UNIVERSITY OF PATRAS
DEPARTMENT OF MECHANICAL ENGINEERING AND AERONAUTICS

Division of Energy, Aeronautics and Environment
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DIPLOMA THESIS 2021

"Detailed propane chemical kinetics scheme reduction and simulation of turbulent bluff-body propane flame under inlet mixture stratification and preheat"

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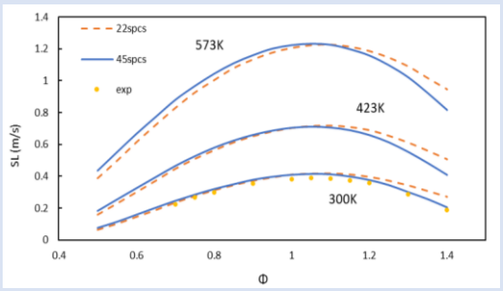
Introduction

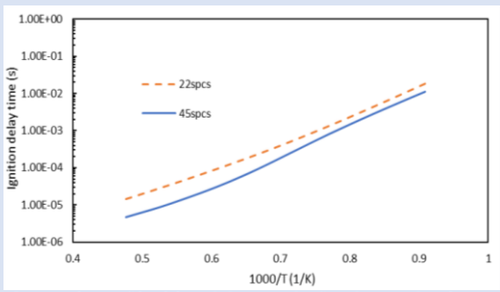
The study of the flame stabilization can provide important information for the combustion phenomenon and therefore help reduce the gas emissions. However, a chemical kinetics scheme is required for the computational simulation that is needed. Yet the detailed chemical kinetics schemes that exist require a high computational cost and they cannot be used in detailed simulations.

Goal

A reduction of a detailed propane chemical kinetics scheme was made, using the Directed Relations Graph (DRG) and Full Species Sensitivity Analysis (FSSA) methods. The resulting reduced scheme was then verified against the original detailed scheme USC Mech II and by comparing parameters such as flame speed and ignition delay. The scheme was later used in the simulation of a turbulent bluff-body propane flame under inlet mixture stratification and preheat. For the simulation, the Large Eddy Simulation (LES) model was used.



Comparison of flame speed results for the mechanisms 22spcs και 45spcs



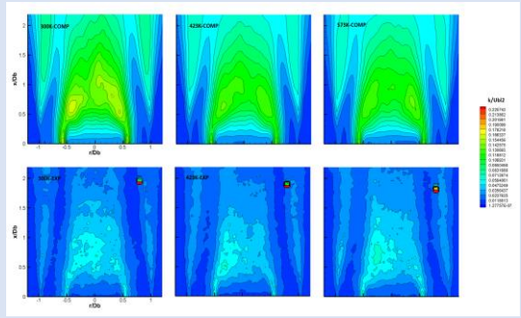
Comparison of ignition delay results for the mechanisms 22spcs και 45spcs Φ=0.8.

Large Eddy Simulation (LES)

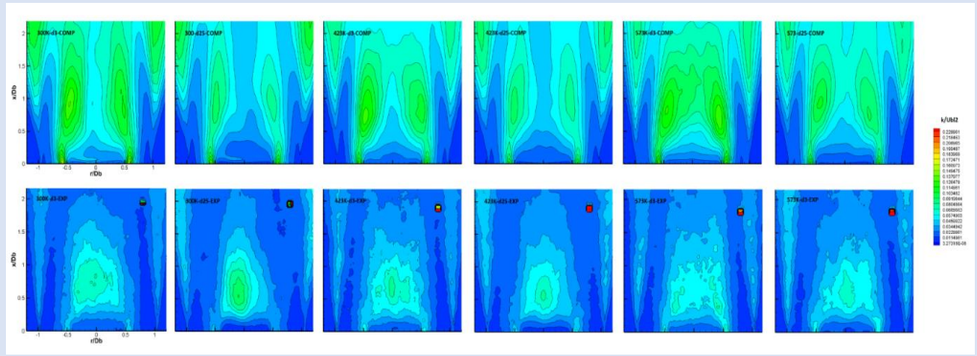
In LES the large eddies of turbulent flow are directly computed and the small sub-grid scale eddies are modeled.

It is considered the most viable numerical tool for the simulation of realistic turbulent flows, due to its good approach of the physical problem that is modeled.

It is the only choice for computing complex flows which are combined with combustion.



