A Numerically Efficient Method for the Prediction of Nitrogen Oxide Emissions in Industrial Furnaces

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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 an optimization of the burners in the furnace using computational fluid dynamics (CFD) methods. Still, state of the art approaches are computationally too expensive for real scale geometries such as industrial furnaces, or can not predict the nitrogen concentrations with sufficient accuracy. Therefore, the development of nitrogen oxides post-processors was defined in K1-Met projects in 2012. Currently, there are three different variations available, where the generation 2.0+ is the latest development.

1. Introduction

Due to constantly increasing environmental requirements, the reduction of nitrogen oxide emissions in industrial furnaces is a permanent topic of interest. End of pipe technologies such as selective catalytic reduction increase the building and operational costs. To reduce nitrogen oxides inside the furnace, a detailed understanding of the chemical kinetics including radical reactions is necessary.[1] A complex chemical mechanism for the modeling consists of several hundred relevant reactions. The kinetic of these reactions is influenced by the turbulence of the flow field. These turbulent reactions are solved using combustion models such as the Eddy Dissipation Concept (EDC)[2] or the Partially Stirred Reactor (PaRS)[3] model, which integrate the reactions in the small chemical time steps. Such approach leads to the averaged reaction source term for each of the species in each computational cell, making it computationally quite expensive. Therefore, the prediction of nitrogen emissions is practically not applicable for the real scale geometries such as the industrial furnaces. Models based on flamelet concepts, such as the laminar flamelet model by Peters,[4] are using a tabulated chemistry in conjunction with a mixture fraction approach and probability functions. In this case, the chemical composition is based on two transport variables: the mean mixture fraction and mixture fraction variance. This concept allows a fast and accurate calculation of the flames in the thin flame regime. Still, some of the reactions in the nitrogen oxides formation have slow reaction kinetics and the thin flame regime is not applicable for such cases. For that reason, a development of a nitrogen oxides post-processor was started in 2012.

2. First Generation of the Nitrogen Oxide Post-Processor

The idea behind the post-processor of the first generation is to solve the global reactions and the according transport equations for the species based on a fixed field for flow, temperature, turbulence, and macroscopic species. The first generation uses the extended Zeldovich mechanism by Heywood[5] under the assumption of a partial equilibrium for the oxygen radicals. Due to the simple reaction scheme, the first generation of the post-processor takes for a furnace with 12 million computational cells ≈2 h on 2 intel Xenon cores. As shown in Figure 2, the post-processor underestimates the formation of nitrogen oxides, but estimates the formation zones and predicts the trends. This simple post-processor is used for optimization processes in the industrial burners because of the calculation speed.

3. Second Generation of the Nitrogen Oxide Post-Processor

The second generation of the nitrogen oxide post-processor for steady laminar flamelet simulations in industrial furnaces was developed by Pollhammer.[6–8] The post-processor uses temperature, turbulence, flow, and predefined species fields from the result of a steady state or quasi-steady-state simulation as constant fields. To model the nitrogen oxide concentrations, a detailed reaction mechanism is used; whereas for the species that are not pre-defined within the mechanism, additional transport equations were solved. The reaction rates were calculated using the PaSR model,

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subsequently stored and calculated again only if at least one of the three predefined criteria is met in a cell. First, if the reaction rates were not solved for the previous 200 iterations, they must be calculated to avoid artificial steady state conditions. It is also necessary to recalculate the reaction rates if the rate of change for any of the species in a cell is more than 2%. To avoid nonphysical conditions, eventual negative values are recalculated and corrected. These criteria are reducing the calculation time of the post-processor by 85%.

4. Generation 2.0+ of the Nitrogen Oxide Post-Processor

To reduce the computational effort of the post-processor further, three possible strategies were investigated: a reduction of floating-point operations (FLOP), due to internal code restructuring, the calculation of initial values for nitric oxide (NO) and oxygen radicals, and then implementing the dynamic mesh refinement to reduce the number of computational cells.

4.1. Reduction of Floating-Point Operations

The second-generation post-processor takes most of the computation time for solving the chemical reactions. As the temperature field during the computation remains constant for the entire calculation, the first strategy was to alter the reaction rate constant calculation method which is mainly dependent on the temperature field. Reaction progress rate Ω_i for every iteration is determined from the forward and reverse reaction rate constants k_f and k_r, respectively, as given in Equation (1) where $[M_\text{k}]$ and ν_k are the concentration and stoichiometric coefficient of the species k.

$$\Omega_i = k_f \prod_{K=1}^{N} [M_k]^{\nu'_k} - k_r \prod_{K=1}^{N} [M_k]^{\nu''_k} \tag{1}$$

$$k_f = AT^\beta \exp\left(\frac{-E_a}{RT}\right) \quad k_r = \frac{k_f}{k_p} \tag{2}$$

The forward and reverse rate constants are determined from the temperature T, pre-exponential constant A, temperature constant β, activation energy E_a, gas constant R, and equilibrium constant k_p. When the temperature field is differing for every iteration, the rate constants must be calculated for every iteration, cell, reaction, and chemical time step. Moreover, single calculation of forward rate constant consumes nearly 30 FLOP, repeating this calculation for every iteration and every chemical time step is unnecessary when the temperature field remains unchanged. To reduce this computational effort, the chemistry model in OpenFOAM was modified to determine the rate constants in the first iteration of the simulation and store the rate constants for each cell and each reaction as a volScalarField. In further iterations, instead of computing the rate constants, they will be accessed from the stored data. At first, only the forward rate constant calculation was modified and subsequently modification for both forward and reverse rate constant calculation was implemented. The modified v2.0+ code was analyzed with the experiments of Sandia Flame D[9] with a mesh size of 204 800 cells using GRI 3.0 mechanism with 325 reactions on a 8 core AMD Ryzen 7 3800× processor and the performance was investigated and compared with the second-generation post-processor. When only the forward rate constant was modified, the code was 35% faster than the second-generation post-processor and modifying both rate constants resulted in only 8% faster calculation process, due to the available memory bandwidth. Although only the calculation method was modified, the accuracy of the results remained unaffected.

