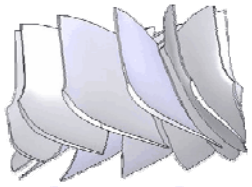

Multiprocessor Simulation of Turbulent Diffusion Flames

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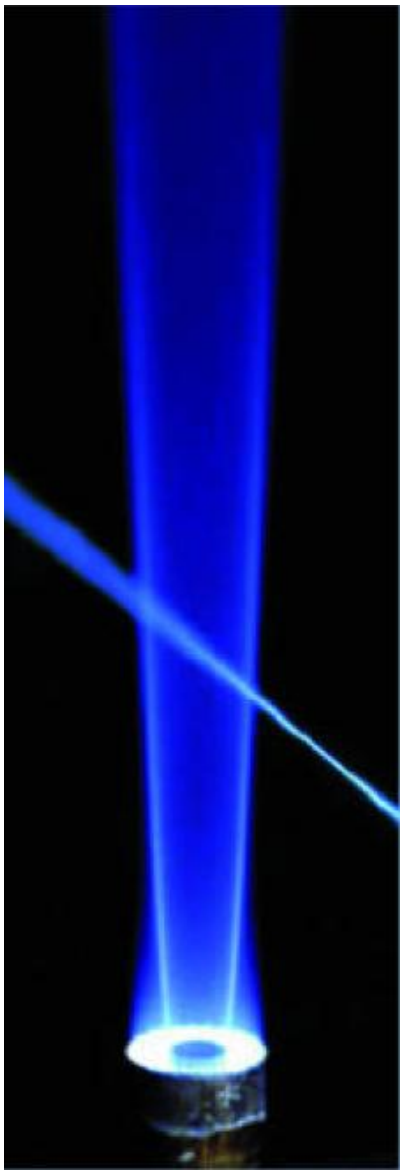


Computational combustion is the most difficult and most complex area of Computational Fluid Dynamics (CFD) due to tight interaction between phenomena of different nature: turbulence, chemistry and radiation. On the other hand this area is very important in engineering applications and industry like modelling furnaces, engines, turbines and predicting prejudice from fires.

In addition, there is a wide spectrum of powerful commercial software that is capable of solving such problems and multiprocessor computers that allow these problems to be solved very efficiently.

In this context the problem of accurate modelling of real-life problems using commercial software arises. All computational experiments must be carried out on model problem that satisfies the requirements of detailed statement and experimental data. As much physical models as possible should be validated on this problem starting from conventional engineering models and finishing with advanced state-of-the-art models.

After these validating simulations it would be possible to proceed to complex chemistry modelling like pollutant emissions.

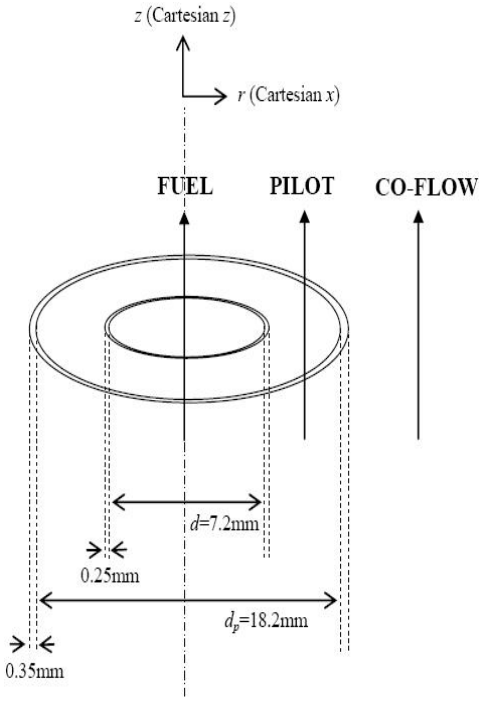
1 Problem Statement

1.1 Object of research

Sandia Piloted Flame D from Sandia National Laboratories (California, USA) was chosen as a model problem (model flame). This flame satisfies two requirements of detailed problem statement and verbose experimental data of mean and root-mean-square profiles of temperature, velocity components and concentrations of 9 major species through axial and 8 radial profiles.

Flame D is a jet flame with pilot-stabilizer and premixed methane-air mixture. This configuration allows to highly reducing pollutant formation and flame extinction and to obtaining accurate experimental measurements. Despite mixture premixing this flame can be treated as non-premixed one due to the fact that mixture ratio is situated above upper flammability limit, so that chemistry reactions won't occur. Finally, this flame expected to have fully developed turbulence due to Reynolds number based on speed (Re = 22400).

