STSM Report in the frame of SMARTCATs Cost Action CM1404

DEVELOPMENT OF COMPUTATIONAL TECHNIQUES FOR THE COUPLING OF COMBUSTION CHEMISTRY WITH CFD CODES FOR REALISTIC MODELLING AND PREDICTION OF COMBUSTION PHENOMENA IN INTERNAL COMBUSTION ENGINES

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1. INTRODUCTION

The present report was prepared for the fulfilment of the requirements of the Short Term Scientific Mission (STSM) program of the 2nd Grant Period of the SMARTCATs Cost Action CM1404 "Chemistry of smart energy carriers and technologies". The STSM stay of Dr. C. Chasos took place for five days during the period 10 to 14 April 2017, inclusive, when Dr. Chasos collaborated with the research team of Prof. L. Kaiktsis. The STSM of Dr. Chasos initiates the collaboration between a home institution, Frederick University in Cyprus with the research team of Prof. L. Kaiktsis at the host institution, National Technical University of Athens in Greece. In the present report the purpose of the STSM is stated first. Next, the work carried out during the STSM is described. Furthermore, the contribution of the STSM to the Action's aim is explained. Finally, the expected future collaboration with the research team of Prof. L. Kaiktsis, along with possible future publications resulting from the STSM are outlined.

2. PURPOSE OF THE STSM

The main purpose of the stay at the Home Institution was to closely interact and collaborate with the research team of Prof. L. Kaiktsis, in order to strengthen collaboration and establish mutual research work in the field of internal combustion engine (ICE) modelling and simulation. The first objective was to use a state-of-the-art CFD code in order to define the simulation setup for methane combustion simulations, and the second objective was to study detailed chemical kinetics mechanisms for the modelling of syngas and methane combustion.

3. DESCRIPTION OF WORK

The work carried out during the STSM included, firstly, the CFD modelling simulation of methane injection into constant volume chamber, and secondly, the chemical kinetics calculations of methane combustion with two detailed mechanisms, namely Aramco [3] and Creck [4]. For the simulation of methane combustion in a constant volume chamber, first the simulation of methane injection in a constant volume chamber was investigated in order to characterize the flow phenomena which are present. A computational mesh of around 70000 cells was generated in the automatic mesh generation of the CFD code STAR-CD [1]. The computational mesh and the boundary conditions are illustrated in Figures 1 and 2.

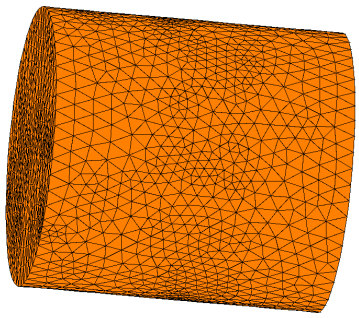

Figure 1: Constant volume chamber computational mesh

For the characterisation of methane injection, increasing injection velocities were used as the initial condition of the methane injection velocity at the tip of the methane injector mounted vertically at the surface of the chamber. The injection velocity is indicated by arrows in Figure 2, where the fuel inlet boundary and the pressure boundary condition are shown in red and green colour, respectively.

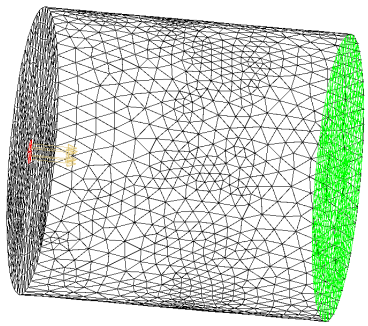

Figure 2: Boundary conditions for methane injection into constant volume chamber

Test simulations were carried out at increasing methane injection velocities, for 300, 600 and 800 m/s. It was found that at high injection velocities supersonic velocities are present adjacent the injector tip which substantially influence the air fuel mixing and the established flow field. Figure 3 presents the simulation results for the predicted methane/air field at injection velocities. As it can be observed in Figure 3, the methane concentration adjacent the injector for the maximum injection velocity is different than the lower injection velocities fuel pattern. A high methane concentration jet which attenuates is present adjacent the injector, and this can be attributed to the supersonic flow phenomena.

