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Study of Methane Oxidation in a Monolith Reactor: Comparison between a 1D and a 3D Modelling Approach

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Highlights

- Study of methane oxidation reaction in a monolithic reactor using a computational approach
- Comparison of results for a CFD-based model with a conventional 1D+1D model
- Good agreement between the two approaches

1. Introduction

CFD based modelling including diffusion and reaction within a meshed porous solid to represent a heterogeneous catalyst has seen a rapid growth in interest over the last decade. Early attempts to do this essentially represented the reaction simply as a heat source terms [1]. Developments in commercial and open source CFD sub-models and methods allowed meshing of the porous solid and the development of functions to model species diffusion and reaction within the porous phase. This approach, sometimes referred to as "hi-fidelity" reactor modelling, is now being widely published [2][3][4][5]. There remains though a shortage of rigorous model validation and verification. A significant number of published validations apply only a single "global" result to the validation (e.g. temperature, reaction conversion etc.) [6] which does not address the validity of the complex substructure of the overall model [7].

2. Methods

This presentation will report on a detailed comparison of results for a CFD-based model of a catalyst coated channel (a single square 1mm channel of a washcoated monolith with length of 1 cm) with those from a conventional chemical reaction engineering (CRE) 1D+1D model. Methane oxidation, at low concentrations, was used as an example reaction and experimental data for methane oxidation over a 1 wt.% Pd/Al_2O_3 catalyst were used to derive a Langmuir Hinshelwood kinetic model. The same kinetic expression was used in both the CFD and CRE reactor models.

Steady state conditions were assumed and the reaction was modelled at different temperature (400 ºC, 425 ºC and 450 ºC) and different feed compositions (dry feed and wet feed). The CRE 1D + 1D model was developed in Athena Visual Studio while the CFD model, with the catalyst meshing, diffusion and reaction aspects based largely on that reported by Partopour & Dixon [8] was compiled in OpenFOAM. For the most part this made use of existing verified folders available within OpenFOAM (e.g. reactingFoam solver) although additional coding for diffusion models and complicated kinetic models was required.

3. Results and discussion

Figure.1 shows the comparison between the two approaches for the methane oxidation reaction conducted at 400 ºC and dry feed conditions.

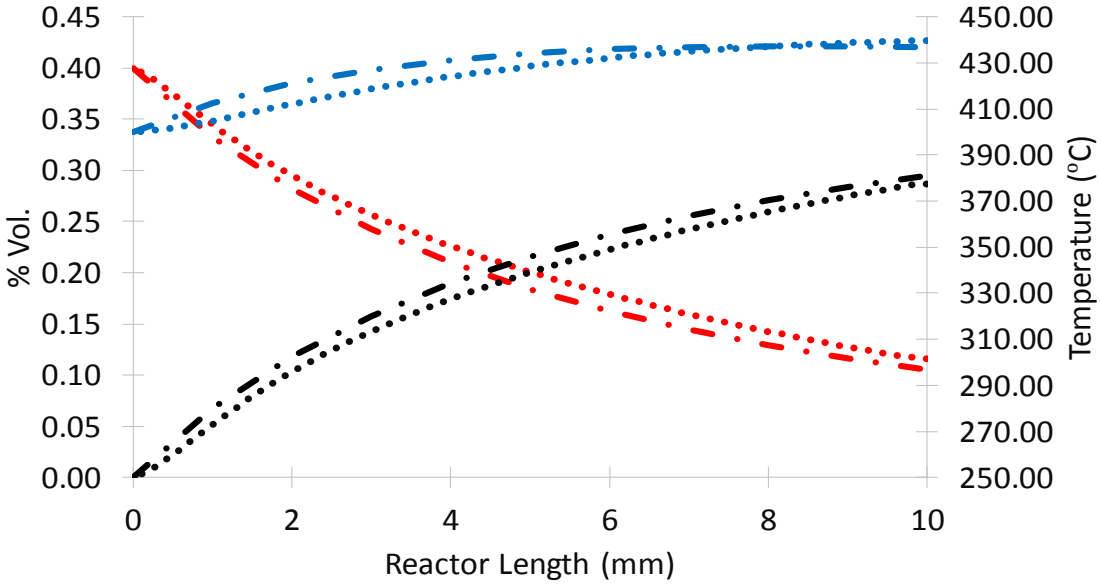

Figure.1 Comparison between 1D + 1D and CFD results for CH_4, CO_2 and temperature trend along the reactor channel. (●—) CH_4 1D + 1D, (●) CH_4 CFD, (●—) CO_2 1D + 1D, (●) CO_2 CFD, (●—) Temp. 1D + 1D, (●) Temp. CFD

4. Conclusions

The two modelling approaches showed comparable concentration and temperature profiles along the modelling channel allowing the validation of the implemented CFD package and growing confidence in its use to simulate diffusion and reaction systems.

References

The reference format is provided below [1 – 3]. [Times New Roman 10].

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Keywords
Methane oxidation; CFD; 1D + 1D; Modelling