Implementation of a 19 Species Methane Global Mechanism into FLUENT

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Gas Turbine Need

✓ In gas turbine applications, notably in combustion devices, the flow is very turbulent and the interaction between the chemical kinetics and turbulence is significant.

✓ Modeling turbulent combustion requires expensive computational resources, whose cost increases with the number of species in the chemical kinetic mechanism. The complexity increases even further when three dimensional full scale computational grids are used resulting into millions of nodes.

✓ Reduced mechanisms are often used in order to decrease the computational cost. One major concern with using reduced mechanism is loosing accuracy and therefore making the simulations unpractical.

✓ Various methods have been developed for mechanism reduction, with the two major methods being the skeletal reduction and time scale analysis.

✓Skeletal mechanisms are stiff in nature. Stiffness is eliminated by the means of the Linearized Quasi Steady State Approximation (LQSSA) using a Directed Graph approach (QSSG). This last approach promises efficient and accurate results.

Objectives

✓ Implement a 19 species-15 step global Methane mechanism (Law), previously derived from the GRI-Mechanism 3.0 using the method of directed relation graph (DRG) and quasi steady state assumption (QSSA), into the CFD solver FLUENT.

✓ Link the precompiled mechanism to the solver by the means of a User Defined Function (UDF). The UDF communicates the chemical source terms to the solver through the subroutine "Define Net Reaction Rates".

✓ Test the implementation of the UDF using the 19 species Law mechanism with two challenging cases; the Berkeley lifted CH4/Air jet flame in a vitiated co-flow and the two-D backward facing step expansion flow.

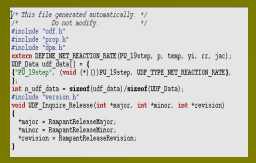
✓ Investigate the effect of coupling detailed chemistry with turbulence models on the computational time and accuracy of the results.

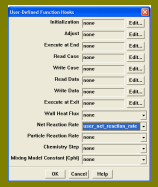
✓ Introduce means by which the chemistry calculations are accelerated in order to overcome the massive computational efforts demanded by the inner iterations of the global mechanism elementary reactions.

Approach

Implementation of the Reduced mechanism into FLUENT

1. Create the User Defined Function which uses the "Define_Net_Reaction_Rate" Macro to compute the net reaction rates of the species.
2. Link precompiled object files from non-FLUENT sources
3. Load the UDF library into the Fluent Solver





Modeling Chemistry-Turbulence Interactions
Eddy Dissipation Concept (EDC)

✓ The EDC model is an extension of the eddy-dissipation model to include detailed chemical mechanisms in turbulent flows.

✓ It assumes reaction occurs in small turbulent structures, called the fine scales over a time scale τ.

$$\gamma = 2.1377\left(\frac{\nu\varepsilon}{k^2}\right)^{1/4} \propto \mathrm{Re}_t^{-1/4} \qquad \tau = 0.4082\sqrt{\frac{\nu}{\varepsilon}} \propto t_{Kolmogorov}$$

✓ The EDC model can become computationally demanding due to the nonlinearity of the chemical kinetics mechanism, therefore the ISAT (In-Situ Adaptive Tabulation) is used to integrate the reactions.

✓ **ISAT** can accelerate the chemistry calculations by two to three orders of magnitude, offering substantial reductions in run-times.

Communication between the FORTRAN subroutine and The FLUENT solver

✓ Once the reduced mechanism is constructed and executed, the subroutine that computes the chemical source terms is automatically generated. A coupled set of nonlinear QSS species equations are numerically solved within the subroutine to provide the necessary elementary reaction rates for the reduced mechanism.

✓ The EDC uses the reaction rates computed from the FORTAN as an input to the turbulent reaction rates.

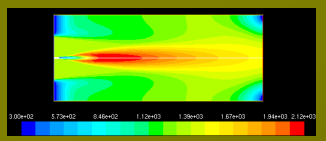
✓ The "Define Net Reaction Rate" macro returns the molar production rates of the species given the pressure, temperature, and mass fractions.

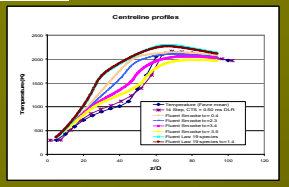
Results

The Berkeley lifted CH4/Air jet flame in a vitiated co-flow

Experiment

CFD Model: Temperature contours (K)

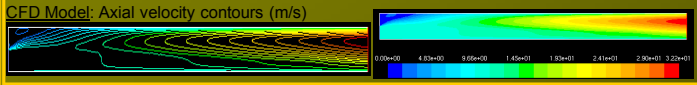




Two-D backward facing step expansion flow

Experiment

CFD Model: Axial velocity contours (m/s)



Conclusions

➢ The 19 species global mechanism was successfully implemented and tested into the CFD solver FLUENT. FLUENT has UDF capabilities to allow for such implementation.

➢ The precompiled mechanism was linked to the solver by the means of a User Defined Function (UDF) which communicates the chemical source terms to the solver through the subroutine "Define Net Reaction Rates".

➢ The Implementation of the UDF was tested with two validation cases: The Berkeley Methane/Air flame and the 2D backward facing step experiments.

➢ The model was capable of capturing the maximum mean velocities and recirculation zone for the 2D backward facing step case.

➢ The model reproduced the shape of the lifted CH_4 jet flame successfully. Accurate temperature profiles were attained by modifying the turbulent time scale of the EDC model.

➢ The computational time was greatly reduced by ISAT (In-Situ Adaptive Tabulation), which accelerated chemistry calculations up to a thousand- fold.

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