**LES SOFTWARE FOR THE DESIGN OF LOW EMISSION COMBUSTION SYSTEMS
FOR VISION 21 PLANTS**

Quarterly Technical Progress Report for

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by

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ABSTRACT

Further development of a combustion Large Eddy Simulation (LES) code for the design of advanced gaseous combustion systems is described in this seventh quarterly report. CFD Research Corporation is developing the LES module within the parallel, unstructured solver included in the commercial CFD-ACE+ software. In this quarter, the Localized Dynamic subgrid Kinetic energy Model (LDKM) was improved and an initial Turbulent Artificial Neural Net (TANN) was developed. Validation and testing of the combustion LES code was performed for the Vanderbilt lean premixed combustor and the Loughborough University combustor port flow experiment.

Next quarter, LES software development and testing will continue. Alpha testing of the code will continue to be performed on cases of interest to the industrial consortium. Optimization of the subgrid models will be pursued, particularly with the In Situ Adaptive Tabulation (ISAT) approach. Also next quarter, the demonstration of the TANN approach in CFD-ACE+ will be accomplished.

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1. INTRODUCTION

Vision 21 combustion systems will require innovative low emission designs and low development costs if Vision 21 goals are to be realized. In this three-year project, an advanced computational software tool will be developed for the design of low emission combustion systems required for Vision 21 clean energy plants. The combustion Large Eddy Simulation (LES) software will be able to accurately simulate the highly transient nature of gaseous-fueled turbulent combustion so that innovative concepts can be assessed and developed with fewer high-cost experimental tests. During the first year, the project has included the development and implementation of improved chemistry (reduced GRI mechanism), subgrid turbulence (localized dynamic), and subgrid combustion-turbulence interaction (Linear Eddy) models into the CFD-ACE+ code. University expertise (Georgia Tech and UC Berkeley) has been utilized to help develop and implement these advanced submodels in the unstructured, parallel CFD flow solver. Efficient numerical algorithms that rely on *in situ* look-up tables or artificial neural networks have been implemented for chemistry calculations. Now, in the second year, the combustion LES software will be evaluated and validated using experimental data from lab-scale and industrial test configurations, including important benchmark data from DOE-NETL. During the last year, seven industrial and academic partners will take the combustion LES code and exercise it on problems of their choice. Final feedback and optimizations will then be implemented in the final release version of the combustion LES software.

2. EXECUTIVE SUMMARY

Work in this seventh quarter (April - June 2002) has included further development of the LDKM and LEM subgrid models. Georgia Tech has extended the laminar ANN to include turbulent fluctuations. This TANN has been tested in their stand-alone LEM code and will be implemented and tested in the CFD-ACE+ code during the next quarter. Combustor LES validation has been carried out on Vanderbilt University's lean premixed combustor and Loughborough University's combustor port experiment.

Next quarter, completion of the following tasks are planned:

1. Optimize and refine ISAT for multi-step chemistry.
2. Finish Vanderbilt lean premixed combustor validation case.
3. Implement and test TANN on lean premixed SimVal combustor test case.

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS AND DISCUSSION

4.1 Localized Dynamic Subgrid Kinetic Energy Model (LDKM)

In this reporting period we have revisited the Localized Dynamic Ksgs-Equation model (LDKM), both in implementation and validation. This step was initiated to ensure that the LEM model is fed with the proper subgrid turbulent kinetic energy levels. The implementation work included the addition of a new test filter and the modification of the wall boundary conditions.

In order to keep the computational costs at a minimum, the LES test filter was initially implemented as a vertex type filter. What this means is that for a given cell we accumulate the values of the neighboring cells which contain the vertices of the current cell and average it out. This produces a filter based on a weighted average, in which the current cell has the biggest weight. The weights in the filter depend on the geometry of the cell. Thus, for hexes the current cell has a weight of 9/65 as opposed to 1/27 for the uniform average test filter. This introduces a bias towards the current cell and could result in an increased smoothing effect. The biased filter can be considered as the upper end estimate of the actual (uniform) test filter. Please note that we are working with an unstructured grid formulation and computing a uniform test filter would be more expensive.

For this reason we have implemented a test filter that is at the opposite end in terms of averaging, with no significant increases in the computational costs. This test filter averages only the face neighbours, resulting in a lower end approximation of the uniform test filter. Preliminary results show that this new filter reduces the smoothing effect.

New validation tests have been chosen to insure that the LDKM produces correct results. Among the cases considered are homogeneous box flow, channel flow and revisitation of the lid driven cavity. The evaluation of the results is still ongoing and final conclusions will be reported next quarter.

Typical results for the homogeneous and isotropic LES simulations are presented in Figures 1 and 2. Figure 1 shows the contours of the U velocity component averaged over time along with the instantaneous velocity vectors. Figure 2 shows contours of the subgrid turbulent kinetic energy. The simulation exhibits the time decay of the turbulent energy of the flow. In the next reporting period we will finalize the validation cases and close any outstanding issues regarding the implementation and the performance of the LDKM model.

Figure 1. Average U-velocity and Instantaneous Velocity Vectors

Figure 2. Subgrid Turbulent Kinetic Energy

4.2 Application of ANN in Engineering LES

An extension of the Linear Eddy Model (LEM) in conjunction with the Artificial Neural Network (ANN) approach is being developed to simulate turbulent flames within LES. In this approach, being developed at Georgia Tech, an additional ANN that contains turbulence parameters such as the subgrid intensity and range of turbulent eddies in the flame zone ($f(l)$) is being developed. For example, the F1-F3 and B1 flames all have different u' and $f(l)$. Therefore, by combining the thermo-chemical ANNs for these flames with the fluid mechanical ANN for u' and $f(l)$, it will be possible to directly obtain the filtered reaction rates. Here, we consider the filtered reaction rate as an average over all the turbulent eddies that have perturbed the chemical state. Thus, mathematically this can be written as: $\bar{\dot{w}}_m = \langle \dot{w}_m \rangle$ where $\bar{\dot{w}}_m$ is the LES filtered reaction rate and $\langle \dot{w}_m \rangle$ indicates the reaction rate averaged over the local eddies. The latter term can be approximated from the LEM approach as: $\langle \dot{w}_m \rangle = \int \dot{w}_m(l) f(l) dl$. This approach allows the inclusion of detailed kinetics into LES solvers without the associated (enormous) increase in computational effort since the term $\langle \dot{w}_m \rangle$ can be determined and stored in the ANN. This approach is denoted Turbulent ANN (TANN) and is briefly described below.

