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Towards the design of a supercritical combustion chamber for combusting H_2 in supercritical CO_2 and Xe

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ABSTRACT

Faced by modern technological advances and the automation of industry, the increasing demand for energy production poses a major challenge. While the energy sector has developed significantly, still the combustion processes remain crucial. Therefore, it is important to adapt current energy technologies to protect the environment, and to make them as efficient as possible. In this context, supercritical fluids are increasingly becoming the focus of interest due to their specific properties. Meanwhile, the optimization of devices, their shapes and parameters is being improved by modern numerical methods. Numerical modelling, particularly computational fluid dynamics (CFD), offers insight into the complex processes interacting within modern devices. Visualizing process parameters across the geometric volume during simulation helps to create superior equipment designs. Despite the many advantages of the supercritical fluids and the benefits they give to the combustion process, there is a gap in the fundamental understanding of this subject, especially in the energy aspects.

The main objective of this study is to design a combustion chamber for burning hydrogen (H_2) using supercritical carbon dioxide (CO_2) and xenon (Xe) as the working medium. The combustor will operate on thermal power of 30 kW and maximum pressure of 100 bar. The design process involves conducting numerical analyses using commercial CFD software. Multiple geometries are evaluated with various inlet configurations and injection angles. The results show different mixing characteristics influenced by the designed geometries. Finally, the most optimal design is selected based on the mixing parameters and will be manufactured to perform further experiments.

This research brings new data on the mixing and combustion process of renewable fuels with supercritical fluids. Additionally, it provides directions to design a supercritical combustor.

INTRODUCTION

The growing global demand for power supply has resulted in significant advances in energy technology. These innovations cover a spectrum of approaches, including improved renewable energy sources, novel power generation techniques and enhanced energy storage solutions. Despite the progress, some challenges represent bottlenecks for these technologies. Stabilising energy generation, reducing emissions and making the systems efficient remain challenges. In addition, the performance of electricity and heat storage systems needs to be improved further to meet the demands of modern energy consumption patterns. Many challenges remain, particularly in terms of environmental protection and reduction of the overall environmental footprint associated with these methods. Addressing the aforesaid issues is key to developing sustainable and efficient energy solutions in the face of constantly increasing global energy demand. Therefore, it is essential to acquire fundamental knowledge of modern energy technologies along with the possibility of integrating renewable sources into energy systems, thereby building clean and efficient energy systems. [1-4]

Highly Efficient Super-Critical ZERO eMission Energy System (HERMES) addresses these challenges. It is a complex and ambitious project to analyse renewable energy sources, fuel synthesis methods and energy storage. The project aims to make the plant independent of peak hours, which is achieved by using an efficient gas turbine operating in supercritical conditions and using renewable fuels (hydrogen and methanol). The products of the combustion process i.e. carbon dioxide and/or water, are reused to generate new fuel via electrolysis and synthesis process.

In the current study, we focus primarily on development of the supercritical combustor based on Computational Fluid Dynamics (CFD) calculations.

A proper mixing of the fuel and oxidizer is a key parameter for the ignition and combustion process. This is especially important when the gas is mixed with a supercritical fluid. For the presented work, a supercritical xenon (sXe) was selected due to its superior properties (e.g. density and heat capacity ratio) and relatively low critical pressure. Hydrogen and oxygen obtained from the electrolysis process of water are used as a fuel and oxidizer, respectively.

Modelling

This study concentrates on the CFD analysis of hydrogen-oxygen mixing with sXe or sCO_2, and combustion with system thermal power of 30kW.

The impact of various parameters on the mixing process is explored, including:

- The angle of oxidant inlet, i.e. axial vs tangential flow
- The number of fuel inlets i.e. 1, 3 and 6 injection inlets
- The substance used as the working fluid, i.e. supercritical Xe and supercritical CO_2

The computations are executed using software ANSYS Fluent 2023 R1 and employing the k-omega SST turbulence model and Soave-Redlich-Kwong equation of state. Calculation are conducted assuming steady state conditions. For combustion simulations, the eddy dissipation model was used. The mixing process analysis was conducted at 10 bar, while combustion simulations were performed at the designated geometry and a pressure of 100 bar.

RESULTS AND DISCUSSION

The calculation of the influence of abovementioned parameters was preceded by a grid convergence test.

Mesh convergence test

A mesh convergence test was performed to ensure that the results were independent of the grid size. Four tetrahedral meshes with different element sizes and consequently various numbers of elements i.e. 0.18M; 0.65M; 1.50M; 2.00M respectively, were investigated. We chose velocity as a comparison parameter obtained at 200 points allocated along the lines at different heights in the combustor (close to injection inlet, in the middle of the combustor and close to the outlet). Comparison of the received data is presented in Fig 1.

