北京航空航天大學
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Numerical simulation on gas combustion and spray flames

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能源与动力工程学院
SCHOOL OF ENERGY AND POWER ENGINEERING

Beihang University

- It was established in 1952. Last year, it is the 60 anniversary！
- It comprises 27 schools, 17 academician and 3759 faculties. The enrollment is over 27800, including 14428 UG, 4015 Ph.D candidates, 668 oversea.

Ranking and the School

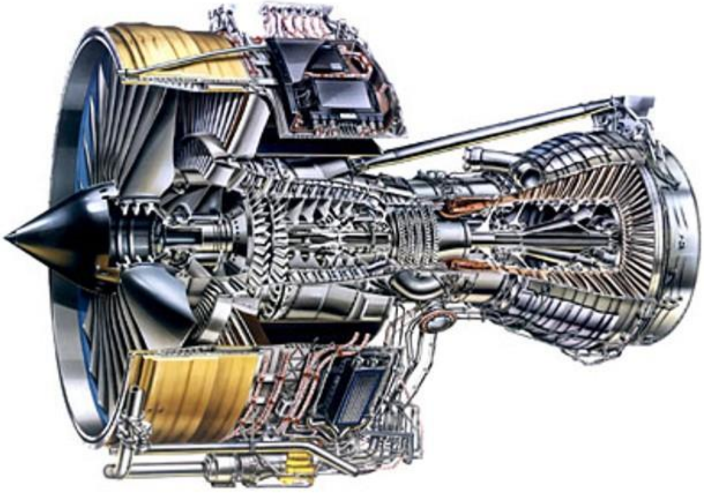
- General ranking: 7-15 in China;
- Aerospace propulsion Theory and Engineering, No.1, Power Engineering and Engineering Thermal Physics, No.7.
- Our school has four departments and one national key laboratory: Department of Aviation propulsion, Department of Fluid Machinery, Department of Engineering Thermophysics, Department of Thermal Engineering, The National Key Laboratory on Aero-Engines.

能源与动力工程学院
School of Jet Propulsion

Content

- Numerical simulation on
  - gas combustion : An algebraic sub-grid scale turbulent combustion model
  - spray flames : An droplet burning model

Gas turbine combustor



- Gas-liquid two phase turbulent combustion
- Droplets tracing, chemical kinetics, turbulent flow in complex geometry, turbulent reaction rate, radiation, …

Turbulent combustion rate

- **RANS, LES, DNS are the three strategies…**
- **Turbulent combustion rate is a big problem in combustion simulation, because of the exponential part.**

$$w_i = B\rho^2 Y_1 Y_2 \exp(-\frac{E}{RT})$$

- **The average reaction rate is not the function of the averaged value**
- **Couple with turbulence…another big problem**
- **Turbulent combustion models are needed for engineering applications.**

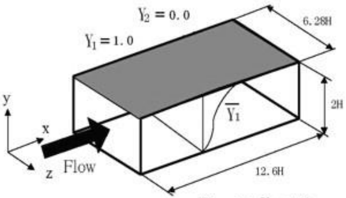
Backgroud – about SGS combustion model

- **Recently, Large eddy simulation (LES) is becoming used in engineering applications.**
- **For gas turbine combustion chambers, it is used to solve the flow topology, emission, compressor/turbine interaction, cooling, ...problems**
- **The sub-grid scale (SGS) combustion model is one of the key aspects of LES method.**
- **There are various SGS combustion models: the *laminar flamelet* model (Pitsch et al., Senoner et al. and Mattsson et al.), *assumed PDF* combustion model (Moin et al, James et al.), *linear eddy* model (Menon et al.), *EBU* model (Menon et al.), *PDF equation* model (James et al.), *Dynamically Thickened Flame* combustion model (Poinsot et al.) …**
- **The SGS turbulent combustion model is still in developing**