To implement TANN, it is necessary to combine thermo-chemical and fluid-mechanical effects within a single formulation. To use it within the context of LEM, the F_{stir} terms in the species and temperature transport equations are not implemented which means that the reaction diffusion equations are identical to the *laminar* case. In order to capture the effect of turbulent eddies on the flame, eddies are sampled from the eddy size pdf, $f(l)$ at the local time scale, and the eddy event rate and event location are determined as in the original LEM approach, except that, now the reaction rates in these eddy locations are implemented in an averaged sense. Figure 3 shows some preliminary results of the TANN prediction. The results when compared to the direct integration result show that there are regions where the local structure is getting smothered by this averaging procedure. This is expected since in the TANN implementation, detailed sub-structure of the flame (i.e., structure within eddies of size l) is not captured and only the integrated effect is included. In spite of some errors due to the implicit smoothing of the flame structure, the “filtered” profile shows the gradual temperature rise in the preheat zone (which is characteristic of a thin-reaction-zone flame). Further improvements of this TANN approach to obtain more accurate prediction are still underway.

(a) CH₄ Profile

(b) T Profile

Figure 3. Instantaneous Profiles for F1 Flame Using TANN

Although the above study appears unrelated to LES, note that we are attempting to estimate the “filtered” reaction rate by TANN. So far, only the eddy size distribution $f(l)$ for a single flame F1 has been incorporated. However, once other relevant parameters, such as turbulence intensity u' , equivalence ratio, and inlet temperature are included (by using the LEM model simulations), TANN will essentially predict the filtered reaction rate as a function of these parameters. In other words, TANN will contain the joint pdf of thermo-chemical and fluid mechanical variables. To mathematically explain this approach, consider the filtered scalar equations that are typically solved in a conventional LES. (Note we are not considering the subgrid simulation model (Chakravarthy and Menon, 1999) here since this approach is considered too expensive for engineering-level LES):

$$\frac{\partial \bar{\rho} \tilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_i} \left[\bar{\rho} \tilde{Y}_m \tilde{u}_i - \bar{\rho} \bar{D}_m \frac{\partial \tilde{Y}_m}{\partial x_i} + \Phi_{i,m}^{\text{sgs}} + \theta_{i,m}^{\text{sgs}} \right] = \bar{\dot{w}}_m$$

for $m = 1, N$ species. In this equation, the subgrid scalar flux, $\theta_{i,m}^{\text{sgs}} = \bar{\rho} [V_{i,m} Y_m - \tilde{V}_{i,m} \tilde{Y}_m]$ and the filtered reaction rate term, $\bar{\dot{w}}_m$ require closure. In engineering LES, a gradient approximation: $\theta_{i,m}^{\text{sgs}} \approx -\bar{\rho} v_t \nabla \tilde{Y}_m / Sc_m$, where Sc_m is a turbulent Schmidt number (assumed to be unity), can be employed for the subgrid scalar flux. This approach is acceptable since the large-scale motion is resolved in the LES, and therefore, any large-scale counter-gradient processes (if they occur) are resolved (even when a gradient closure is employed for $\theta_{i,m}^{\text{sgs}}$).

The closure for $\bar{\dot{w}}_m$ is the key problem in LES. For example, the most popular approach is the assumed pdf approach in the mixture fraction space but this approach is not considered appropriate when complex kinetics and pollutant formation have to be predicted. The subgrid LEM model (Menon and Calhoon, 1996; Chakravarthy and Menon, 1999) avoids this assumed pdf approach by simulating the actual local evolution of the joint-scalar pdf and therefore, provides an elegant closure for the scalar field. However, this approach is too expensive for engineering application. In the new TANN approach, the joint pdf for the thermo-chemical and fluid mechanical processes will be stored and accessed on-line to directly obtain $\bar{\dot{w}}_m$. As noted earlier, this results in $\langle \dot{w}_m \rangle$ which is stored in the TANN.

There is another subtle advantage of TANN. Since it is built using the 1D species and temperature transport equation, it contains within it the molecular diffusion (and differential diffusion) process (the term $\Phi_{i,m}^{\text{sgs}}$ in the above equation). Since the molecular process occurs in the small-scales, it cannot (and should not) be modeled at the LES scale. The TANN database contains within it molecular diffusion (in effect simulates $\Phi_{i,m}^{\text{sgs}}$) and therefore, does not have to be modeled.

Furthermore, the diffusion term in the above equation, $\bar{\rho} \bar{D}_m \frac{\partial \tilde{Y}_m}{\partial x_i}$ is a special term in the TANN approach since it incorporates diffusion across LES cell faces only under special circumstances (e.g., molecular diffusion when there is no flow). However, in high-Re turbulent flows (where $\theta_{i,m}^{\text{sgs}}$ is likely to dominate at the resolved scales), this term could be neglected.

Further development of TANN is still underway in order to make this approach robust and applicable to a wide range of problems within the LES context. An approach we are now exploring is to implement the subgrid LEM model within each LES cell as a surrogate to obtain information on the eddies and their consequence on stirring. In this approach, the scalar fields are still solved on the LES grid (as done for the earlier TANN) but the subgrid field is

interrogated between each LES time-step to determine how many eddies from the distribution $f(l)$ contribute to turbulent mixing. The chemical ANN is then evolved within each local eddy of size l in-between the LES time-step and the final states are ensemble-averaged to obtain $\langle \dot{w}_m \rangle$ in each LES cell. This filtered reaction rate term carries the subgrid scale information of turbulent stirring and reaction, to the coarser LES grid. Since the frequency and number of stirrings are still decided based on the 3D scaling laws of LEM, this approach will capture the effects of turbulent mixing and the filtered reaction rate without significantly increasing the computational cost. This approach combines the strengths of TANN and on-line LEM and may be general for wide applications. We hope to report on these studies very soon.

4.2.1 Computational Cost of TANN in a LES

The primary reason to use TANN is to reduce the computational cost (memory and runtime). As our recent studies have shown, ANN drastically reduces the memory requirement by an order of magnitude or more (Kapoor et al., 2001). For example, a 150 MB ISAT table for a 19-species mechanism reduces to less than 2 MB for ANN. Also, the computational time for ANN retrievals can be orders of magnitude less than that for ISAT, especially for more complicated mechanisms, like the 15-step, 19-species mechanism. Furthermore, since the ANN can be built using a different time-interval beforehand, the cost for direct integration is completely eliminated. It is expected that once the TANN approach has been fully developed and integrated into the LES methodology, an engineering level LES with detailed kinetics will become feasible since the cost of obtaining the filtered reaction rate has been reduced to just the TANN access cost.

4.3 Combustor Port Flow Validation Case

Experimental data from a combustor port flow at Loughborough University is being used for validation of the combustion LES code. Adrian Spencer, assistance professor at Loughborough University, was responsible for acquiring the data and is now at CFDRC doing the validation work. The air admission ports of most conventional combustors can be categorized as annulus fed ports issuing jets into a confined crossflow. Isolating the flow mechanisms associated with such a configuration provides a method of understanding phenomena particular to this setup without introducing complications of studying fully featured combustors (such as interaction with swirl from fuel injectors or liner cooling flows etc.). Simplifying the geometry also allows parallel computational-experimental studies to be performed in such a way, that not only are the flow physics better understood, but high quality experimental data can be captured which is ideal for LES code validation.