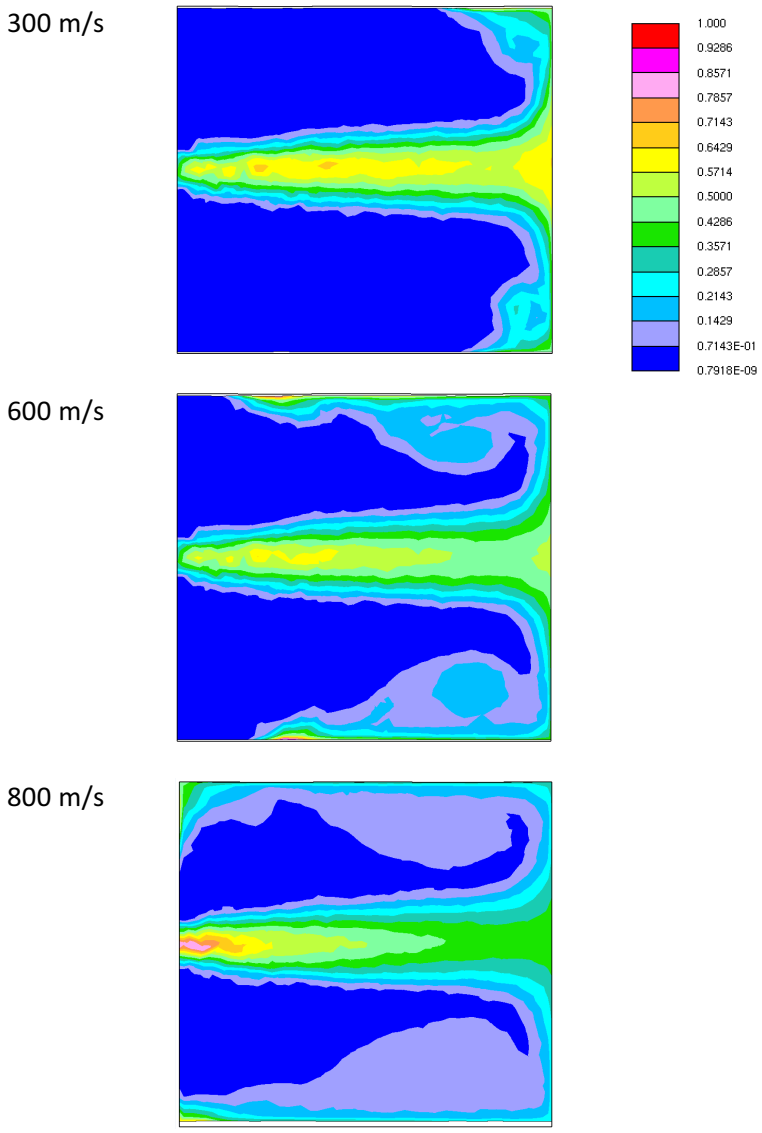

Figure 3: Methane and air fuel mixing prediction at injection velocities 300, 600 and 800 m/s.

However, further CFD modelling and simulations are required in order to fully characterize the methane injection flow phenomena, for particular engine application. A relevant research work [2] was found in literature, which describes in detail the subsonic and hypersonic methane injection flow phenomena which are present. For particular engine combustion modelling and simulation, it is required to model the full gas injector geometry and assemble it with a constant volume chamber for very fine mesh structure. The detailed simulations will provide the data for setting up the initial conditions for methane injection into the cylinder of the internal combustion engine for which the full simulation setup is required to be defined in future work. This setup includes the modelling of fuel injection, fuel properties, and the numerical aspects (including time step size and mesh size), as well as the user coding requirements for the implementation of special chemical kinetics mechanisms for the modelling of combustion.

Furthermore, two detailed chemical combustion mechanisms were selected from literature, namely Aramco [3] and Creck [4]. The two mechanisms were studied and used for chemical kinetics test calculations of syngas combustion. The results from the test calculations with Aramco [4] mechanism for the combustion of

syngas in a perfectly stirred reactor at temperature 790 K, pressure 1 atm and residence time 120 ms are included in Figures 4, 5 and 6.

