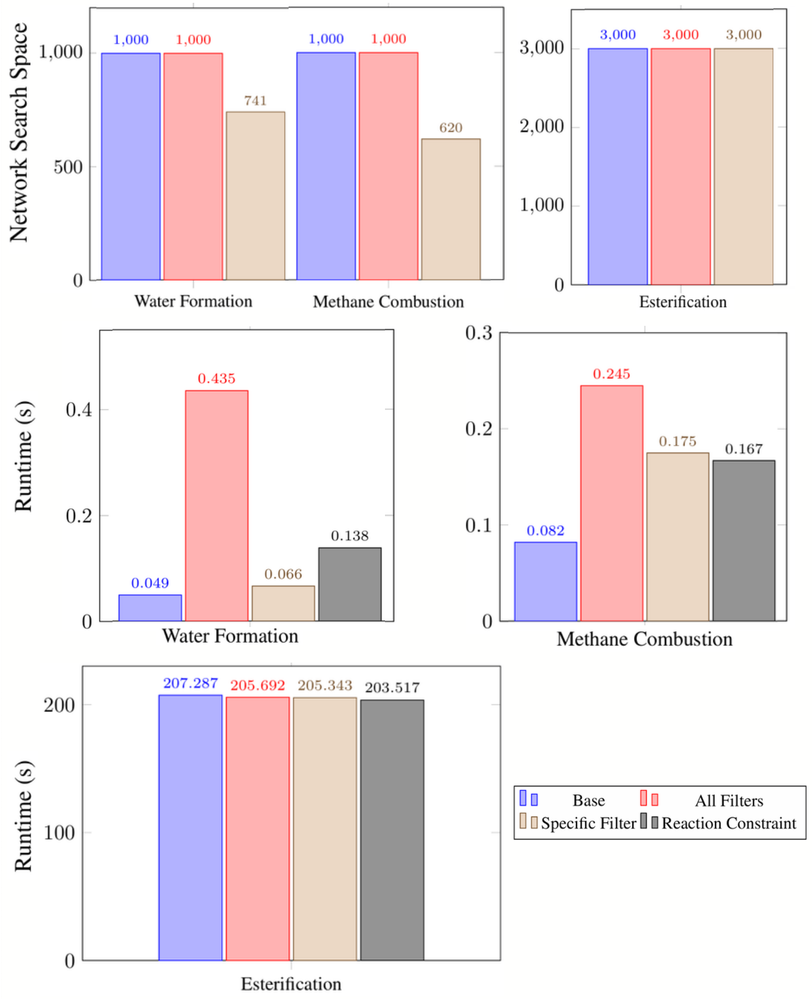


Reaction Template Filter Example

Oxidation	$A + O_2 \rightarrow AB$ Exactly 2 reactants, 1 product. O_2 must appear as an isolated reactant.

04 RESULTS





05 CONCLUSIONS AND FUTURE WORK

- Does it work? ⟶ **Yes! ...** But there are some limitations:
  - Limited amount of CRNs benchmarked.
  - 5 general reaction templates modelled.
  - high overhead for small networks.

- Future Work:
  - more reaction templates, perhaps a database.
  - general reaction templates are helpful for reaction structure, but what about more specific reactions? ⟶ enhance molecule generation or even replace it altogether!

References:
[1]: Program synthesis library written in Julia: arXiv:2510.09726
[2]: Automated Discovery of Chemical Reaction Networks using Program Synthesis: https://resolver.tudelft.nl/uuid:f70ee49d-d0e6-4938-af11-7c6770a38502