

Modelling of differential diffusion with sparse particle methods in detailed H_2 - O_2 reactions

Motivation

The pursuit of clean energy sources requires the search for novel methods for generating, storing and transporting these. Among them, hydrogen has emerged as a solution capable of addressing society's growing demands and the call for more environmentally friendly substitutes. However, accurately and efficiently simulating hydrogen combustion, as well as appropriately modeling its underlying physical phenomena, remains a significant challenge.

Project description and research goals

Multiple Mapping Conditioning (MMC) is a method to simulate combustion reactions which combines the use of an Eulerian flow field and a set of Lagrangian particles. It is a more efficient method than traditional numerical approaches for combustion. A new technique, known as "Side Stepping", capable of modelling differential diffusion phenomena within MMC framework was developed and tested for very simple H_2 - O_2 reactions. Further studies with more complex chemical mechanisms need to be carried out to assess the model performance in the presence of multiple high diffusing species and more than one global reaction.



Tasks

- Conduct a literature review about differential diffusion and flow modelling with sparse PDF methods.
- Simulate the differential diffusion effects of detailed H_2 Figure 1: Temperature field for O_2 combustion using a DNS fluid flow filtered solution H_2 - O_2 one reaction mechanism and MMC methods
- Simulate the differential diffusion effects of detailed H_2 -O₂ combustion using an LES approach with MMC methods
- Evaluate and analyze the simulation results
- Write a thesis and present your results

Prerequisites

- Basic knowledge in fluid dynamics and combustion reactions
- Beneficial: knowledge in C/C++ and Python, experience with computational fluid dynamics (CFD), OpenFOAM

Contact

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