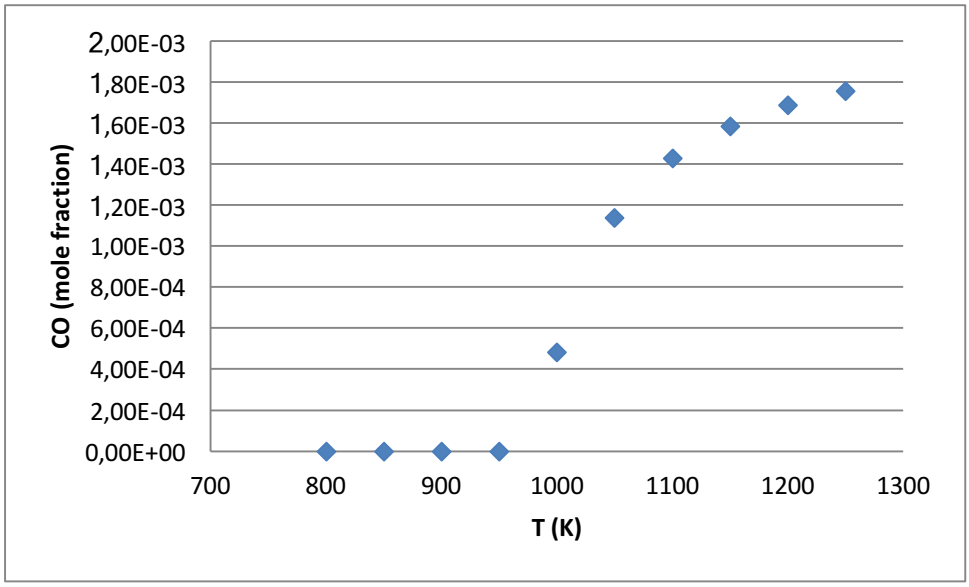

Figure 4: Estimation of CO mole fraction as function of temperature with Aramco mechanism [3].

The two mechanisms will be validated against experimental data from literature. The validation work is required for meeting the objective for the selection of detailed chemical kinetics mechanisms for the modelling of syngas and methane combustion, and then producing skeletal and reduced validated combustion mechanisms for the modelling and simulation of methane combustion in the cylinder of internal combustion engines.

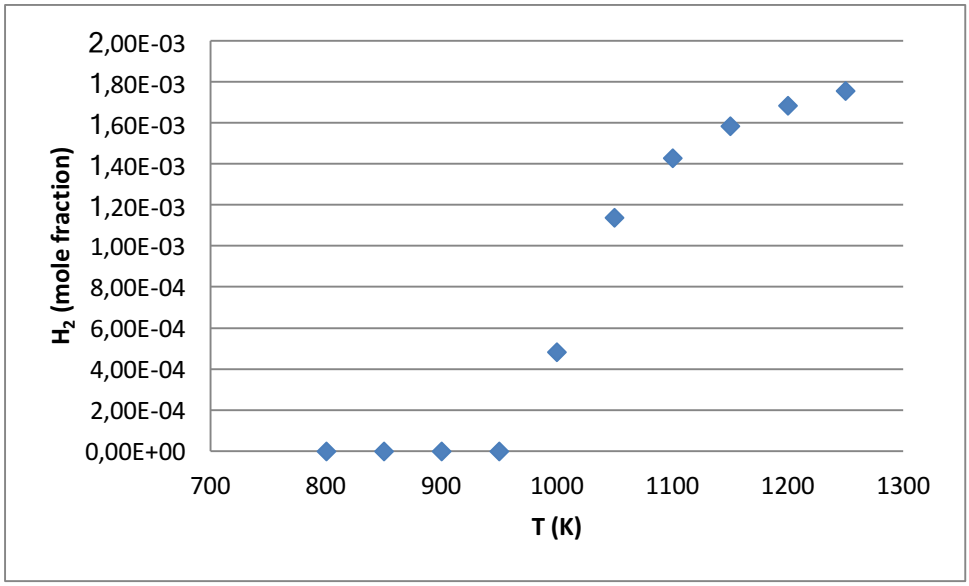

Figure 5: Estimation of H_2 mole fraction as function of temperature with Aramco mechanism [3].