At Loughborough University such a study has been carried out on generic combustor port flow scenarios. This has been done on a water flow rig which is scaled to match typical jet Reynolds numbers found in combustors. The use of water is advantageous for various reasons, but in particular it was chosen for the ease in which measurements can be made using optically based techniques. Isothermal, constant density flow is a good description of the annulus feed flow. However, it is a poor description of a combustor flow, but, before testing CFD codes on fully reacting combustor flows it is important to have faith in the underlying aerodynamic models, particularly when the flow field contains phenomena challenging to turbulence models, e.g. jet on jet impingement. RANS based predictions of jet impingement have had mixed success, but

for this type of configuration they typically under predict turbulent kinetic energy by a factor of 2. This can be improved slightly by choosing different model constants or discretization schemes, but it is rare that such *a priori* knowledge is available to *tweak* the calculation. The high levels of turbulence, presence of bi-modal PDFs and evidence of coupling between the annulus feed flow and internal flow fields suggest that LES methodology may be well suited to predicting such a flow. As yet none are presented in the open literature.

The test case comprises of two concentric pipes. The inner pipe has a row of 6 equi-spaced ports which allows flow from the annulus feed to enter the inner pipe, or core, see Figure 4. By using various valves it is possible to set the following parameters; jet Reynolds number, annulus bleed flow fraction and jet to core flow velocity ratio. These three bulk flow parameters fully define the test condition, and may be varied to represent primary zone or dilution zone type port flows. Measurements of an impinging flow are available for a jet to cross flow ratio of 5 and an annulus bleed flow of 50%, with a jet Reynolds number of around 24000. It is this case which will be simulated using LES.

Figure 4. Co-Ordinate System Used for the Test Section

4.3.1 Setup and Boundary Conditions

With strongly impinging jets there can be significant reverse flow in the core. Time average measurements show that the reverse flow penetrates to around $x = -60\text{mm}$ (3 port diameters upstream of the port centreline). It is important to ensure that instantaneous reverse flow does not approach the inlet plane so the computational domain was positioned at $x = -200\text{mm}$. For the annulus $x = -100\text{mm}$ was sufficient. LDA measurements are available for the inlet planes of the rig and these are shown in Figure 5. The given axial velocity profiles were scaled to give the correct inlet mass flow rates and the other inlet velocity components were set to zero. Random Gaussian fluctuations were specified, having a uniform rms value representative of a mass weighted average value available from the LDA measurements. The annulus exit velocity was fixed to set the correct bleed flow and the core exit plane was specified as constant pressure.

Figure 5. Inlet Axial Velocity Profiles

The solid model of the computational domain is shown in Figure 6. Flow enters left and exits right, the area reduction at the exit planes was used to ensure that no back flow occurred through these planes, and the core inlet and exit planes were extended as far as possible from the impingement point. The downstream extension was used to reduce any effects of the constant pressure boundary condition on the impingement. PIV measurements of the flow show that reverse flow can penetrate to $x = -150\text{mm}$ instantaneously thus the upstream extension was employed to $x = -200\text{mm}$.

Grid density was chosen based on previous RANS grid refinement studies. With a RANS approach only $1/12^{\text{th}}$ of the domain requires modeling by using implied circumferential symmetry, and, since the reverse flow regions of the time averaged flow are known from experimental evidence the axial domain can also be reduced to $-90\text{mm} < x < 90\text{mm}$. A modest 100,000 cells for a grid independent RANS calculation thus requires 2,200,000 cells for a full 3D LES study at a

similar grid density. One advantage of modeling the full 360° however is that the poor cells associated with centrelines of sector domains are removed along with the stiffness they impose on the solution. Here, in Figure 7, a butterfly grid is used in the core and an O-grid in the annulus. Each port contains $15 \times 15 \times 5$ cells connecting the core and annulus domains.

Figure 6. Solid Model

Figure 7. Surface Grid

4.3.2 Preliminary Results

It is common practice to start LES predictions from a steady state RANS prediction, and this was generated using a standard $k-\epsilon$ model. A solution was obtained which contained the expected symmetry as has been forced in previous RANS studies. Figure 8 shows isosurfaces of high velocity magnitude and contours of the same parameter on a diametral plane. Clearly the six jets can be identified, along with the impingement point indicated by a small cluster of contour lines. Downstream of the impingement point the jets merge and continue along the core centreline. Some of the jet fluid is deflected upstream also creating a toroidal recirculation zone. + marks the time-averaged stagnation point ($|V|=0$) at the head of this recirculation.

Figure 8. Velocity Magnitude - RANS $k-\epsilon$

Despite expecting near grid independence for this setup it was found that this point (+) was very sensitive to the discretization scheme employed. Upwind and 2nd order upwind under and over predicted the size of the recirculation by similar amounts (-5,+7mm) compared to the experimentally found $x = -57\text{mm}$. Central differencing however significantly under predicted the size of the recirculation positioning + at around $x = -20\text{mm}$. In other regions of the domain the solutions from the 1st and 2nd order differencing schemes produced similar results, helping to confirm that the grid provides adequate resolution. The sensitivity of the size of the recirculation is likely to be due to the prediction of the impingement point, since slight changes in the flow at this point will influence the mass flow rate fraction of the jets which is deflected back upstream and feeds the recirculation zone. As with previous predictions the turbulent kinetic energy at impingement was under predicted by close to 50% using the $k-\epsilon$ turbulence model.

The LES prediction of this flow has only just commenced. Initially the Smagorinsky model has been used with a time step of 100ms with Crank-Nicolson temporal differencing. Using a cluster of 16 1,000 MHz PCs each time step takes approximately 160s. For this incompressible flow some non-physical spiking was seen in the pressure field, with it oscillating between user-set high and low limits for the first few iterations. After around 500 time steps this behaviour had settled down and sensible results were obtained for the pressure field: the spiking appears to be a start-up problem.

A comparison of the RANS time averaged and LES instantaneous velocity fields can be seen in Figure 9. This comparison confirms previous statements about implied symmetry - clearly the assumption is valid for RANS predictions, but not so for LES. Also the need to increase the domain size can be seen, with reverse flow regions (blue) penetrating much further upstream in the LES prediction. Looking closely at the LES prediction shows a region of reverse flow attached to the upper wall of the core pipe very close to the inlet. For this reason the inlet plane has been moved further upstream for future calculations. This phenomena has been witnessed experimentally, where the flow in the recirculation zone flips to one side and interacts with the boundary layer, allowing jet fluid to penetrate far upstream as shown in Figure 10. This figure shows instantaneous velocity vectors and contours of axial velocity, where reverse flow is indicated as black. The reverse flow does extend (just?) beyond the measurement plane of $x=-140\text{mm}$ and is indicative of the most extreme extent witnessed for a jet to crossflow velocity ratio of 5. It may be surprising that an LES calculation would capture this event considering the question marks surrounding near wall treatments in LES models.

