Development of optimisation strategies to enhance the performance of NOx Postprocessor

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Nitrogen oxides emissions are a concern in industrial furnaces, due to constantly increasing environmental requirements. A cost-effective way to reduce emissions is the optimization of burners using Computational Fluid Dynamics methods. Predicting these NOx emissions in CFD with detailed chemistry models and turbulent combustion requires immense computational effort. To reduce the calculation time, an efficient method (v2.0) for determining the NOx emissions was developed by Pollhammer et. al [1]. This method first calculates the flame properties such as temperature and velocity of the flame. Subsequently the converged results are then used for the prediction of NOx emissions with detailed chemistry model, where the calculation is performed only if the change in species concentration in the computational cell is more than 5%. The current study (v2.0+) proposes three optimisation strategies to the existing method, by modifying the reaction rate constant calculation method, by initializing the species mass fraction values from extended Zeldovich mechanism [2] and by using dynamic mesh refinement. These proposed strategies reduce the computation time further and improve the efficiency of existing postprocessor.

As a first optimisation strategy, the chemistry model in OpenFOAM was modified to calculate and store the forward and reverse reaction rate constants. This approach was used since the temperature field remains constant throughout the calculation and the reaction rate constants are mainly dependent on the temperature field as in Eq. (1).

$$k_f = A\,T^{\beta}\exp\left(\frac{-E_a}{RT}\right) \qquad k_r = \frac{k_f}{k_p} \qquad (1)$$

In general, the reaction rate constants are calculated for every cell and every reaction for all iterations and all chemical time steps which was unnecessary for the current postprocessor (v2.0) and hence, storing the reaction rate constants in the first iteration reduces the FLOPS (Floating Point Operations Per Second) magnificently. The code was developed in OpenFOAM and analysed with experimental results of Barlow and Frank [3].

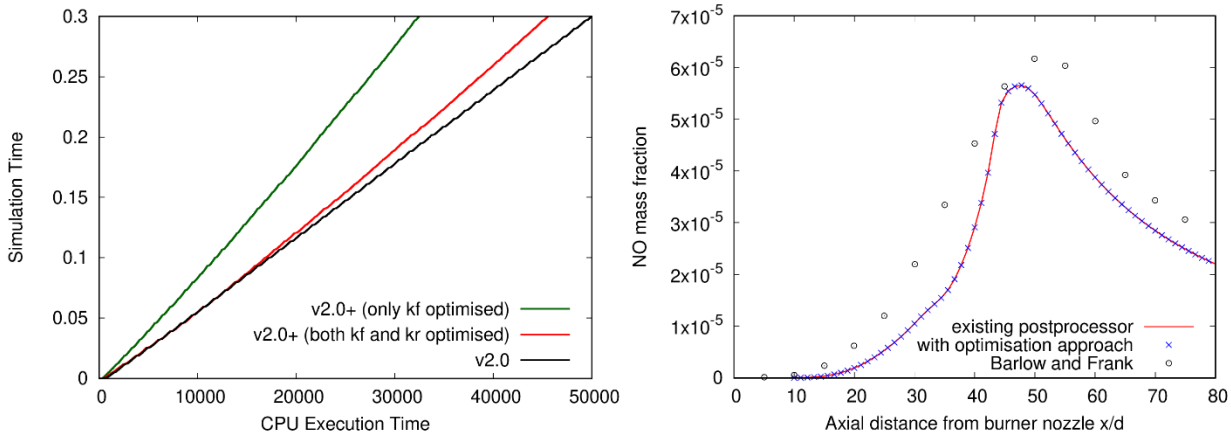

Fig 1: Comparison of computation time and accuracy between the existing and optimised code.

The optimised code, when only the forward reaction rate constant was calculated and stored, completes the computation in 32,459 s for a real time simulation of 0.3 s. Whereas the existing code takes 49,983 s and the accuracy of the postprocessor remains unchanged. But modifying both the forward and reverse rate constants resulted in increased computational effort due to high memory consumption by the data storage.

Further reduction of computation time was achieved by initializing the postprocessor using extended Zeldovich mechanism [2]. In the existing postprocessor (v2.0), the nitrogen oxide species concentration obtained from the flamelet model was not used and the initial values are set to zero.