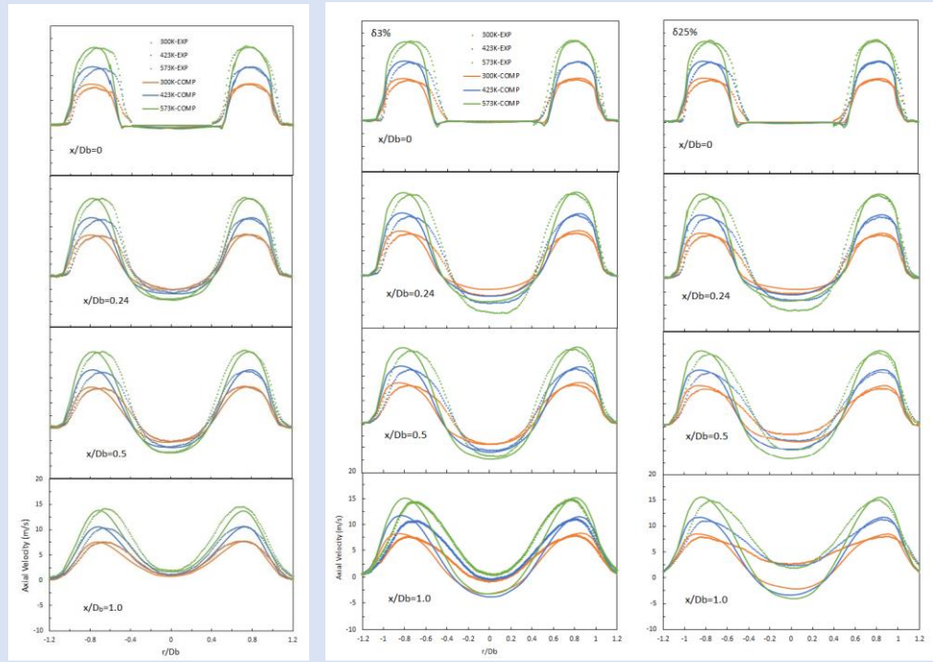
Comparison of computational and experimental results of the Turbulent Kinetic Energy of the non-reactive field.



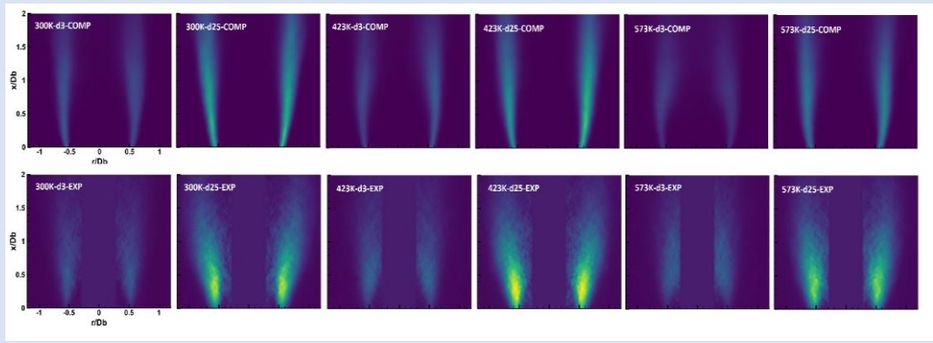
Comparison of computational and experimental results of the Turbulent Kinetic Energy of the reactive field.

Results

- The reduced mechanism gives good results on the flame speed form ultra lean up to stoichiometric. Moreover, it has a good prediction on ignition delay results.
- From the contours of the Turbulent Kinetic Energy, it is apparent that there is an overestimation of the results by 30-40%, while the topology is correctly predicted. The deviations are probably the result of the deference between the sampling rates of the computational and experimental data.
- At the non-reactive field, there has been a good estimation of the axial velocity, especially at the shear layers, where the deviation of the maximum velocities does not surpass 2% at 300K, 3% at 423K and 5.5% at 573K.
- At the reactive field there has been a good estimation of the axial velocity at the shear layers, but there has been an overestimation of the recirculation.
- The OH* chemiluminescence is estimated well, with the computational emissions a little closer to the axis.



Comparison of computational and experimental results of the mean axial velocity of the non-reactive field (left) and the reactive field (right)



Concentration of the OH* chemiluminescence

Conclusions

The reduced chemical kinetics scheme that was developed, has given good results in several important parameters from lean up to stoichiometric mixtures. In addition, the results of the simulation of the propane flame have small deviation from the experimental results at the non-reactive field, while the deviation at the reactive field is larger.