Figure 9. Axial Velocity, (a) $t=0.1s$, LES (b) RANS $k-\epsilon$

Figure 10. PIV Measurement of Instantaneous Velocity

In addition to LDA and PIV, some preliminary LIF is also available for this case. To compare LIF and LES results a conserved scalar has been solved for, which is set to 1.0 at the core inlet and 0.0 at the annulus inlet. In this way seeding is introduced to the core flow and the mixing of the jets with the core stream can be observed. Unfortunately a problem with the boundary conditions has meant that all of the flow entering the LES calculation has a scalar value of 0.0. However, since the calculation was started from a RANS prediction containing a scalar field, a useful indication of the flow through time can be seen. Figure 11 shows that after a time interval of 0.1s most of the core fluid has passed way downstream of the jets. It is evident that some pockets of the scalar, albeit at low concentration, exist upstream of the jets, and in particular along the upper core wall as previously discussed. Knowledge of this type gives a good indication of the required period for averaging of the LES simulation to obtain stationary statistics.

Figure 11. Conserved Scalar Concentration

Predicted instantaneous radial velocity can be seen on a plane containing all of the port centre-lines in Figure 12. (Blue indicates high negative V_r , and red indicates high positive.) The symmetry of jet strength witnessed in the RANS prediction (see Figure 8) is far from evident in the instantaneous velocity field here. It is not surprising that with such a distribution, and hence lack of a fixed impingement point, that RANS predictions are not able to predict the impingement mechanisms accurately. Indeed, many of the large scale unsteady flow features witnessed in combustors that are usually attributed to combustion instabilities could have much more humble origins.

Figure 12. Radial Velocity $t=0.1s$, LES

In conclusion, CFD-ACE+ RANS results agree well with previous RANS predictions. Core recirculation as predicted by k- ϵ RANS is highly sensitive to discretization method. The initial LES prediction has indicated a few areas which can be improved before running the case for a significant time period:

- need to increase LES domain size (upstream inlet plane);
- need to be able to set inlet scalar in LES; and
- useful to understand start-up problem with pressure field.

4.4 Vanderbilt Lean Premixed Bluff-Body Combustor Test Case

Detailed temperature and emissions measurements from the Vanderbilt/Sandia (Nandula et al., 1996) lean premixed bluff-body combustor are being used to validate the combustion LES software. This test case was chosen by the industrial consortium and was described in the last quarterly report. Last quarter the results were reported with reaction rates that were increased by an order of magnitude to prevent blow-off. After closer inspection it was found that the upstream reactant velocity entering the combustor was inadvertently set to a higher value than was used in the experiment (15 m/s instead of 12.2 m/s). Also, the modified LDKM now predicts higher subgrid kinetic energy levels in the shear layer (~ 2 times higher) compared to the

previous LDKM. The new modeling of the lean premixed combustor now shows an attached flame with the standard CH₄-air reaction rates.

Steady-state computations were first performed and are shown in Figure 13. A 2D axisymmetric grid was utilized with 5,278 cells. The combustor operating conditions correspond to an equivalence ratio of 0.586, an inlet velocity of 12.2 m/s, an inlet temperature of 300 K, and a combustor pressure of 1 atm. The bluff-body temperature was set to 600 K and the downstream combustor sidewalls were set to 500 K. Radiative heat transfer was ignored in the steady-state calculations. The steady-state calculations at these conditions had a difficult time predicting a stable flame. As can be seen, the hot combustion product region narrows closer to the centerline with downstream location. As will be shown later, the experimental data shows different behavior, with a widening of the hot product zone at far downstream combustor locations. The recirculation zone length is approximately 3 bluff-body diameters in length. The use of an assumed pdf method to account for turbulence-chemistry interactions actually caused the flame to be less stable and a non-reacting steady-state solution was obtained.

LES calculations were then performed for the same 2D axisymmetric configuration. The grid parameter and Kolmogorov time in Figure 13 for the steady-state calculations give some indication that the grid is appropriate for LES. A grid parameter less than 0 indicates that a finer grid should be utilized to capture the energy-containing scales. Only along the walls, would a finer grid be needed. Since a relatively coarse grid was used near walls, wall functions were utilized for the steady-state and LES cases. The local Kolmogorov time indicates that a time step of less than 2E-5 seconds would adequately resolve the eddy turnover times of the smallest energy-containing scales. A time-step of 7.5E-6 seconds was utilized in the LES runs.

The LDKM was used to describe the subgrid turbulence in the combustor. The Linear Eddy Model was used to describe the subgrid chemistry and turbulence-chemistry interactions. Radiative heat transfer was accounted for using the Discrete Ordinates method with wall temperatures of 500 K downstream of the bluff-body and boundary condition emissivities of 0.2. Gas-phase absorptivities were computed locally as a function of the mass fraction of CO₂ and H₂O. Figure 14 shows the time-averaged temperature and axial velocity predicted using the LES code. It is easy to see that the hot product region fills up almost the entire combustor area at downstream locations, in contrast to the steady-state predictions. Also, the recirculation zone length is now ~1.1 bluff-body diameters, much shorter than the 3 diameter length predicted with the steady-state model. The use of LES with the Linear Eddy Model allows enhanced reaction rates and more turbulent mixing than the steady-state model.

Figure 13. Steady-State Predicted Flowfield for Bluff-Body Combustor

Figure 14. Time-Averaged and Instantaneous LES-LEM Predicted Flowfield for Bluff-Body Combustor

Comparisons of experimental mean temperature data with predictions are shown in Figure 15. These results indicate that near the bluff-body, the predictions are similar and in good agreement for all three models. The far downstream location, on the other hand, shows the LES-LEM model to do much better at predicting the large scale mixing that distributes the hot products across much of the combustor cross-section. The LEM allows the filtered reaction rate, at downstream locations, to be higher than the laminar (non-filtered rate) due to the effect of subgrid turbulent fluctuations. Comparisons of major species predictions and measurements will

show similar agreement as observed in the temperature results. The predictions of minor species are currently being performed. A 5-step mechanism that predicts CO and NO has been used with the LES and laminar chemistry approximation. These 5-step predictions blew out. The 5-step with LEM is also being used. These calculations will be reported next quarter. In addition, a 3D LES calculation with LEM is being performed. This case has proved to require significant amounts of memory due to the LEM. The ANN and TANN approach will be required to replace the on-line LEM for design calculations of 3D combustor configurations.

Figure 15. Comparisons of Predicted and Measured Mean Temperature in Bluff-Body Combustor

A comparison of predicted and measured mean axial velocity are shown in Figure 16. Very near the bluff-body ($x/d=0.1$), the SS RANS results do a good job of matching the data. But, at further downstream locations, the SS RANS predictions deteriorate significantly. The LES with laminar chemistry overpredicts the recirculation zone negative velocities at all axial locations. The LES-LEM predictions do a pretty good job of matching the data at all axial locations.