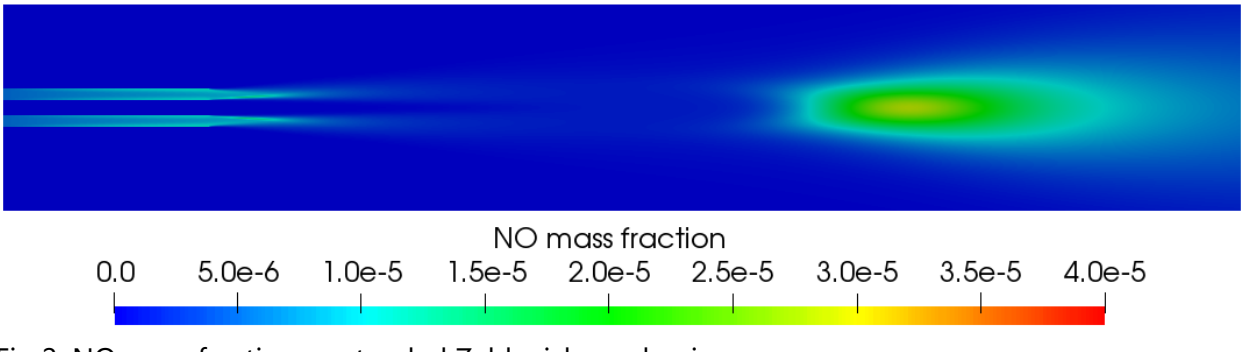

Fig 2: NO mass fraction – extended Zeldovich mechanism

In the current approach, extended Zeldovich mechanism was used to predict the concentration of NO and Oxygen atoms and then the postprocessor was initialized with the predicted values. The convergence of this approach was analysed by integrating reaction rate for the NO species over time. The existing postprocessor converges around 0.004 s and the optimised postprocessor converges around 0.002 s. Calculation of species concentration using extended Zeldovich mechanism requires very less computational effort and using these predicted values have reduced 31.8% of the computation time.

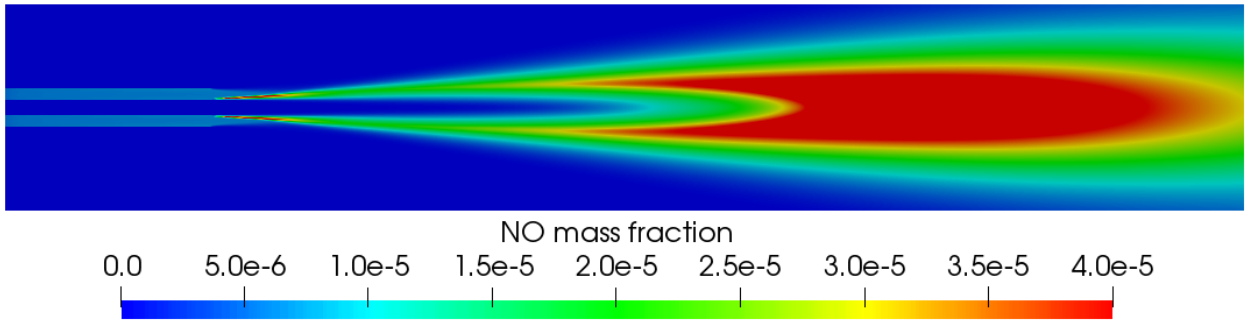

Fig 3: NO mass fraction – optimised postprocessor

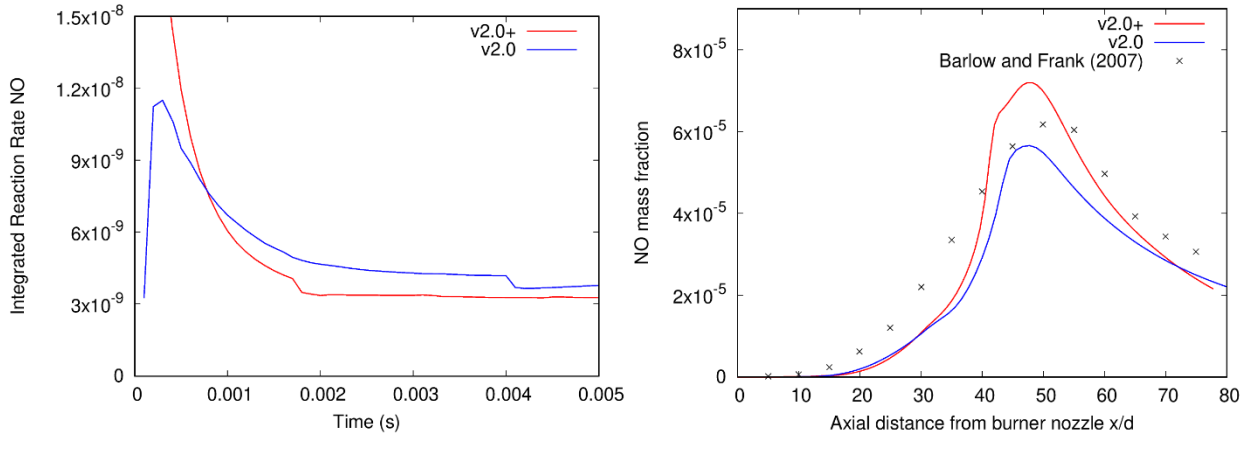

Fig 4: Convergence and accuracy comparison between existing and optimised postprocessor based on extended Zeldovich mechanism.