1.2 Computational Statement



The computational domain is modelled as an inverted and truncated cone. The lower cone base diameter is *6d* and the burner is located in the centre of this base. The greater cone base diameter is *38d*, and the truncated cone height is *80d*.

The mean mass-weighed velocity magnitude of the fuel is 49.6 m/s, of the pilot bulk – 11.4 m/s and of surrounding co-flow – 0.9 m/s. The temperatures are 294, 1880 and 291 K for main jet, pilot bulk and co-flow correspondingly. The composition of fuel is 25% CH4 and 75% air by volume, co-flow is 100% air and the pilot composition is obtained from experimental data.

2 Physical models

Navier-Stokes equations for multi-component reacting medium are used for combustion problems. It includes filtered momentum, species (of mixture fraction) and enthalpy transport equations and continuity equation:

$$\begin{cases} \dfrac{\partial \overline{\rho}}{\partial t} + \dfrac{\partial \overline{\rho}\widetilde{u}_j}{\partial x_j} = 0 \\ \dfrac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \dfrac{\partial \overline{\rho}\widetilde{u}_j\widetilde{u}_i}{\partial x_j} = -\dfrac{\partial \overline{\rho}\,\widetilde{u_j''u_i''}}{\partial x_j} - \dfrac{\partial \overline{P}}{\partial x_j} - \dfrac{\partial \overline{\tau}_{ij}}{\partial x_j} + \overline{\rho} g_i \\ \dfrac{\partial \overline{\rho}\widetilde{Y}_\alpha}{\partial t} + \dfrac{\partial \overline{\rho}\widetilde{u}_j\widetilde{Y}_\alpha}{\partial x_j} = -\dfrac{\partial \overline{\rho}\,\widetilde{u_j''Y_\alpha''}}{\partial x_j} - \dfrac{\partial \overline{F}_{j,\alpha}}{\partial x_j} + \overline{\dot{r}_\alpha} \\ \dfrac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \dfrac{\partial \overline{\rho}\widetilde{u}_j\widetilde{h}}{\partial x_j} = \dfrac{\partial \overline{P}}{\partial t} - \dfrac{\partial \overline{\rho}\,\widetilde{u_j''h''}}{\partial x_j} - \dfrac{\partial}{\partial x_j}\left(\overline{F}_{j,h} + \overline{u_i\tau_{ij}}\right) - \dfrac{\partial \overline{q_j^r}}{\partial x_j} + \overline{\rho u_i} g_i \end{cases}$$

Some terms are unclosed and have to be modeled. We used *k*-*ε*, *k*-*ω* and Reynolds stress turbulent model families (Reynolds-Favre Averaged Navier-Stokes models, RANS) and Large Eddy Simulation model (LES) to model turbulence. Chemistry was modeled with Eddy Break-up model family (EBU) and Mixture-fraction-based statistical model family (PDF). Radiation impact wasn't investigated but it was modeled with Discrete Transfer (DTRM) and Discrete Ordinates (DO) radiation models.

Additional transport equations for turbulence parameters were introduces in Navier-Stokes equations in RANS turbulence approach. When using LES turbulence model only subgrid viscosity needs to be modeled and we used Smagorinsky subgrid model.

Eddy Break-up model defined mean reaction rate explicitly assuming fast chemistry and slow turbulence and defining characteristic reaction time scale through turbulence scale. This is the main defect of this model, since the flame front is very thin and grid is unable to resolve it. Despite this fact this model is widely used by engineers. Statistical model based on mixture fraction approach transpose this problem into 1D space, associated with flame front, where it can be resolved precisely. And mixture fraction acts like the fuel mass quantity variable (it is unity in fuel and zero in oxidizer). Different chemistry submodels can be applied under this model (e.g. equilibrium chemistry or flamelet model).

3 Test simulations

In this section simulation factors that impact the flame were considered. First, we tested the impact of domain dimensions and side boundary conditions were investigated. Conditions of undisturbed co-flow were set on cone sides. When we widen the base diameter of the cone in 1,5 times and set the same condition, a very slight discrepancy was observed, but computational time was much more higher. So this widening was considered unreasonable.