Figure 16. Comparisons of Predicted and Measured Mean Axial Velocity in Bluff-body Combustor

5. CONCLUSION

The combustion LES code has been further developed and tested for predicting turbulent reacting flows. The accuracy of the LDKM subgrid turbulence model was improved and modeling of the Vanderbilt lean premixed combustor now shows good predictions with the updated LES model. Initial modeling of the Loughborough University combustor port flow has also been performed. The use of a Turbulent Artificial Neural Net (TANN) will be required for 3D LES simulations that include the Linear Eddy subgrid chemistry model. Georgia Tech is currently testing and trying to improve the TANN approach before it is implemented in the combustion LES code.

6. REFERENCES

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APPENDIX A — WORK SCHEDULE

Key Milestones

1 Complete In-Situ Adaptive Tabulation Module	7 Complete Tabulation Schemes
2 Complete LES Framework Modification to CFD-ACE+	8 Complete Parallelization of LES Code
3 Complete Reduced Mechanisms	9 Complete Implementation of LEM Model
4 Complete Selection of Cases	10 Complete Alpha Testing of LES Code
5 Complete Implementation of Turbulence Models	11 Complete Beta Testing of LES Code
6 Complete Implementation of Initial Version of LEM Model	12 Final Release of LES Code

Performance Targets

- A Alpha Release of LES Code
 B Beta Release of LES Code
 C Final Commercial Release of LES Code

Planned
 Performed

APPENDIX B — FUTURE PLANS

During the next quarter, the following work is planned:

1. Optimize and refine ISAT for large chemical mechanisms (> 19 species).
2. Continue validation of LES code for predicting emissions and instability in selected cases from industrial consortium.
3. Develop, implement, and test turbulent artificial neural net on lean premixed SimVal combustor test case.

APPENDIX C — GEORGIA TECH ATTACHMENT

LES of Premixed Combustion in the DOE-HAT Combustor

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Abstract

The present effort is to simulate and predict the pollutant emission in the so-called DOE-HAT combustor. The simulation are carried using Large-Eddy Simulation (LES) under the axisymmetric conditions but with correcting terms that take into account the azimuthal component. Hence, this approach resolves the swirl motion, albeit in an axisymmetric assumption. The pollutants tracked are the carbon monoxide (CO) and Unburnt Hydrocarbons (UHC). A flamelet approach and a library obtained from the CHEMKIN program are used in order to treat the chemical mechanisms (laminar flame speed, the pollutants reaction rates, etc.). The flame is tracked using the G-equation model. Preliminary emission predictions are carried for different equivalence ratio.

1 Introduction

Recent more stringent emission regulations have pushed for the development of more fuel efficient and low- NO_x gas turbine systems. However, design studies of new devices will require accurate prediction of emissions (CO , NO and UHC) as a function of the operating conditions. Recent measurements in a full-scale combustor (denoted DOE-HAT hereafter) [Bhargava et al.,

2000] showed that, as the equivalence ratio is decreased, the *CO* emission first decreases and then, suddenly increases exponentially. In the present effort, a new LES model is being developed to study this problem with the goal of predicting the emission from typical gas turbine combustors. The DOE-HAT combustor data is being used for the present effort as a baseline problem to demonstrate the new technology.

We will first describe the swirl correction method then describe the method used to predict the *CO* and *UHC* rate of formation. Results will then be presented and discussed.

2 Geometry - Operating Conditions

The geometry of the combustor is shown on figure 1. The grid resolution is 250x80. The length of the combustor is 60 cm, its radius is 5.3 cm. The inlet is located between 1.73 cm and 3.14 cm from the centerline. The length of the combustor was chosen such that emissions prediction can be performed at 38.1 cm (15 in).

The inflow characteristics chosen for the present study are: a temperature of 533K, a pressure of 13.78 atm. (200 psi), a mean inflow velocity of 68.6 m.s⁻¹. Different equivalence ratio in a range going from 0.52 to 0.70 are used. A random turbulent field is added to the inflow mean velocity and a subgrid turbulence intensity of around 7 percent is used to initialize the subgrid kinetic energy. The fuel considered is methane (*CH*₄).

3 Simulation Model

The simulation model is based on the LES model for a fully compressible flow. The filtered LES equations contain terms that represent the effects of the unresolved scales on the resolved motion. These unresolved subgrid terms in the momentum and energy transport are modelled using a transport equation for the subgrid kinetic energy. A second-order accurate numerical scheme is used and the constants used by the LES model are constant at this time. We also have a scheme fourth-order-accurate spatial scheme and a dynamic approach to compute the LES model coefficients. We plant o use this version later on once the current preliminary implementation and validation effort is completed.

3.1 Swirl Correction

The advantage of using an axisymmetric configuration to simulate the reacting flow in the DOE combustor is to dramatically reduce the computation cost and time in the initial development phase. Eventually, we plan to redo all these calculations using the full 3D LES model once the model issues are resolved. However, since the flow of interest is swirling, some corrections have to be made in order to take the swirl effects into account. We therefore employ the full 3D compressible equations but with all azimuthal variations neglected (this is sometimes called the 2.5D approach as opposed to the 2D or 3D approach). Thus, all three velocity components are simulated except that all properties are axisymmetric. In this approach, no azimuthal instability is allowed but on the other hand, effect of swirl on streamwise vortex breakdown and spreading is captured reasonably well.

3.2 Flamelet Approach

The basic idea of flamelet modelling is to treat locally the turbulent flame surface as a laminar flame surface, i.e., we consider that the flame structure can be decomposed into a succession of laminar flame elements. This approach is valid when the flame thickness is smaller than the Kolmogorov scale (high Damkoeler number). The main purpose in considering the flame structure as a laminar flame wrinkled by turbulent eddies is that laminar flame properties can be easily computed using programs like CHEMKIN ([Kee et al., 1992]).

The main parameter for the chemistry processes is the mixture fraction $\tilde{Z}$ (the symbol $\tilde{\cdot}$ represents the LES resolved variables). In order to take into account the influence of the subgrid turbulence upon the mixture fraction, the variance of the mixture $\widetilde{Z''^2}$ is used (in the LES approach, a variable ϕ is decomposed as the sum of the resolved variable $\tilde{\phi}$ and the subgrid variable ϕ'' , thus $\phi = \tilde{\phi} + \phi''$). These two parameters are chosen because CHEMKIN can deliver flame characteristics (Laminar diffusion speed, pollutants formation, etc...) as a function of $\tilde{Z}$ and $\widetilde{Z''^2}$.

Once filtered using the LES spatial filter, the mixture fraction governing equation is closed using a turbulent eddy diffusion assumption to take into account the turbulent convection mechanism at the subgrid scale.