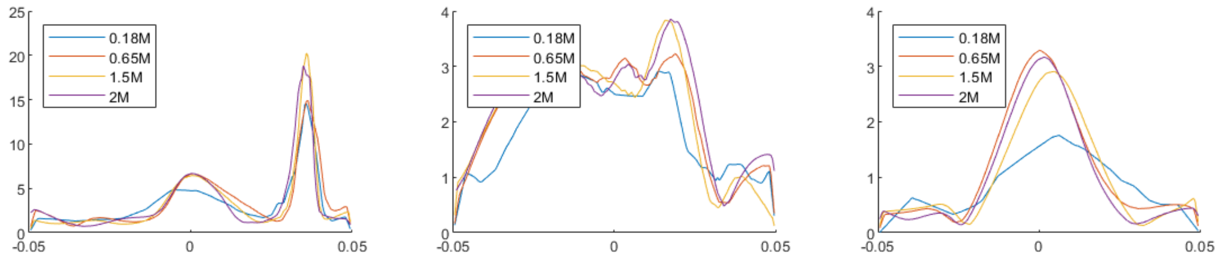

Fig 1. Velocity [m/s] for different mesh sizes for three selected lines near the inlet (left), center (middle) and outlet (right).

On the basis of the results we selected a grid with 0.65M elements for the further calculations, This is due to the speed of the calculations and a good agreement with the reference grid of 2.0M elements, as well as taking into account that the purpose of the simulation is comparative and not quantitative analysis of the investigated processes.

Impact of oxidant and fuel inlets

Based on the velocity profiles for the axial and tangential oxidizer inlets (Fig 2), it is visible that the axial injection exhibits a higher velocity at the center of the combustion chamber, whereas the tangential profile reveals a circular pattern with a higher velocity at the wall. Given the importance of achieving a proper substance mix in the combustion process without overheating of the walls, only the axial inlets were selected for further analysis.

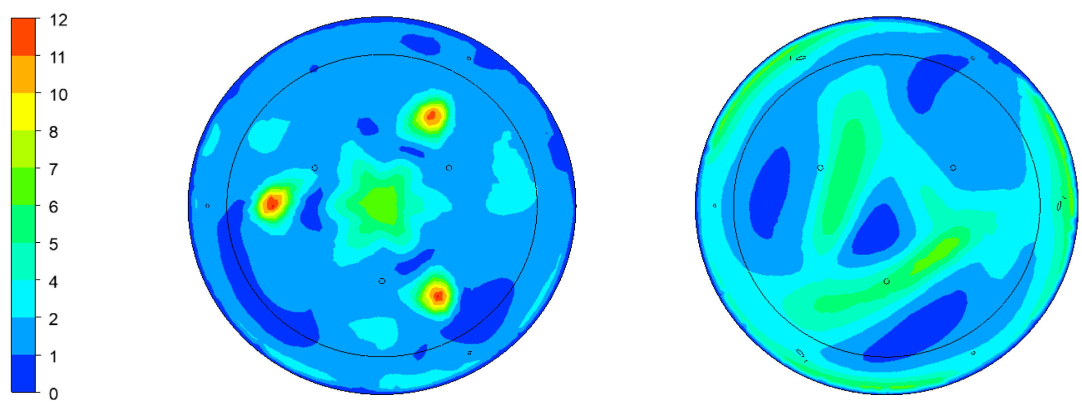

Fig 2. Comparison of the effect of oxidizer inlet angle: axial injection (left), tangential injection (right), on the cross sectional velocity profiles [m/s].

Comparing the velocity profiles (Fig. 3) for cold mixing of H_2 with O_2 in CO_2 and Xe at 10 bar, it can be seen that there is no significant difference in the velocity pattern. This resemblance allows for a similar combustion chamber design for CO_2 and Xe as working fluids. In contrast, for the combustion in Xe at 100 bar, the velocity, although still resembling the former cases, is significantly reduced. This discrepancy can be attributed to the effect of pressure on density, which in turn affects velocity. In practice, this will lead to positioning the flame upstream of the combustor.

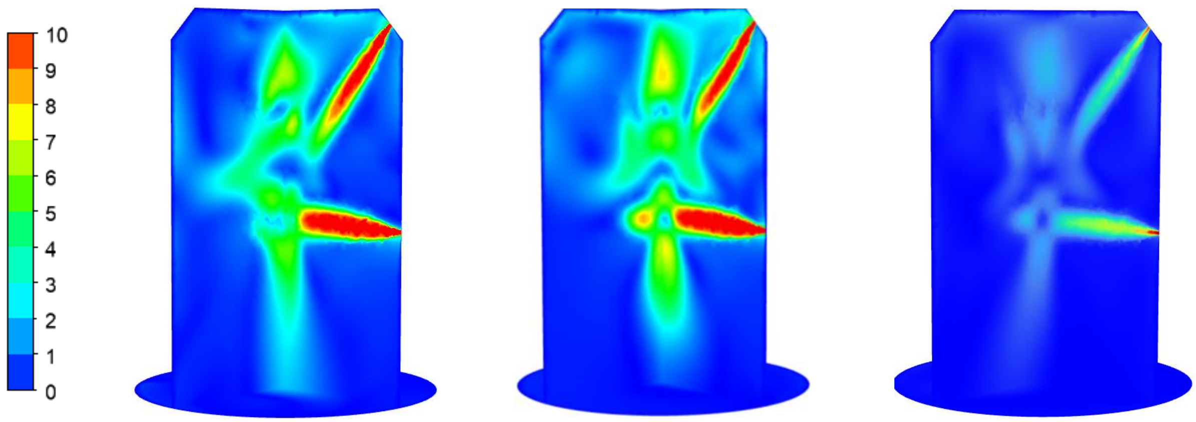

Fig 3. Velocity profiles [m/s] for: cold mixing in CO_2 at 10 bar (left), cold mixing in Xe at 10 bar (middle) and mixing and combustion in sXe at 100 bar (right).