The final optimisation strategy was performed based on the dynamic mesh refinement utility. In the first step, the current mesh size of 204,800 cells was manually coarsened to 60,175 cells and afterwards the mesh was refined, where the temperature field is greater than 1200 K with dynamic mesh refinement. This approach coarsens the mesh in the regions where the temperature is low and refines the mesh where the temperature is high, thereby resulting in a refined mesh which perfectly captures the flame region. Through this approach, the mesh size was reduced to 105,780 cells.

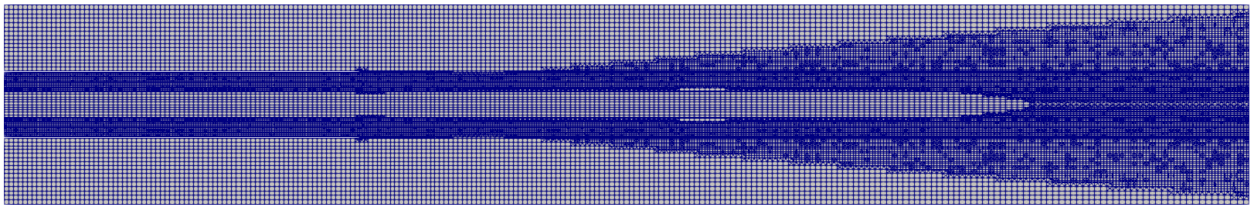

Fig 5: Mesh generated using dynamic mesh refinement utility.

Using the generated mesh, resulted in 36.5% reduction of computational time. In the existing postprocessor, when divergence is detected, the code automatically reduces the current time step. Refining the mesh in the flame region, results in lesser divergence and the computation is comparably faster if the time step is not reduced.

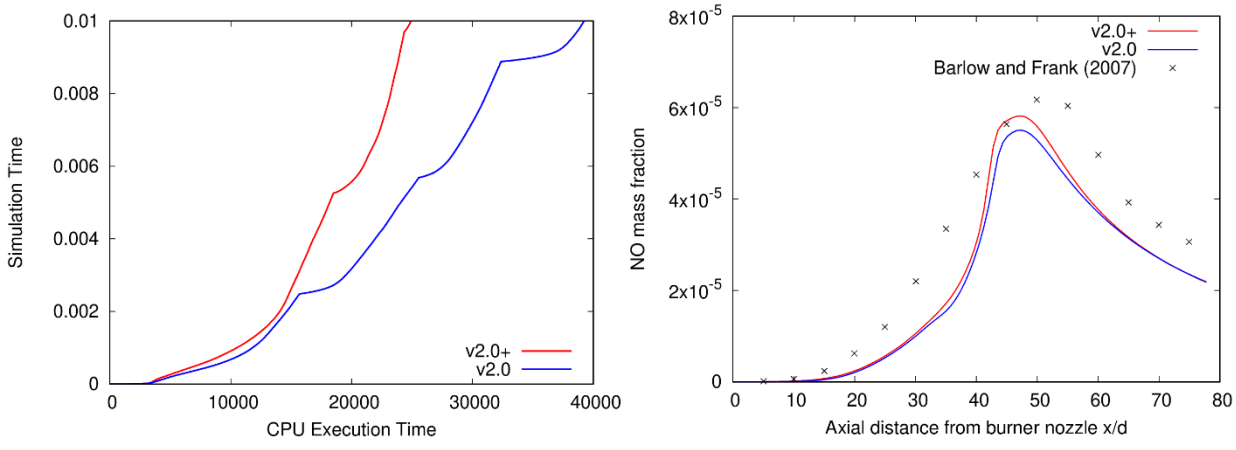

Fig 6: Comparison of computation time and accuracy between the existing and optimised postprocessor based on dynamic mesh refinement

Furthermore, the proposed optimisation strategies will be combined, with an aim to develop a rapid and efficient postprocessor. Using all the proposed strategies together would approximately reduce half of the computation time in predicting NOx emissions.

References

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