The variance of the mixture fraction is described by N. Peters ([Peters, 2000]) and, once filtered, has the following form:

$$\bar{\rho} \frac{\partial \widetilde{Z''^2}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \widetilde{Z''^2} = -\nabla \cdot (\bar{\rho} \mathbf{v}'' \widetilde{Z''^2}) + 2\bar{\rho} D_t(\nabla \tilde{Z}) - 2\bar{\rho} D \nabla \widetilde{Z''^2} \quad (1)$$

The left hand side is the material derivative of the variance of the mixture fraction. The first term of the right hand side represents the mixing by turbulent convection at the subgrid scale, the second term is a source term taking into account the effect of the gradient of the mixture fraction on the variance of the mixture fraction and the third term represents the mean scalar dissipation rate (χ). The mixing by convection at the subgrid scale is, again, modelled using a gradient diffusion assumption. The scalar dissipation rate is modelled as follow:

$$\tilde{\chi} = 2D \nabla \widetilde{Z''^2} = 2 \frac{\tilde{\epsilon}}{\tilde{k}_{sgs}} \widetilde{Z''^2} \quad (2)$$

3.3 Flame Propagation Speed

The laminar flame speed is obtained from the CHEMKIN library. The effect of thermal expansion, flame curvature and strain can be taken into account in this approach. If S_{fl} is the laminar flame speed with respect to the unburnt gas, the effective flame speed S_L is:

$$S_L = S_{fl} \frac{\rho_u}{\rho} \quad (3)$$

where ρ_u is the unburnt gas density and ρ is the actual gas density. The effect of curvature and strain upon the laminar flame speed is modelled as follow:

$$S_c = S_{fl} - S_{fl} L \kappa - L S \quad (4)$$

where S_c is the corrected flame speed, L is the Markstein length, which is set to be equal to the flame thickness and κ is the flame curvature ($\kappa = \nabla \cdot \mathbf{n}$ and $\mathbf{n} = -\frac{\nabla G}{|\nabla G|}$), and S is the strain rate ($S = -\mathbf{n} \cdot \nabla \mathbf{u} \cdot \mathbf{n}$).

We should also take into account the effect of turbulence on the flame speed. Pocheau's Model is used ([Pocheau, 1992]) in the present study to compute the turbulent flame speed as a function of the laminar flame speed and the turbulence level u' . It should be noted that the turbulent flame speed S_t is a function of the ratio of the turbulence level (u') over the laminar flame

speed, S_L . Thus, when the laminar flame speed goes to zero, the turbulent flame speed goes to infinity. To avoid this problem, the value of (u'/S_L) is bounded by a maximum value. This implies that when S_L goes to zero, S_t goes to zero also.

3.4 Heat release

The product temperature T_p is a function of Z and Z''^2 and is computed by the CHEMKIN program. Because we track the energy as a conserved scalar, we defined the amount of chemical energy (E_c) that will be released during the chemical reaction by:

$$E_c = C_p(T_p - T_{ref}) \quad (5)$$

If (F_b) is the fraction of burnt product, the amount of chemical energy released (E_r) is:

$$E_r = F_b C_p(T_p - T_{ref}) \quad (6)$$

Thus, the temperature obtained from CHEMKIN is not used to set the temperature of the post flame region. This temperature just allows us to compute the amount of chemical energy that will be released by the reaction and thus transformed into thermal energy.

3.5 Flame description - G-equation approach

To track the flame without using finite-rate kinetics, a flame front tracking model is employed. In this approach, the flame front is tracked as a infinitely thin surface that is convected by the flow and also propagates normal to itself at a characteristic flame speed S_f . In laminar flow, $S_f = S_L$, where S_L is the laminar flame speed, which contains within it all the thermochemical state of the fuel-air mixture. For a given equivalence ratio, S_L is well defined. However, in turbulent flow, the turbulent flame speed S_T is still required to be modelled. Typically, $S_T = S_T(u', S_L)$, where u' is subgrid turbulence intensity. In the present study, a model employed in our past studies for gas turbine simulations [Kim et al., 1999, Kim and Menon, 2000] is used to obtain the turbulent flame speed as a function of u' (which is obtained using the subgrid kinetic energy, k^{sgs}) and S_L .

The mathematical model for the flame front considers a progress variable G which is governed by a transport equation which in the LES model is of the following form:

$$\frac{\partial \rho G}{\partial t} + \frac{\partial \rho G u_i}{\partial x_i} = -\rho_0 S_T |\nabla G| - \rho_0 D_G |\nabla G| \quad (7)$$

Here, ρ_0 is the reference density in the reactant mixture and ρ is the LES filtered density. Also, G and u_i are respectively, the LES-resolved progress variable and flow velocity. The last term represents a closure of the convective subgrid flux related to the LES filtering. It is modelled using a gradient diffusion at the resolved scale and D_G is the effective subgrid diffusion which is obtained using the subgrid eddy viscosity model (which is also used for the momentum transport closure) and using a turbulent Schmidt number of unity. Further details are in the cited references.

Note that in the present implementation, the LES-resolved variable G can range from 0 to 1 and represents a measure of the flame brush thickness. This is in contrast to the original "laminar" interpretation of the G field where $G = 0$ denotes burned product and $G = 1$ denotes reactants and the flame is an infinitely thin interface between $G = 0$ and $G = 1$. In the LES implementation, the filtered G represents the resolved flame brush which is an average location of the instantaneous thin flames.

3.6 Unburnt Hydrocarbons (UHC) Emission Prediction

UHC is formed at the flame front due to an incomplete consumption of the fuel through the flame front. At high temperature, UHC will be oxidized due to the presence of oxygen (because the DOE-HAT combustor uses the lean premixed technology, oxygen is present in the post flame region).

In typical gas turbines engines, turbulence controlled flame are unlikely to produce UHC except in localized regions where flame quenching is a result of aerodynamic stretch. The model we adopted in this study was the one developed by Meneveau and Poinso ([Meneveau and Poinso, 1991]) and is known as the Intermediate Turbulent Net Flame Stretch Model. In this model we assume that the interaction between the flame front and the eddies is equal to the sum of the interactions of the flame front and all eddies considered separately, i.e., the non-linear effects are not taken into account. This method will output the fraction of the flame that is quenched due to aerodynamic stretch.

