~ 6 MONTHS INTERNSHIP (2023-2024)

Title: Hydrogen combustion in heterogeneous media using an Euler-Euler approach

Supervisors:
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Laboratory: IMFT - UMR 5502
Internship stipend: ~600 Euros/month.

This work deals with the numerical modeling of hydrogen combustion in heterogeneous media using an Eulerian approach. It is a part of the project MIMOSAH [1], which aims at modeling the hydrogen combustion in fluidized beds to safely produce thermal energy from hydrogen while reducing the risks related to the high reactivity and wide range of flammability of such a fuel. In fact, fluidized beds allow to ensure well-controlled temperature and combustion stability by a relatively low-temperature fuel conversion. This makes the use of hydrogen possible to replace conventional fossil fuels to contribute meeting the challenge of climate change.

The Euler-Euler approach allows the Computation Fluid Dynamics (CFD) to reproduce the two-phase flow behavior regardless of the particle number since both the phases are solved in an Eulerian framework accounting for interphase momentum and energy transfers. The Euler-Euler approach accounting for reactions is implemented by IMFT (Institut de Mécanique des Fluides de Toulouse) in collaboration with EDF (Électricité de France) R&D in the neptune_cfd code by appropriate models and closure laws [2]. The code neptune_cfd is a multiphase CFD code developed in the framework of the NEPTUNE project, financially supported by EDF, CEA (Commissariat à l'Énergie Atomique), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and Framatome. The code solves the coupled partial differential equations by a finite-volume approach using an adaptive time step. The solver is based on a cell-center type finite volume method and an elliptic fractional time-step method. The latter relies on a volume fraction-pressure cycle, which is an iterative method to ensure mass and energy conservation [3].

In the frame of a previous internship [4], several numerical approaches for the treatment of stiff chemical reactions, such as those used for hydrogen combustion, were analyzed and evaluated for the implementation in neptune_cfd. One effective way to solve the highly non-linear reactive system is to use a splitting approach, which first integrates in time implicitly a set of ODEs for species and energy variables using a backward differentiation formula (BDF) method, and then solves for the reactive system by a semi-implicit method using updated quantities. This approach makes it possible to decouple chemistry, which is constrained to very small characteristic times, from hydrodynamics, which is subject to larger times imposed by the CFL constraint. The goal of the present internship is to realize the practical evaluation and implementation of this approach by coupling neptune_cfd with the implicit stiff ODE solver CVODE [5], and also with the code Cantera [6] to update thermodynamic and transport properties, as well as chemistry, during the numerical integration.
This approach will be compared in terms of efficiency and accuracy with alternative approaches proposed by [4]. Several kinetic schemes will be tested to validate hydrogen/air combustion in 0D/1D flames [6]. Then, numerical simulations of combustion in a heterogeneous medium characterized by inert particles will be carried out to study the flame response in the presence of a solid phase.

The internship would ideally lead to a PhD thesis in the frame of a PEPR French project on the carbon capture by eco-efficient oxycombustion processes. This project aims at improving knowledge and skills in oxycombustion which is considered as a key process to decarbonise heat production in industry. IMFT is

participating in the project because of its expertise in high-performance numerical simulation and modelling of reactive gas-particles flows, in particular in 3D unsteady numerical simulations of chemical looping combustion (CLC) [7].

Requirements:

The candidate is ending the academic year of graduation (Master's degree or Engineering School) in mechanics or applied mathematics and is interested in pursuing a PhD thesis. The candidate is familiar with numerical methods and numerical simulations in fluid mechanics. Knowledge of the C programming language is recommended. Knowledge of combustion is a plus.

References:

[1] Agence Nationale de la Recherche, Funded projects, MIcro to macro-scale MOdeling for SAfe Hydrogen combustion in fluidized beds, https://anr.fr/Projet-ANR-19-CE05-0004

[2] Hamidouche, Z., Masi, E., Fede, P., Ansart, R., Neau, H., Hemati, M., Simonin, O. Chapter two - numerical simulation of multiphase reactive flows. In: Bridging Scales in Modelling and Simulation of Non-Reacting and Reacting Flows. Part I. Vol. 52 of Advances in Chemical Engineering. Academic Press, pp. 51–124, 2018.

[3] Neau, H., Pigou, M., Fede, P., Ansart, R., Baudry, C., Mérigoux, N., Laviéville, J., Fournier, Y., Renon, N., Simonin, O. Massively parallel numerical simulation using up to 36,000 cpu cores of an industrial-scale polydispersed reactive pressurized fluidized bed with a mesh of one billion cells. Powder Technology 366, 906–924, 2020.

[4] Pierre, G., Développement d'un algorithme semi-implicite d'intégration des termes sources réactifs et implémentation dans NEPTUNE_CFD. Rapport de stage, M2 Dynamique des Fluides, Énergétique et Transferts, 2021.

[5] Cohen, S. D., Hindmarsh, A. C., Dubois, P. F. CVODE, A Stiff/Nonstiff ODE Solver in C. Computers in Physics, 10(2), 138-143, 1996.

[6] Goodwin, D. G., Moffat, H. K., Schoegl, I., Speth, R. L., Weber, B. W. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. https://www.cantera.org, 2022. Version 2.6.0.

[7] Hamidouche, Z., Masi, E., Fede, P., Simonin, P., Mayer, K., Penthor, S. Unsteady three-dimensional theoretical model and numerical simulation of a 120-kW chemical looping combustion pilot plant. Chemical Engineering Science, 193, 102-119, 2019.