A NOVEL TOOLBOX FOR KINETIC MODELLING AND CHEMICAL REACTION SIMULATION FOCUSED ON OPEN SCIENCE

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1 INTRODUCTION

We live in the race of the green and digital transition, and shortening the time between research and application of novel technologies is a key target, where CFD has already shown its potential (Papurello et al, 2022; Paris et al, 2022) in the optimization of processes either during the design step or parallel to its use. While CFD software was originally developed for aeronautics applications, it has spread to other sectors, and software platforms must adapt to cover different phenomena. A subject as general as chemical reactions is poorly covered in most CFD platforms, including OpenFOAM, and users usually have to code their own kinetic models. This fact limits the broad application of these simulations and makes it difficult to share the models.

This work presents a novel toolbox for kinetic modelling and chemical reaction simulation. It uses the SBML standard (Hucka et al, 2003), which allows defining species, reactions, constraints, rules and events, to describe a complete mechanistic kinetic model. The toolbox is completely OpenSource and includes a web GUI to create and modify SBML files, an application to fit kinetic parameters using experimental data based on a metaheuristic specially designed for kinetic modelling, and an OpenFOAM model able to load a SBML file and insert it in the simulation without any coding. The use of a standard that also stores and maintains a public repository of models allows sharing easily models, reactions and kinetic parameters between users.

The web GUI was entirely developed in JavaScript, fully reactive (it updates the SBML model as the user introduces data) and lacks server side, meaning that it can be downloaded and used locally. It uses MathLex and MathJax Open Source codes to parse, preview, and transform the raw text of mathematical expressions in the ContentMathML format used by SBML.

A C++ parser of SBML models reads and transforms in objects the SBML files, with some special considerations for the final use of the file. Non-constant parameters are treated as the target to be fitted in the metaheuristics software, while the OpenFOAM model reads them as references to fields out of the model (temperature or incident radiation, for example). The SBML compartments are associated with OpenFOAM regions and patches, and the parser checks the compatibility of the model before starting the simulation.

The main challenge in the design of the metaheuristic is to cover a wide range of kinetic models without any previous adaptation of the problem or the metaheuristic parameters by the users. This was intended to ease and spread its use. Too large ranges for parameter values create regions of flat gradient and discontinuities in the error function, while the error function itself could be tunned to avoid preferred paths of the gradient to undesired solutions. Simplest models can be easily fitted using linear regression or even human guided heuristics, and thus, the metaheuristic is thought to be used in complex models with slow evaluations of the error at each proposed solution. All those challenges are tackled in the metaheuristic, including a novel channeled random generator that quickly learns to avoid flat regions and exploit those where the error function shows variations, a couple of local search methods that minimize the evaluations of the error function, and a solution recombination algorithm to further explore the best regions of the whole solution space.

Finally, the OpenFOAM model reads and uses the kinetic laws and stoichiometric parameters of the defined reactions, allows introducing rules to assign dynamic values to fields or species, algebraic rules that are solved as additional equations of the model, constraints for fields and species, and temporal events or delayed expressions. The parser of ContentMathML equations in the SBML file was carefully designed to allow and interpret operations between scalars and scalar fields. It includes a reactivePatch boundary that can read and solve surface reactions or even model species transfer mechanisms between regions.

The metaheuristic was validated using a complex kinetic model of photo-Fenton water disinfection including 13 kinetic parameters and more than a hundred species (Casado et al, 2021) which involves three submodels that can be fitted separately, of growing complexity. It achieved a better solution than the originally found using a human-guided Squared Programming Optimization software in a fraction of time.

The OpenFOAM model was validated using a model of photocatalytic degradation of methanol in three different photoreactors (Figure 1) with two different models of kinetic dependence on incident radiation. Results were compared to those of equivalent simulations in ANSYS Fluent, that required User Defined Functions to introduce the dependence on incident radiation (Figure 2). Minor differences were observed between either software and experimental samples.