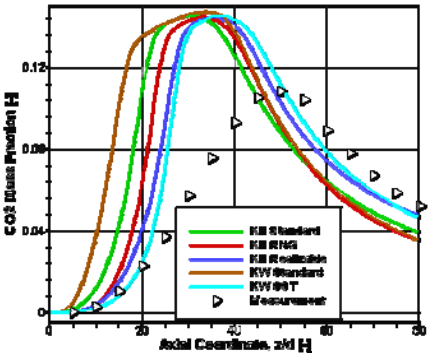
Second, we investigated inlet boundary velocity profile impact at flow entrance. Initially we used mass-weighed piecewise-linear profile, but we observed unphysical step near fuel entrance. This defect was corrected using experimental velocity boundary profile. Boundary profiles of other variables do not affect flame structure a lot.

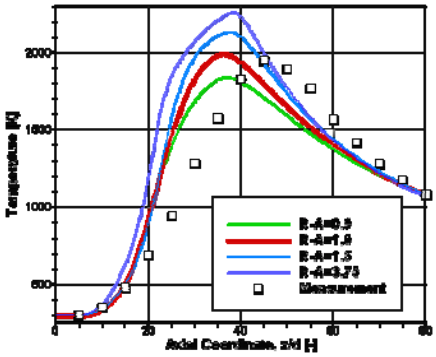
Third, we made test simulations with different order of approximation and determine that it does not make serious effect on the flame.

And finally, we investigated radiation impact on the flame. It was discovered that radiation consideration affects only temperature field by decreasing peak temperature by 100 K, other scalar fields do not seriously affected by radiation. Nevertheless, radiation was considered in all simulations.

4 Simulation results

4.1 Eddy Break-up chemistry model

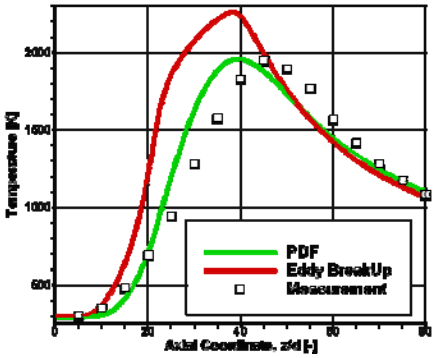




First of all, we investigated Eddy Break-up model on different turbulence models. The results were very disappointing: peak temperatures and peaks concentrations of main reaction products were greatly overestimated by 300 K and by 15-40% correspondingly. In addition, flame was significantly smaller and wider, than in experiment (left figure).

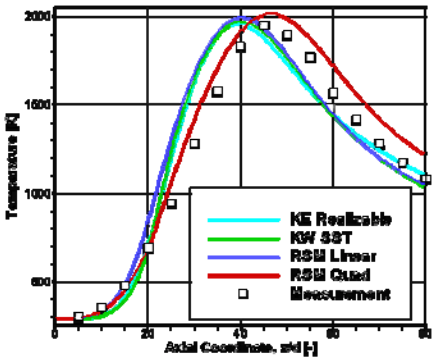
We decided to improve this model and to select satisfying constant in reaction rate expression. The default generally accepted constant value is 4,0, but we discovered that the optimal value for this task is 1,0 (right figure). This significant variation of the constant means poor model adaptability to different types of reacting flows.

4.2 Statistical chemistry model



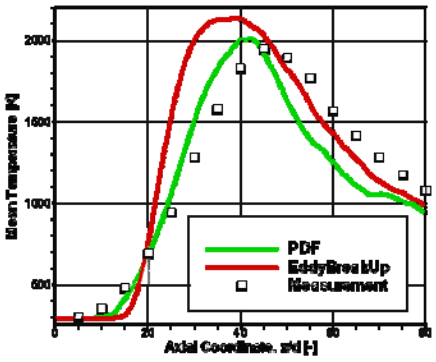
As simple chemistry model failed to accurately predict flame structure, more complex models were involved. Statistical model based on mixture fraction approach showed significantly more accurate flame prediction. Peak values of temperature and main reaction products are significantly improved. The flame became more narrow and long than in EBU predictions, but still is smaller and wider (left figure).

4.3 Turbulence comparison



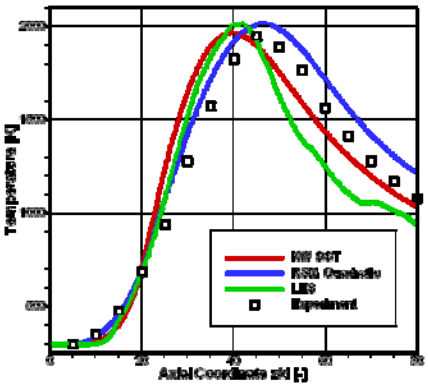
Then we decided to compare turbulence models on the statistical chemistry model. Standard *k-ε*, *k-ω* and *k-ε RNG* models predictions were unsatisfactory. Best models among turbulence models with two additional equations for turbulence parameters were *k-ε Realizable* and *k-ω SST*. The most accurate *RANS* turbulent model is Quadratic Reynolds Stress model (left figure).

