RESOLVING TURBULENCE-CHEMISTRY INTERACTIONS IN MIXING-CONTROLLED COMBUSTION WITH LES AND DETAILED CHEMISTRY

Convergent Science White Paper
**OVERVIEW**

Although the SAGE detailed chemistry solver has demonstrated success in a host of gas turbine, internal combustion engine, and other applications, it has been questioned for not employing a model to account for turbulence-chemistry interaction (TCI). In this study, we demonstrate that CONVERGE CFD (with LES, detailed chemistry, and sufficient grid resolution) can account for turbulence without explicitly assigning a sub-grid model to account for those interactions. We simulate the Sandia Flame D case, which is a canonical turbulent partially premixed flame. Because LES and detailed chemistry can be computationally expensive, these CONVERGE simulations include Adaptive Mesh Refinement (AMR) and adaptive zoning as acceleration strategies.

**TURBULENCE-CHEMISTRY INTERACTION**

There are two components that comprise TCI: (1) enhanced mixing in momentum, energy, and species due to turbulence and (2) the commutation error in the reaction rate evaluation. A good turbulence model, whether RANS or LES, should account for the enhanced mixing due to turbulence. The commutation error is more difficult to address.

In a RANS simulation, the commutation error is the difference between evaluating the reaction rates using the ensemble average quantities and evaluating the reaction rates by ensemble averaging the reactions using un-averaged quantities (the latter is exact and the former is an approximation). In an LES simulation, the commutation error is the difference between evaluating the reaction rates using the spatially filtered quantities and evaluating the reaction rates using spatially filtered reactions that use the un-filtered quantities. Unfortunately, in a typical CFD simulation, we do not know the un-averaged or un-filtered values to evaluate the reaction rates correctly. Thus it is convenient to use the averaged or filtered values to evaluate the reaction rates. Mathematically, the commutation error can be expressed by

\[
\text{Commuation Error} = \omega(T, \bar{Y}_m) - \omega(T, \hat{Y}_m).
\]

*Equation 1. Commutation error*

In the above expression, \(\omega\) is the species reaction rate, \(T\) is the temperature, and \(Y_m\) is the species mass fraction vector. The overbar indicates an ensemble average for RANS or a spatial filter for LES.

For LES, the commutation error reduces as the cell size is reduced, and thus, with sufficient grid resolution, the commutation error becomes negligible. In a RANS simulation, the commutation error does not reduce as the cell size is reduced.
There are also sub-grid effects that are a consequence of insufficient grid resolution rather than true turbulence-chemistry interaction. These sub-grid errors can result in significant error in combustion simulations, which are often incorrectly attributed to TCI effects. Combustion models are often tuned using TCI as justification when the true problem is that the simulation is under-resolved.

CASE SETUP

The Sandia Flame D case consists of a main jet with a mixture of 25% methane and 75% air by volume surrounded by a hot pilot jet to stabilize the flow. The Reynolds number for the main jet is 22,400; the nozzle diameter (D) is 7.2 mm; and the bulk jet velocity is 49.6 m/s.

The methane-air chemical mechanism used in this paper is a 30-species skeletal mechanism based on GRI-Mech 3.0. A dynamic structure LES model is used to simulate sub-grid turbulence.

The inflow variables, including the inlet profiles of mean velocity, temperature, species mass fraction and turbulent kinetic energy, are set to match the experimental measurements. To excite the jet development in LES, synthesized turbulent fluctuations based on the Von Karman turbulence spectrum model are used to match the turbulence intensity at the inlet.

DETAILED CHEMISTRY

The finite rate detailed chemistry model employed by the SAGE detailed chemistry solver has several advantages over other combustion models in CONVERGE. First, the SAGE detailed chemistry solver is directly coupled to the flow solver. Second, SAGE does not restrict the species to a low-dimensional manifold, which gives the model a broader applicability to more challenging combustion regimes such as ignition, extinction, and emissions formation. Third, you can easily include a detailed chemical mechanism, which may have hundreds or even thousands of species. A well-designed mechanism that is accurate over the full range of conditions in the simulation can allow you to predict complex chemical kinetics (e.g., to predict soot).

To accurately predict non-premixed turbulent combustion, both turbulent mixing and the chemical reactions must be solved correctly. Assuming that the burned region is resolved (see the Grid Convergence section for more detail), accurate results for diffusion flames can be achieved without a term for the commutation error.
The SAGE detailed chemistry solver evaluates the chemical source term in each cell at each time-step. The detailed chemistry solver can be computationally expensive, and so this study includes adaptive zoning\textsuperscript{15}, which accelerates the simulation by grouping similar cells into zones and then performing detailed chemistry calculations once per zone rather than once per cell. CONVERGE can group cells based on several flow field variables—here the adaptive zoning is based on temperature and progress equivalence ratio. The number of zones for each of these variables changes dynamically, and we specify a fixed size for each zone (5 K for temperature, 0.05 for progress equivalence ratio). Adaptive zoning has been shown to reduce computational expense without significantly affecting simulation results\textsuperscript{16}.