The number of fuel inlets has no significant effect on the overall velocity profile. However, we see that the highest velocity near the wall occurs for 1 inlet, while for 6 it is more concentrated in the center. The cross section with 3 inlets has the most uniform velocity profile and the velocity remains low near the wall. In the combustion process, mixing in the central part is crucial, hence the geometry with 3 inlets was chosen.

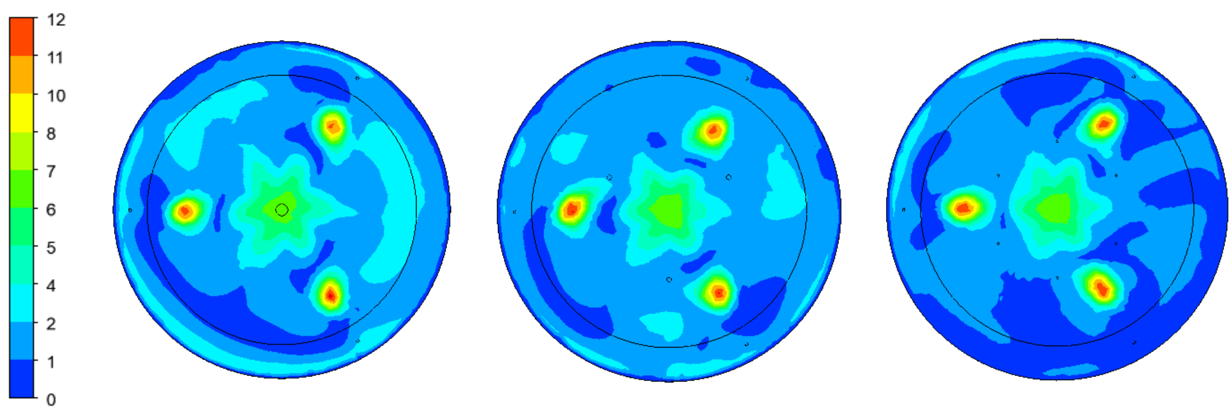

Fig 4. Comparison of the effect of number of fuel inlets: 1 (left), 3 (middle), 6 (right) on the cross sectional velocity profiles [m/s].

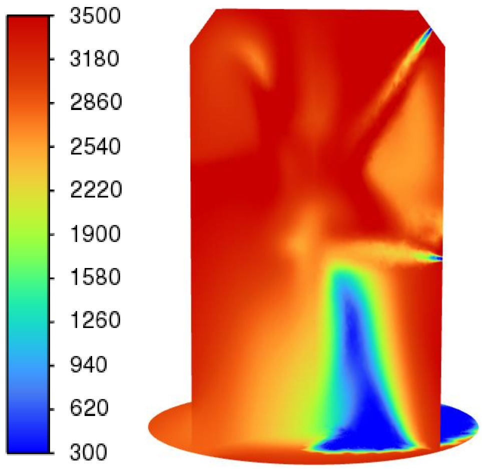

Fig 5. Temperature profile [K] for combustion in sXe at 100 bar.

The temperature profile of the combustion process reveals exceedingly high temperatures across the entire volume. This is a consequence of the investigated conditions and the assumption of the adiabatic walls in the CFD simulation. However, the excessive temperature near the walls, being consequence of combustion products blown there, is problematic, as the stainless steel under consideration cannot withstand such elevated conditions, even when including cooling flow. Additionally, an ununiform mixing of the supercritical fluid injected via the secondary cooling holes in the combustor and the combustion product is visible. This could be also an effect of the recirculation region formed close to the outlet of the combustor. Such conditions may lead to high thermal stresses in the material and its final failure, thus further optimization in the combustor geometry design is needed.

Conclusions

The CFD simulations performed for various fuel inlets, oxygen injector angles and supercritical fluids show that the general velocity profiles for the CO_2 and Xe are similar, however, increased pressure has significant effect on the overall velocity magnitude. The simplified combustion model already shown a risk of walls overheating and non-uniform mixing profile at the outlet of the combustor. Therefore, upcoming work will focus on solving these issues. The redesign of the supercritical fluid cooling system will include designing part of the inlets such that a cooling film along the walls is created. Lower oxygen velocities will be used to reduce the likelihood of hydrogen blowing off the walls.

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