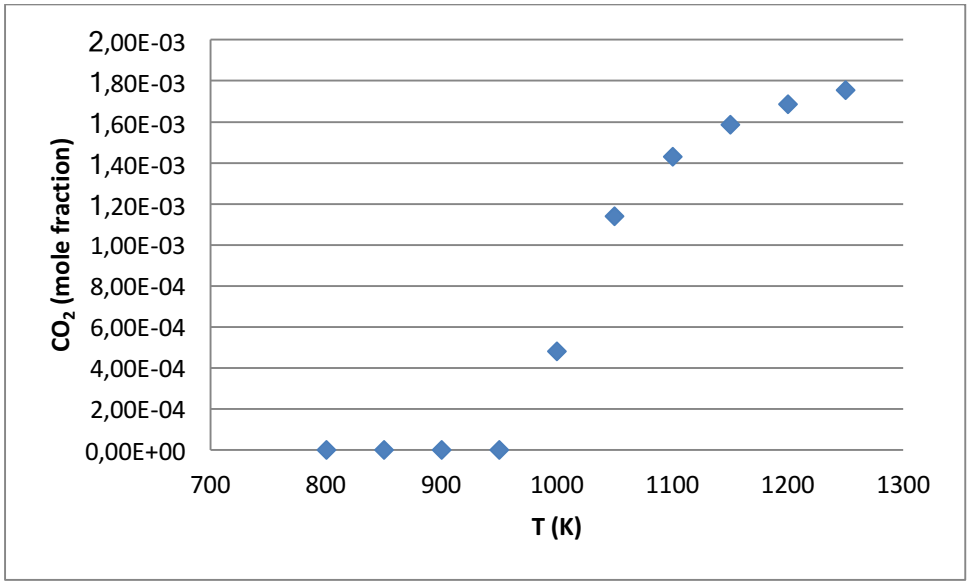

Figure 6: Estimation of CO_2 mole fraction as function of temperature with Aramco mechanism [3].

4. CONTRIBUTION OF THE STSM TO THE ACTION'S AIM

The present STSM proposal is mostly related to the activities of the Working Group 5 (WG5) "Integration of the fundamental knowledge towards technology application for Smart Energy Carriers Exploration". The study of different types of fuels (syngas and methane), regarding fuel utilisation and injection, as well as combustion mechanisms investigations contribute in the aims of the COST Action CM1404, which include the increase of fuel flexibility and carbon efficiency, which can be reached by the improved ICE design based on realistic modelling and simulation.

5. FUTURE COLLABORATION

Firstly, the existing combustion modelling methodology in the STAR-CD CFD code [1] will be used for test simulations of methane (CH4) combustion in a constant volume chamber, first for atmospheric and then for high temperature and pressure conditions resembling the engine cylinder conditions towards top dead centre during compression stroke. The results from the test simulations will be used for future comparisons with special chemical kinetics mechanisms of combustion.

Secondly, it is envisaged to adapt the existing frameworks of combustion modelling in state-of-the-art CFD codes, namely KIVA and STAR-CD, which are currently adopted in both industry and academia for the simulation of ICE engine processes including combustion. The CFD codes methodology both from modelling and numerical respects be examines, in order to define the simulation setup and user coding requirements for the implementation of special chemical kinetics mechanisms for the modelling of combustion.

Third, it is aimed to understand and use the methodology of validation and optimisation of detailed chemical kinetics mechanisms for both gas and liquid fuels, with the use of special computational tools, including CHEMKIN and OptimaPP tools. The determination of skeletal chemical kinetics mechanisms, along with the use of computational tool, notably SEM tool will be accomplished in future work.

Finally, based on the aforementioned future work, the implementation of validated and/or optimised reduced order chemical kinetics mechanisms in CFD codes will be carried, for reacting flow processes that are present in industrial and transportation systems in general.

6. FORESEEN PUBLICATIONS

It is aimed that the complete methane injector geometry assembled with the constant volume chamber for very fine mesh up will be employed for detailed injection simulation of methane, and the results will be published in a journal. Furthermore, upon progress on the implementation of validated and optimised reduced combustion mechanisms in the CFD codes, then CFD simulation of combustion and validation studies from constant volume chambers will be published in a journal.

7. CONFIRMATION BY THE HOST INSITUTION

The confirmation letter from the host institution is attached.

8. ACKNOWLEDGEMENTS

I am grateful to the COST Action CM1404 for the financial support of my STSM. I would also like to express my gratitude to Prof. L. Kaiktsis for the collaboration with him and his research team and hosting my STSM.

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