Challenges in industrial implementation of global reaction schemes for simulation of MILD combustion with LCF

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In detailed 3D CFD combustion simulations both the chemical kinetics and the interaction between turbulence and chemical reactions have to be modeled accurately to predict the combustion process. Increasing computer capacity have made it possible to use more advanced turbulence models and more species and reactions included in the chemistry. However, the need for simplified chemistry and hence global reaction mechanisms is still important for effective product development work.

The addition of a large number of chemical species complicates the turbulent reaction modeling since the chemical reaction rates depend non-linearly on the species' concentrations, [1]. An assumption of fast chemistry is often made for turbulent reacting flows, implying that reaction rates are solely controlled by turbulent motion and thus reducing it to a mixing problem. In MILD combustion conditions, where the reaction paths are altered and some reaction rates are slowed down significantly by large amounts of inert diluents in the combustion zone, the assumption of fast chemistry is not valid, [2]. Use of more elaborate chemistry/combustion models which take into account finite-rate chemistry together with global reaction mechanism that accurately capture the altered combustion behavior in MILD conditions are prerequisites to efficiently simulate industrial burners in MILD conditions. The questions that come to mind now are of course:

- How should the reactions in the Global Mechanism be chosen?
- Which combustion model, or rather chemistry/turbulence interaction model, is best?
- How accurate need the turbulence modeling be (RANS vs URANS/LES)?

Furthermore, are there any commonalities, best practices and truths within the various 3D CFD simulations of MILD combustion out there? This is the topic that will be looked at and hope to initiate a discussion about.

Based on the MILD combustion burner produced by Cleanergy AB, Sweden, an initial numerical investigation and partial validations with test data has been performed. The investigation includes a comparison between two similar four step global reaction mechanisms optimized for LCV (Low Calorific Value) Landfill gas (24.2% CH4, 21.6% CO2, 2.0% O2 and 52.2%N2 by volume) in MILD conditions. The first mechanism, called AAT4NR, includes 4 irreversible reactions while the second, called AAT4R, includes 1 irreversible and 3 reversible reactions. Both mechanisms were evaluated using Ansys CFX. It is apparent that the modelling of reversibility in chemical reactions using CFD is a topic to consider and that it has a large effect on the results, see Figure 1. The investigation will in the future be continued by looking into software dependencies, how chemical reversibility is handled in different software and the effect on this specific MILD combustion case.

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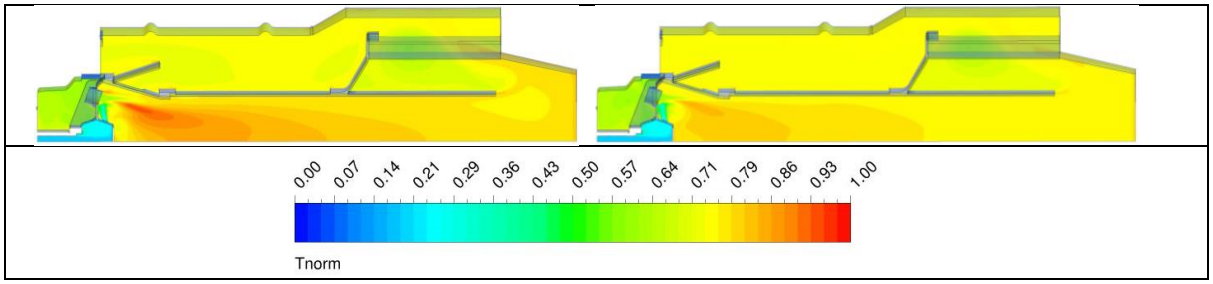

Figure 1. Temperature for AAT4NR (left) and AAT4R (right)

Following this first comparison, attention shifted to the question of the turbulence model. Is a steady-state two equation RANS turbulence model sufficient to model MILD combustion? The differences in results for the same case run with k-ω SST steady-state turbulence and transient hybrid SAS / k-ω SST indicates that this might be an issue at least for the Cleanergy burner, see Figure 2.

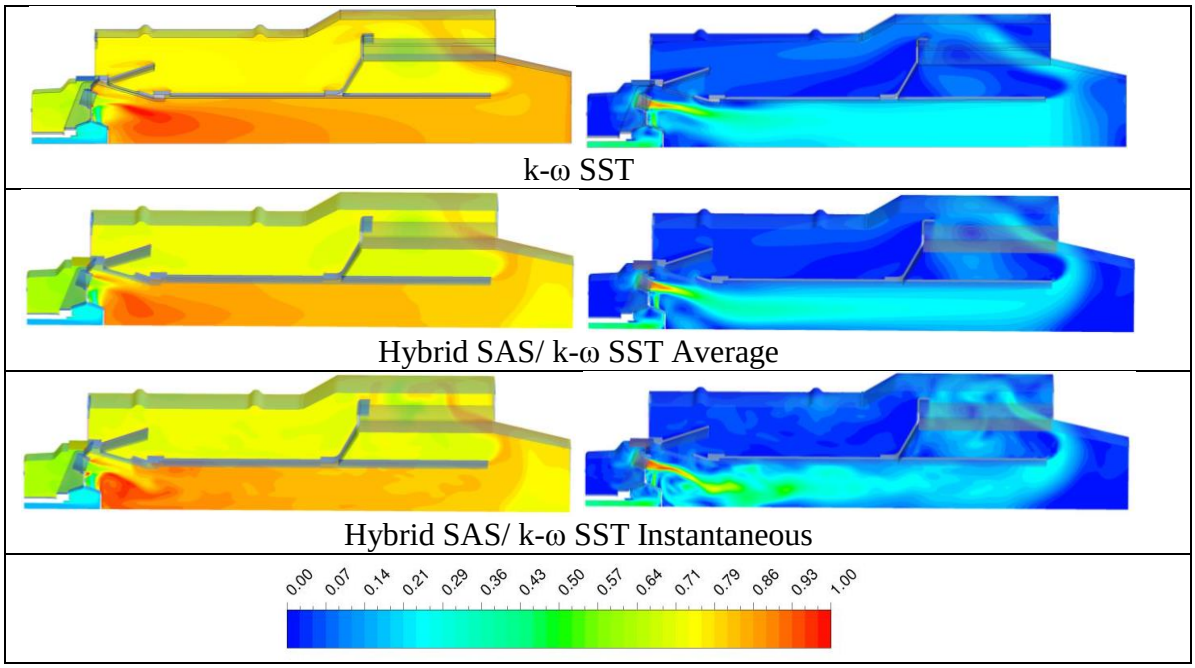

Figure 2.Normalized temperature (left) and normalized velocities (right) for k-ω SST, Hybrid SAS/ k-ω SST Average & Hybrid SAS/ k-ω SST Instantaneous.

Given the differences and limitations in commercial CFD codes regarding the setup and the possibility to combine chemical reversibility and combustion models including finite rate chemistry (EDC, PSR, EDM/FRC etc) there is substantial work to be done looking into all combinations and their effect. This is a task that is planned to be executed together with the investigation of Open-Source alternatives without some of the apparent black box features of commercial codes.

References

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