**ADAPTIVE MESH REFINEMENT (AMR)**

AMR automatically adjusts the grid at each time-step based on curvature (second derivative) of a field variable such as temperature or velocity. This feature adds cells in areas with complex phenomena and eliminates cells that are not needed to yield accurate results. In this study, we use velocity- and temperature-based AMR. In these simulations, AMR places additional cells at the burning region, which provides a significant reduction of the commutation error in the LES simulation.

To study the grid convergence of the Sandia Flame D case, we ran simulations with minimum cell sizes from 0.25 mm (case A) to 2.0 mm (case E). Refer to the Grid Convergence section below for more details.

In Figure 1(a), you can see instantaneous distributions of velocity, mixture fraction, mass fractions of CO\textsubscript{2} and CO, and sub-grid scale (SGS) velocity (which is defined as the square root of sub-grid scale TKE) for the case with a base grid size of 0.25 mm. You can see spatial fine-scale structures for all of these quantities, which implies that a substantial range of turbulent scales has been resolved.

With AMR, additional cells are added to the shear layer and to any local regions that have large velocity gradients resulting in an effective grid size of 0.25 mm, while far away from the shear layer the grid size remains 2 mm. Figure 1(b) expands the area of the small white box (12 mm × 36 mm) from Figure 1(a) so that you can see the mesh around the flame.
Figure 1(a): Instantaneous distributions of velocity, mixture fraction, mass fractions of CO2 and CO, and SGS velocity at the y = 0 plane from case A (0.25 mm).

Figure 1(b): Small subsection [white box from Figure 1(a) above] of the instantaneous distributions of velocity, mixture fraction, mass fractions of CO2 and CO, and SGS velocity at the y = 0 plane from case A (0.25 mm).
RESULTS

To obtain sufficient time-averaged statistics, LES is run for 0.35 $s$ since flow through the domain takes 0.02 $s$. Time-averaged values for mean and RMS values of velocity, temperature, mixture fraction, and species mass fractions are calculated. Here we present the results for the centerline of the jet and at radial positions, and we compare these simulation results to experimental data\textsuperscript{17,18}. Please see Liu et al., 2017 for additional results\textsuperscript{19}.

GRID CONVERGENCE

To study the grid convergence of the Sandia Flame D case, we ran simulations with minimum grid sizes from 0.25 mm (case A) to 2.0 mm (case E). Table 1 below gives grid information for these five cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base grid size (mm)</td>
<td>2</td>
<td>3</td>
<td>8</td>
<td>16</td>
<td>32</td>
</tr>
<tr>
<td>AMR refinement level</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Minimum cell size (mm)</td>
<td>0.25</td>
<td>0.375</td>
<td>0.5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Cell number (million)</td>
<td>50</td>
<td>25</td>
<td>10</td>
<td>3</td>
<td>0.5</td>
</tr>
</tbody>
</table>

*Table 1. Grid information for cases A-E*

Figures 2 and 3 show the instantaneous and mean temperature distributions from cases A through E on the symmetry plane. Cases A, B, and C have a fully developed jet inside the simulation domain, while the jet core length in case D is too large for the domain (though we see some local turbulent structures). Case E is unphysical as it is extremely under-resolved—the jet does not develop at all in the domain. The difference between cases A and B is relatively small, which suggests that we have reached grid convergence.

Figure 4 shows centerline profiles (mean) of axial velocity, temperature, and mass fractions of CO\textsubscript{2} and CO for cases A through D. Overall the results from cases A and B match the experimental data quite well. The results from case C show good agreement with measurements at $x/D = 30$, but the centerline and radial profiles at $x/D = 45$ indicate a slower jet development. The statistics of velocity, temperature, and species mass fraction match experimental measurements. Although there is a small difference between the results of cases A and B, from these results we expect grid convergence at a minimum grid size of 0.25 mm.
**Figure 2**: Instantaneous temperature distribution at \( y = 0 \) plane from case A (far left) to case E (far right).

**Figure 3**: Mean temperature distribution at \( y = 0 \) plane from case A (far left) to case E (far right).
Figure 4: Centerline (a, b, c, d) and radial profiles at $x/D = 30$ (e, f, g, h) and $x/D = 45$ (i, j, k, l) of velocity (row 1), temperature (row 2), and mass fractions of CO$_2$ (row 3) and CO (row 4) from LES with different grid resolutions.
COMPARING LES TO EXPERIMENTAL DATA

The detailed results from the finest grid resolution (case A) are shown in Figure 1 above and Figures 5, 6, and 7 below. From Figure 1, we can see that the maximum SGS velocity is approximately 0.55 m/s, which is far less than maximum RMS of axial velocity along the centerline. The small amount for which we use the dynamic structure turbulence model tells us that we resolved most of the velocity fluctuations directly through LES in the case with the finest mesh size (A).

