

# Sensitivity Analysis of Simulation Parameters on Premixed Propagating Flames: Impact of XiFOAM Discretization Schemes

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## Extended Abstract

This paper uses the OpenFOAM Computational Fluid Dynamics (CFD) code to study the turbulent premixed flame propagation characteristics inside a partially open duct filled with obstacles. The simulation results were validated across the experimental results by Patel et al.[1], the experiments were carried out in a rectangular duct of small scale with dimensions of 500×150×150mm, which was open from one end and filled with three equally spaced rectangular obstacles along the centreline. All the simulations were performed using a two-dimensional model with realizable k- $\epsilon$  turbulence modeling and the Flame Surface Density (FSD) model proposed by Weller et al.[2] for Combustion modeling. The solver uses an adaptive time-stepping method coupled with a maximum value of the Courant number.

Initially, the simulations were carried out with a first-order upwind scheme (limited linear with a limiting coefficient of one [3]) for divergence terms, a second-order Crank Nicolson method for time discretization, and a PIMPLE solver (with outer correctors set to 200 with residual for outer correctors set to  $10^{-4}$ ) for pressure-velocity coupling. The solution with these schemes resulted in impractical dependence of pressure peak on the initial values of simulation parameters: turbulent kinetic energy 'k', initial time step size ' $\Delta t$ ', mesh size ' $\Delta x$ ' as well as the maximum value for Courant number of the flow 'maxCo'. The k values tested are 0.5, 0.1, 0.05, and 0.01, as at 0.01 the pressure peak was negligible and far delayed. Similar results have been obtained for the above-mentioned parameters, whereupon reducing  $\Delta x$ ,  $\Delta t$  or maxCo, the flame failed to propagate, resulting in no pressure peak at all. For some cases, the pressure plots have shown oscillatory behavior, and correspondingly, the flame structure was also seen to be more wrinkled compared to the experimental results. The discretization schemes were updated to a second-order linear scheme (limited linear with a coefficient of zero) for divergence terms and a first-order Euler method for temporal terms. The pressure velocity coupling was updated to an iterative PISO algorithm (PIMPLE in OpenFOAM, with outer correctors of three). The updated solver was then tested against the experimental results to analyze the dependence of pressure peak on the above-mentioned simulation parameters. It was found that the unexpected dependence was eliminated, and the solver provided reasonably good qualitative agreement with the experimental results for k=0.01. The solution became independent of the other parameters as well, and grid independence was also obtained for the results. The effect of each of the discretization schemes is also tested individually, and it was found that the significant effect was found to be of the Crank Nicolson method due to its diffusive nature and difficulty in accurately resolving the discontinuity across the flamelet.

## References

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