4.4 Large eddy simulation



Large eddy simulation enables explicitly resolve energy-bearing long-wave part of vortex spectrum through a very high computational cost. It allows obtaining instant, mean and root-mean-square characteristics; in addition, it allows observing vortex development.

The same chemistry models were validated on Large Eddy Simulation model and results were quite the same (left figure).



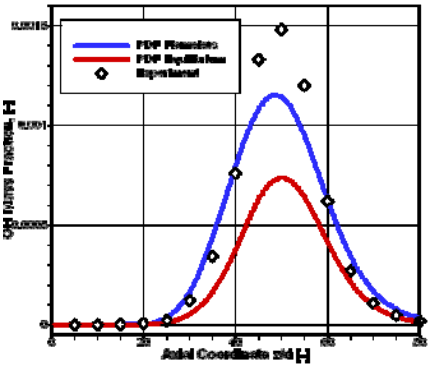
The Statistical chemistry model showed better results than Eddy Break-up model, but it is necessary to underline that peak values were not so greatly overestimated. This is due to different time scale used in reaction rate for LES than for RANS, for LES it is based on strain-rate tensor.

In comparison to the RANS turbulence models LES showed good accuracy and is inferior only to the most complicated model – Quadratic Reynolds Stress model.

We used the simplest Smagorinski subgrid viscosity model; we did not generate perturbations according to turbulence parameters at flow entrance into the domain and still Large Eddy Simulation model shows good prediction of flame shape (upper figure). Second order statistics was in good agreement with experimental data.

4.5 Laminar flamelet chemistry model

Laminar flamelet model is a submodel for the statistical chemistry model that allows including slow chemistry reactions and detailed chemistry mechanisms. Two different mechanisms were investigated in this model: test and complicated mechanisms. Flamelet is a non-averaged dependence of temperature, density and species concentrations of mixture fraction for certain value of scalar dissipation. This variable characterises the disturbance of velocity field, the more disturb flow field is the further chemistry reactions are from equilibrium conditions. Scalar dissipation variation does not seriously affect temperature and major species profiles but seriously influence on intermediate species. That's why this model is capable of pollutant predictions.



First calculations with this model showed very significant improvement (figure left) for intermediate species predictions. In addition, flow, scalar and major species fields are quite the same as in equilibrium chemistry. This model seems to be promising and further investigation will be performed.

5 Computational efficincy

5.1 Model efficiency

We tested efficiency of different turbulence and chemistry models. Eddy Break-up models family is significantly faster than Statistical models family in chemistry models comparison. Along turbulence models more accurate turbulence model require more computational time. All three mentioned accurate turbulence models require quite the same computational time. The general conclusion is the more accurate results you want to obtain the more computational time you have to spend.

5.2 Cluster efficiency

We made all Large Eddy Simulations on two clusters of Laboratory of Applied Mathematics and Mechanics. Technical characteristics of these clusters you can observe in the presentation. These clusters are controlled by different operating systems: Linux SUSE and Windows CCS. The comparison showed that these operating systems have equal paralleling efficiency in this type of simulations.

Cluster **ε** does not have sufficient enough capabilities for Large Eddy Simulation, so cluster **λ** was used for these simulations. Each Large Eddy Simulation took 5 weeks on 48 cores on that cluster.

6 Conclusions

First of all it is very important that simple conventional turbulence and chemistry models usage leads to severe errors in turbulent flame simulations. That's why it is recommended to use Statistical Chemistry model with Equilibrium or Detailed chemistry mechanisms that significantly excels Eddy Break-up model. If it is needed to make steady RANS calculations it is preferable to use *RSM Quadratic*, *k-ε Realizable* and *k-ω SST* turbulence models. If it is desirable to obtain detailed computational data, instant scalar peak, observe chemistry dynamics and large computational resources are available then it is preferable to use Large Eddy Simulation model.

Future work is planned to be spend on detailed research of flamelet chemistry models and reaction mechanisms. And finally to investigate accurate pollutant emission models.