The rate of production of UHC will be proportional to the fraction of the flame surface that is quenched (P_Q), the fuel mole fraction (Y_F) and the rate of flame crossing ($S_T | \nabla G |$) ([Held and Mongia, 1998],[Held et al., 2001]). To summarize, the rate of formation of UHC is:

$$\dot{w}_{UHC} = P_Q S_T | \nabla G | Y_F \quad (8)$$

The so-formed *UHC* will then be oxidized in the post-flame region. This oxidation - or re-ignition - will depend upon the oxygen concentration and the rate of oxidation. The oxygen mole fraction is easily determined using the mixture fraction. The rate of oxidation will be controlled either by mixing processes (related to the flow behavior) or by chemical processes. The mixing time scale (τ_{mix}) is proportional to the ratio of the turbulent kinetic energy over the dissipation rate. The chemical time scale (τ_{chem}) depends upon the oxygen concentration, the activation energy and the temperature of the burnt products. More precisely:

$$\tau_{mix} = \frac{k_{sgs}}{\epsilon} \quad (9)$$

$$\tau_{chem} = 6.25 \times 10^{-16} [O_2]^{-1} \exp(23000/T) \quad (10)$$

The time scale controlling the *UHC* oxidation will be the larger of the two time scales previously described. One assumption is that the oxidation of the unburnt *UHC* will be oxidize in *CO* only.

3.7 CO Emission Prediction

CO is formed by three major mechanisms. The first mechanism is the formation of *CO* at the flame front. The second one is the *CO* formed by oxidation of unburned *CH₄* described above. The third mechanism is the *CO₂* dissociation. The CHEMKIN program allows us to determine the fraction of *CO* formed at the front flame as a function of the mixture fraction and the variance of the mixture fraction. The formation of *CO* at the flame front is treated as a jump relationship, i.e. *CO* is produced as fuel (represented using the G-variable) is consumed ([Held and Mongia, 1998],[Held et al., 2001]). Thus, the production across the flame will depend on the fraction of *CO* formed at the flame front and the rate of flame crossing. To summarize, we have:

$$\dot{w}_{CO_{ff}} = S_T | \nabla G | Y_{CO_{ff}} \quad (11)$$

Typically, the flame front formation lies, in terms of mass fraction, between 1 and 3 percent. Once this CO is formed, it will be oxidized. The CHEMKIN program allows us to determine the oxidation time scale as well as the equilibrium mass fraction of CO as a function of Z and Z''^2 . In a well designed combustion chamber the majority of the CO formed at the flame front will be oxidized in the post flame region, and thus, the CO mass fraction at the combustion chamber outlet will be equal to the equilibrium value. The equilibrium value is defined as the CO mass fraction reached when the rate of CO consumption by oxidation equals the rate of CO production via CO_2 dissociation. Again, The CHEMKIN program allows us to determine the equilibrium mass fraction.

Regarding the CO production due to the UHC , one takes the rate of destruction of UHC as the rate of production of CO multiplied by a coefficient corresponding to the ratio of the carbon monoxide molecular mass to the UHC molecular mass (this is required because we are tracking the species mass fractions).

4 Results and Discussion

In the present study, a flamelet library that was developed originally for a GE LM6000 test configuration is employed without any modifications. The test conditions for the LM 6000 did NOT match the test conditions (especially inlet temperature and combustor pressure) of the DOE-HAT combustor. Therefore, no direct comparison with experimental data is carried out at this time. However, our present effort was to implement and evaluate this approach first and therefore, for this only qualitative analysis is sufficient (since the physics should not be drastically different when the combustor pressure is changed). We are currently re-creating a new flamelet library for the DOE-HAT operating conditions and will be revisiting these calculations soon.

4.1 UHC emission prediction

The mass fraction of UHC for various equivalence ratio is shown on figure 2. The mass fraction increases dramatically when the equivalence ratio ap-

proaches the lean blow out equivalence ratio. This observation is consistent with observations made in the experiments. This shows that the occurrence of the quenching of the flame strongly depends upon the flame propagation speed. We know that, in the post flame region, the unburned fuel will be oxidized into CO . Thus, the more the equivalence ratio approaches the lean blow out equivalence ratio, the more UHC is produced in the post flame region.

4.2 CO emission prediction

4.2.1 Post Flame CO

To focus only on the CO production in the post flame region, we did not take into account the oxidation mechanism in the post flame region. We are only tracking the CO formed by the fuel consumption in the flame region. Results are shown on Fig. 3. The smaller the equivalence ratio, the smaller the CO mass fraction produced at the flame front.

4.2.2 CO Production in the Post Flame Region

CO is produced in the post flame region if UHC is produced in the flame region. This oxidation of unburnt fuel is clearly shown in Fig. 4. (Note that the data is taken from a field averaged in time, and along a line parallel to the centerline and located at 2.7 cm from the centerline). Figure 4 shows the CO mass fraction produced by the unburnt fuels, the UHC mass fraction and the flame location (i.e. the G-field). Note that, CO oxidation in the post flame region was again not taken into account in this case. In the flame zone (where G lies between 0 and 1), UHC is produced due to quenching of the flame caused by aerodynamic stretch. A short distance after UHC starts to be produced, CO is produced due to the oxidation of unburnt CH_4 . UHC is produced until $G = 0$ (i.e., until the post flame region is reached). Then, UHC is oxidized in the post flame region (i.e., as the axial location increases). The decrease of the UHC mass fraction corresponds to an increase of the CO mass fraction. Thus, the CO produced in the post flame region should follow the trend of the UHC production as far as the dependance via the equivalence ratio is concerned (i.e., the more UHC is produced at the flame front, the more CO is produced in the post flame region). This production is important for very lean mixtures and negligible once the equivalence ratio

is not in the vicinity of the lean blow out equivalence ratio.

In order to analyze how the formation of CO via the oxidation of UHC influences the emission prediction, we simulate cases with and without taking this source of carbon monoxide into account (i.e., simulations are performed taking the oxidation of CO and dissociation of CO_2 into account). For the test without the CO source from the oxidation of UHC , the predicted CO at 15 inches from the combustion chamber inlet is 23.6 ppm whereas, it is 47.6 ppm when we take UHC oxidation into account. This test was with an equivalence ratio of 0.548, i.e., in conditions where the production of UHC by quenching is not negligible. Results from the simulation described above are shown in Fig. 5. This shows that the amount of CO produced reaches the equilibrium value faster when the CO source from UHC oxidation is neglected. This proves that the amount of CO produced by the oxidation of UHC does not have time to be oxidized before reaching the emission probe placed at 15 inches from the inlet.

Further, we looked at the influence of the equivalence ratio on the CO emission once when taking into account the CO produced by the oxidation of the unburnt fuel. These tests were performed without taking into account both the oxidation of the carbon monoxide in the post flame region and the dissociation of the carbon dioxide. Results are shown in Fig. 6. Again, as we reach an equivalence ratio close to the lean blow-out equivalence ratio, the mass fraction of CO increases dramatically. Results shown in Fig. 6 are in good agreement with results shown in Fig. 2, i.e., the amount of UHC produced at the flame front strongly influences CO emission production at the location of the emission probe.

in Fig. 7 we plot the CO mass fraction prediction produced at the front flame only, the CO mass fraction prediction produced by the oxidation of the unburnt fuel only and the CO mass fraction prediction produced by both these mechanisms. In this case, only CO production was taken into account, i.e., CO oxidation in the post flame region was neglected. If we take the bigger equivalence ratio as a starting point, the amount of CO present at the probe location is decreasing when the equivalence ratio decreases. The CO emission is directly related to the production of CO at the front flame. Because we did not take the CO oxidation into account, the CO production at the flame front increases with the equivalence ratio. When we continue to decrease the equivalence ratio, the mass fraction of CO increases rapidly. This increase is directly related to the increase in CO production via the oxidation of unburnt fuel. Once unburnt fuel is produced, the smaller the

equivalence ratio, the bigger the amount of UHC released by the flame, the bigger the CO produced by the oxidation of UHC . To summarize, for equivalence ratio bigger than a critical value, the front flame production is dominant. For equivalence ratio smaller than a critical value, the CO production from UHC is dominant.