Comparing the axial mean and RMS velocity (Figure 5) between simulation and experimental data, we conclude that the jet decay rate is accurately predicted. Near x/D = 45, the peak temperature from LES is slightly lower than experimental data, but the double peak of temperature RMS is well captured. The peaks for the species mass fractions of CO2 and H2O are slightly under-predicted. This might be due to measurement uncertainties or errors from the chemical mechanism. Although the peak value of the mass fraction of CO from case A was 0.01 lower than the experimental value, the RMS value of CO is very close to the experimental measurement.

Figures 6 and 7 show the radial profiles of statistics from x/D = 15 and 30, respectively. The velocity and major species mean and RMS show very good agreement with measurements. The peak mean value for the minor species CO is under-predicted, but the peak mean and RMS values of CO2 mass fraction are well predicted.

The commutation error becomes smaller as we resolve the temperature and species fluctuations. With LES case A, the finest mesh, we match the mean and RMS to the experimental values. Thus, with sufficient grid resolution, LES with the SAGE detailed chemistry solver can predict mixing-controlled turbulent combustion without a model for the commutation error.
Figure 5. Centerline mean and RMS profiles of (a) axial velocity, (b) temperature, (c) mixture fraction, and mass fractions of (d) CH4, (e) O2, (f) CO2, (g) H2O, and (h) CO from LES case A (0.25 mm).
Figure 6: Radial mean and RMS profiles of (a) axial velocity, (b) temperature, and mass fractions of (c) O2, (d) CO2, (e) H2O, and (f) CO at x/D = 15 from LES case A (0.25 mm).
**Figure 7:** Radial mean and RMS profiles of (a) axial velocity, (b) temperature, and mass fractions of (c) O2, (d) CO2, (e) H2O, and (f) CO at x/D = 30 from LES case A (0.25 mm).
CAPTURING NON-EQUILIBRIUM COMBUSTION PROCESSES

We know from previous studies\textsuperscript{20,21} that Sandia Flame D shows non-equilibrium combustion processes at $x/D = 15$ and $x/D = 30$. To check if LES can predict non-equilibrium combustion processes, we compare 15,000 data points from the experiment to the equivalent points from LES (30 from each of 500 images) for the mass fraction of CO2. Each plot in Figure 8 shows a scatter plot of these data points (15,000 from LES and 15,000 from the experiment) and the conditional mean value of the mass fraction of CO2 at $x/D = 15$ and $x/D = 30$.

![Figure 8: Sample points and conditional mean value in mixture fraction and mass fraction of CO2 in mixture fraction space from experimental data and LES case A at (a) $x/D = 15$ and (b) $x/D = 30$.](image)

It is not surprising that the LES results correctly predict the extinction and reignition trends at both $x/D = 15$ and 30. Accurate prediction of non-equilibrium combustion processes is dependent on two factors: an accurate mechanism over the range of conditions (to correctly predict extinction strain rate and ignition delay time) and a good LES solver with sufficient grid resolution (so that a large portion of velocity, temperature, and species fluctuations are well resolved). With the combination of these two factors, the commutation error can be neglected and good results can be obtained.
CONCLUSIONS

In this study, we demonstrate that CONVERGE (with LES, detailed chemistry, and sufficient grid resolution) can accurately solve a non-premixed flame without an explicit model for the commutation error that is shown in Equation 1.

In our Sandia Flame D simulations, we find that the 0.25 mm minimum grid size is sufficient to resolve most of the velocity, temperature, and species fluctuations. Adaptive Mesh Refinement, detailed chemistry, and LES provide the simulation conditions needed to reduce the commutation error. By resolving most of the velocity, temperature, and species fluctuations and thereby significantly reducing the commutation error, we negate the need for an explicit sub-grid model for the commutation error.

REFERENCES

10 Barlow, R.S. Sandia National Laboratories, TNF workshop website, 2003.


Founded in Madison, Wisconsin, Convergent Science is a world leader in computational fluid dynamics (CFD) software. Its flagship product, CONVERGE, includes groundbreaking technology that eliminates the user-defined mesh, fully couples the automated mesh and the solver at runtime, and automatically refines the mesh when and where it is needed. CONVERGE is revolutionizing the CFD industry and shifting the paradigm toward predictive CFD.

CONVERGENT SCIENCE: WORLD HEADQUARTERS
6400 Enterprise Ln
Madison, WI 53719
Tel: +1 (608) 230-1500

CONVERGENT SCIENCE: TEXAS
1619 E. Common St., Suite 1204
New Braunfels, TX 78130
Tel: +1 (830) 625-5005

CONVERGENT SCIENCE: DETROIT
21500 Haggerty Rd.
Detroit, MI 48167
Tel: +1 (248) 465-6005

CONVERGENT SCIENCE: EUROPE
Hauptstraße 10
Linz, Austria 4040
Tel: +43 720 010 660

CONVERGENT SCIENCE: INDIA
Office #701,
Supreme Headquarters
Mumbai-Bangalore Highway
Baner, Pune, Maharashtra 411021
+91 741-0000-870

For additional information or to contact us, visit convergecfd.com