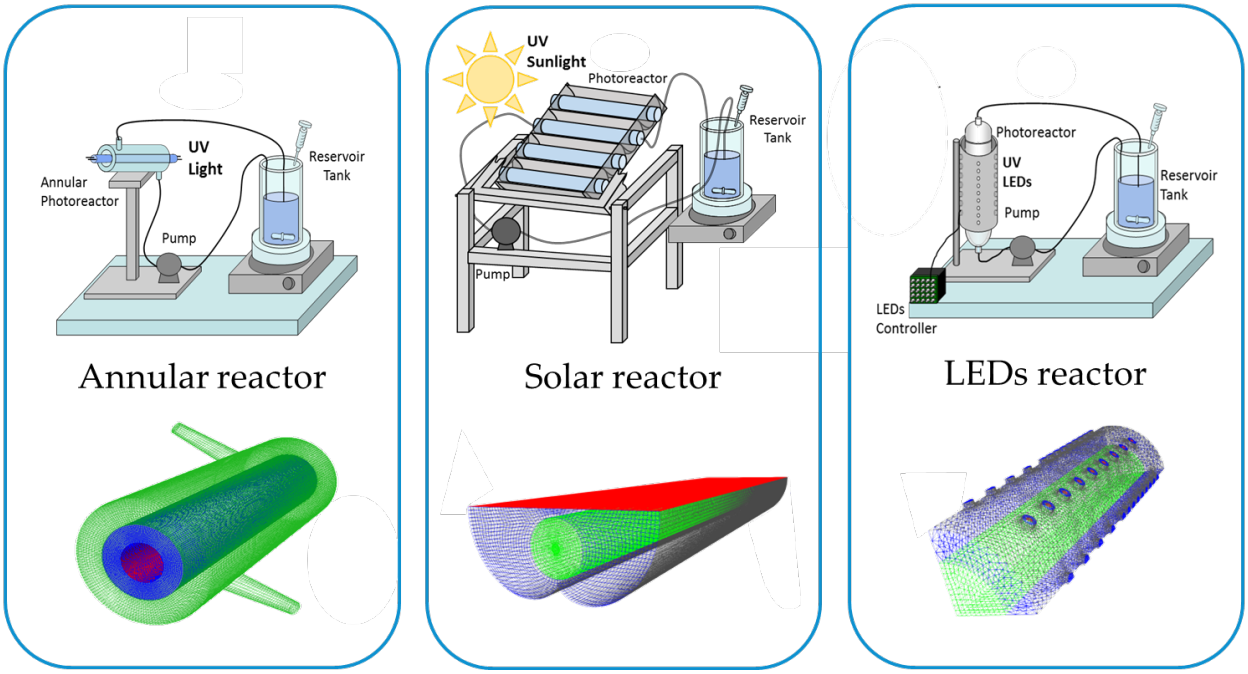

Figure 1. Reactors used in the validation of the OpenFOAM chemical model.

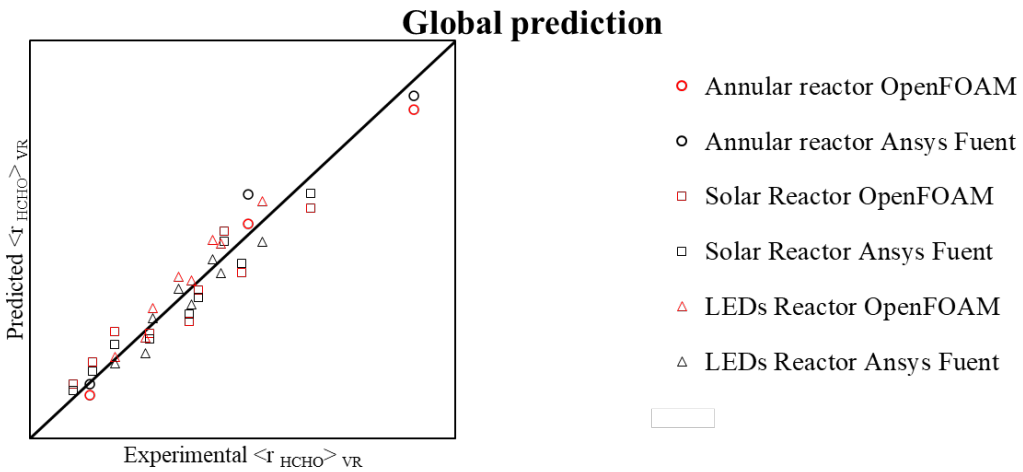

Figure 2. Comparison between experimental and modelled values of average kinetics under different radiation emissions in each reactor.

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