The other source of the formation of CO in the post flame region is the dissociation of CO_2 . Figure 8 shows the equilibrium value (CO equilibrium value was defined in section 3.7) predicted by CHEMKIN. As expected, larger the equivalence ratio, larger the rate of CO production via dissociation of CO_2 . This is due to the fact that at larger equivalence ratio, the burnt gas temperature is also higher and thus, the amount of molecule dissociation is larger.

4.2.3 CO Oxidation in the Post Flame Region

In the post flame region carbon monoxide will be oxidized due to the high temperature of the burnt gases and the presence of oxygen. We performed one simulation taking into account only the CO produced at the flame front, in the second simulation we added the oxidation mechanism of the carbon monoxide. CO mass fractions are plotted in Fig. 9 (the flame location, i.e., the value of G is also plotted). As the fuel is burnt through the flame, CO is produced. In the post flame region CO is oxidized and this mechanism works against the CO formation. This is not the case in the simulation where we neglected the CO oxidation. Furthermore, when the oxidation process is neglected, the CO mass fraction is constant as the axial location increases. If we take the oxidation into account, the CO mass fraction decreases until it reaches its equilibrium value. This figure also proves that the oxidation process can not be neglected. By neglecting it, the CO oxidation will be over predicted by a factor larger than 1000.

4.2.4 Equilibrium CO - CO_2 dissociation

In the post flame region CO is consumed due to the oxidation with the remaining oxygen and is produced via CO_2 dissociation. Once the rate of oxidation equal the rate of production, one can assume that the carbon monoxide has reached the equilibrium value. This value is computed by the CHEMKIN program. In Fig. 10 we plot the CO emission prediction and the value of the CO equilibrium vs. equivalence ratio. We notice that for an

equivalence ratio larger than 0.58, the amount of CO at the measurement probe equals the mass of equilibrium CO computed by CHEMKIN. This means that, for these equivalence ratio, the CO produced at the flame front is totally oxidized before reaching the emission probe (for $\Phi > 0.58$, there is no UHC production and thus, no CO source from UHC oxidation). Thus, for equivalence ratio larger than a certain value, the emissions of CO are determined by the amount of CO at equilibrium.

4.3 Lean Blow Out (LBO) phenomena

LBO phenomena is the name we use to describe the phenomena of the large increase in CO emission once we reach the vicinity of the lean blowout equivalence ratio limit. From the simulations we performed so far, we observe that this phenomena is directly related to the production of CO via unburnt fuel oxidation. The residence time of the burnt gases inside the combustion chamber is large enough to allow oxidation of the UHC in CO . But once this oxidation is done, the remaining time is not large enough to allow the CO formed to be oxidized in CO_2 . Thus controlling or damping the rapid increase in CO production in the vicinity of the blow out equivalence ratio will require the control or damping of the formation of unburnt gases at the flame front, i.e., flame quenching has to be reduced.

This is also shown in Figs. 11 and 12. Both figures represent the unburnt fuel and carbon monoxide mass fraction vs. the axial location in the combustor. Figure 11 corresponds to an equivalence ratio where aerodynamic stretch is an important phenomena. Figure 12 corresponds to an equivalence ratio where aerodynamic stretch is not an important phenomena. Both CO curves peak at the same location and at approximately the same value. This is due to the CO formation at the flame front. After this concentration peak, the CO mass fraction decreases faster for the case where aerodynamic quenching of the flame is a negligible phenomena. In the case described in Fig. 12, the UHC production is limited, and thus the decrease of CO mass fraction is governed only by the oxidation of CO . In the other case, if CO is still oxidized, CO is also formed due to the oxidation of the unburnt fuel. Thus, the net rate of CO mass fraction decrease is slower.

5 Summary and Future Plans

In the range of equivalence ratio that we studied, we can define a critical equivalence ratio Φ_{CR} corresponding to the equivalence ratio where the CO emission reaches a minimum.

For $\Phi \gg \Phi_{CR}$, the carbon monoxide formed at the flame front is entirely oxidized before reaching the emission probe. No UHC is produced via flame quenching, thus no CO is produced due to UHC oxidation. The emission of CO is entirely controlled by its equilibrium value (see Fig. 10).

For $\Phi \ll \Phi_{CR}$, a large amount of UHC is formed via flame quenching. This unburnt fuel is then oxidized into CO in the post flame region. The combustor residence time is smaller than the time required for the oxidation of the CO formed via UHC oxidation. Therefore, CO emission is controlled by flame quenching (i.e. UHC production) and not by the value of CO at equilibrium.

This study allowed us to get a better understanding of the carbon monoxide production as well as the mechanism leading to an exponential increase in the CO emission once we reach the lean flammability limit. The dominant mechanism, for equivalence ratio not located in the vicinity of the lean blow out limit, is the CO equilibrium process. When the equivalence ratio is close to the lean flammability limit, the mechanism controlling the CO emission is the flame quenching that produces unburnt fuels.

In the near future, the new flamelet libraries for the test conditions of the DOE-HAT will be generated and these simulations will be repeated for the DOE-HAT operating conditions. Results will be compared to the results presented in ([Bhargava et al., 2000]). Finally, once all the modeling issues are resolved, we will revisit these studies using the full 3D LES.

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Figure 1: The DOE-HAT combustor dimension.

Figure 2: UHC emission prediction (ppm) vs. equivalence ratio.

Figure 3: CO emission from the flame front (ppm).

Figure 4: CO mass fraction from UHC oxidation and UHC mass fraction vs. axial location.

Figure 5: CO emission prediction (ppm).

Figure 6: CO emission from the UHC oxidation (ppm).

Figure 7: CO emission from both the UHC oxidation and the flame front (ppm).

Figure 8: CO at equilibrium from CO_2 dissociation (Data from Chemkin) .

Figure 9: CO mass fraction with and without post flame oxidation vs. axial location.

Figure 10: CO mass fraction prediction and value of CO at equilibrium.

Figure 11: CO and UHC mass fraction vs. axial location. High occurrence of flame quenching .

Figure 12: CO and UHC mass fraction vs. axial location. Low occurrence of flame quenching .