4.2. Calculation of Initial Values

Using the species concentration values from the flamelet model resulted in increased computational effort, therefore the second-generation post-processor was initialized with zero concentration to reduce the simulation time.[6–8] Therefore, as a second strategy, the second-generation post-processor was initialized with species concentration values from the first-generation post-processor, which uses the extended Zeldovich mechanism by Heywood.[5] NO and oxygen radical concentration obtained from the first-generation post-processor were used as initial values. After initialization, to determine the convergence, the reaction rate of the NO species is integrated for every time step.

The second-generation post-processor needs for convergence double the time steps compared to the generation 2.0+. Furthermore, the NO mass fraction is slightly more precisely determined in v2.0+ for the post combustion zone. Since the initial value calculation using the first-generation post-processor takes only a few seconds for the Sandia Flame D,[9] this strategy drastically reduces the computation time of the post-processor. Real time simulation of second-generation post-processor required 24 069 s of CPU time (4 core) and simulation in Generation 2.0+ required 16 392 s till convergence, due to the initial values change, which is 31.8% faster.

4.3. Dynamic Mesh Refinement

The final strategy to reduce the computational effort was achieved by implementing the dynamic mesh refinement utility. Mesh size was at first reduced from 204 800 cells to 60 175 cells by manual coarsening. In the next step, based on the temperature field, the coarsened mesh was further refined with dynamic mesh refinement by selecting the cells where the temperature field is greater than 1200 K producing a mesh size of 105 780 cells (**Figure 1**). Even though the number of cells is reduced, the mesh is well refined in the flame region compared to the previous mesh. The data from the flamelet model are interpolated to the generated mesh and the computation was performed to analyze the efficiency of the post-processor.

The effectiveness of mesh refinement is analyzed after dynamic mesh refinement. Coarsening the mesh in unnecessary regions and refining the mesh in the flame region results in 36.5% decrease of CPU time. In addition, combining all the above discussed strategies will result in considerable reduction

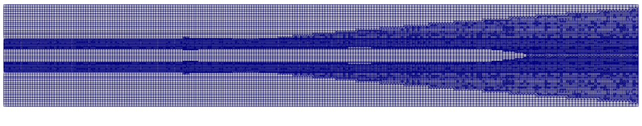

Figure 1. Generated mesh by implementing dynamic mesh refinement based on temperature field.

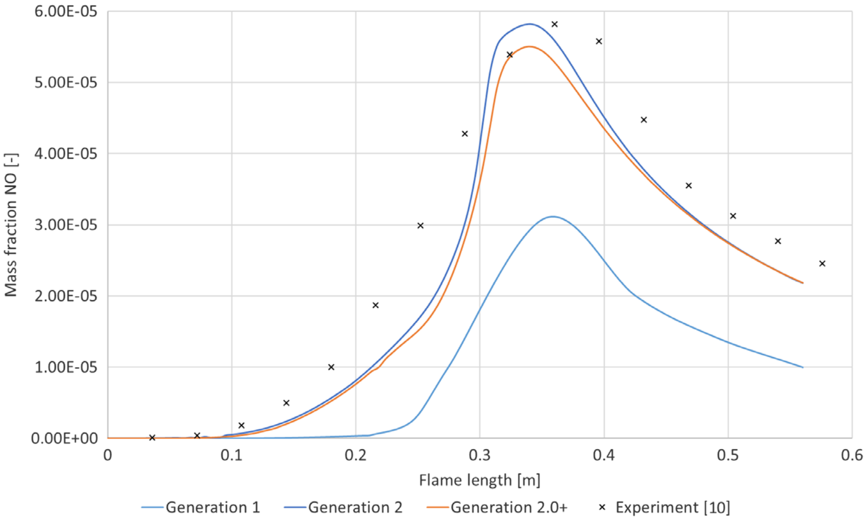

Figure 2. Compression of the NO mass fraction for the Sandia Flame D[9] with different generations of the post-processor.

of computational time and produce an efficient post-processor for determining the nitrogen oxide emissions.

5. Conclusion and Comparison of the Generations

The first generation of the post-processor is not predicting the NO_X concentrations with sufficient accuracy (**Figure 2**), but estimates reaction zones with lower computational effort. So that it can be a useful tool for optimization loops to reduce the nitrogen emissions in flames. As shown, the second generation predicts precise values and is applicable for real scale geometries, but still too slow for optimization loops. With the combined usage of the first- and second-generation post-processor an optimization of burners is possible. Pollhammer[10] was able to reduce the nitrogen emissions of a 500 kW burner for floater furnaces from 46 to 30 ppm. However, this combination is still too time consuming for the optimization of a furnace. Here are only some improvement steps possible, without reaching the optimum. The aim of the generation 2.0+ is to reduce the calculation time, without sacrificing accuracy for an optimization of industrial furnaces. The predicted concentrations are even more accurate compared to the second generation (Figure 2).

Due to three different changes, the calculation time could be decreased to about a third in comparison to the second generation for the Sandia Flame D.[9] Currently, the generation 2.0+ is in use to optimize an 850 kW burner for floater furnaces and a bogie hearth furnace.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

computational fluid dynamics (CFD), combustion, NO_X, post-processor

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