Backgroud - DNS verification and LES validation

- **As an important tool for fundamental studies, direct numerical simulation (DNS) attracted increasing interest in recent years.**
- **Attention is paid to finding detailed instantaneous flow and flame structures, understanding the turbulence/flame interaction (Poinsot et al. , Zhang and Rutland) and verifying RANS and LES models (Zhang and Rutland, Luo, Overholt and Pope, Bedat et al., Sreedhara and Huh, Hawkes and Chen, Chong and Heinz).**
- **So the SGS model should be better verified by DNS before applying to test cases. Thus, in this paper:**
  - **A direct numerical simulation of turbulent reacting channel flows, taking the buoyancy effects account, is performed using a spectral method, and the DNS database is used to verify the SGS combustion model**
  - **This SGS combustion model is tested using methane and *methanol-air* jet flame.**

DNS Governing Equations



$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] - F_i \quad F_y = -g\frac{T - T_w}{T_w}$$

$$\frac{\partial}{\partial t}(Y_i) + \frac{\partial}{\partial x_j}(u_j Y_i) = \frac{\partial}{\partial x_j}\left(D\frac{\partial Y_i}{\partial x_j}\right) - w_i / \rho \qquad i = 1,2$$

The buoyancy effect using Boussinesq approximation

$$\frac{\partial}{\partial t}(T) + \frac{\partial}{\partial x_j}(u_j T) = \frac{\partial}{\partial x_j}\left(\frac{\lambda}{c_p \rho}\frac{\partial T}{\partial x_j}\right) + w_1 Q_1 / (c_p \rho)$$

One-step Arrhenius chemical kinetics

$$w_i = B\rho^2 Y_1 Y_2 \exp\left(-\frac{E}{RT}\right)$$

Numerical Methods

- **Galerkin-Tau spectral expansion method: Fourier transform is used in x and z directions and the Chebyshev transform is used in the y direction;**
- **Uniform grid distribution is used in x and z directions and the Gauss-Lobatto nonuniform grid distribution is used in the y direction. 128×128×129 results in a total of 2.11 million nodes. The time step used is 0.01H/U_m with a third-order scheme.**
- **For all cases the mass fraction of species 1 (fuel) is given as 1.0 at the top wall and 0.0 at the bottom wall, whereas the mass fraction of species 2 (oxidizer) is given as 0.0 at the top wall and 1.0 at the bottom wall. The wall temperature is given as 900K.**
- **Periodic boundary conditions are used in the longitudinal and span-wise directions and solid-wall boundary conditions are used on the top and bottom boundaries.**

Parameters for DNS Cases

$$F_y = -g\frac{T - T_w}{T_w}$$

Case	B	E/R (K)	Q (kJ/kg)	F_y (m/s^2)
1	0	0	0	0
2	0.1	0	0	0
3	1.0	0	0	0
4	10^8	15000	100	0
5	10^8	20000	100	0
6	10^{10}	20000	100	0
7	10^8	20000	100	-0.5
8	10^8	15000	100	F_y
9	10^8	20000	100	F_y

$$\frac{\partial}{\partial t}(T) + \frac{\partial}{\partial x_j}(u_j T) = \frac{\partial}{\partial x_j}\left(\frac{\lambda}{c_p \rho}\frac{\partial T}{\partial x_j}\right) + w_1 Q_1 / (c_p \rho)$$

$$w_i = B\rho^2 Y_1 Y_2 \exp\left(-\frac{E}{RT}\right) = \rho^2 K Y_1 Y_2$$

LES Governing Equations

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho\widetilde{u}_i)=0$$

$$\frac{\partial}{\partial t}(\rho\widetilde{u}_i)+\frac{\partial}{\partial x_j}(\rho\widetilde{u}_i\widetilde{u}_j)=\frac{\partial}{\partial x_j}\left(\mu\frac{\partial\widetilde{u}_i}{\partial x_j}\right)-\frac{\partial\widetilde{P}}{\partial x_i}-\boxed{\frac{\partial\tau_{ij}}{\partial x_j}}$$

Smagorinsky-Lilly's eddy viscosity model

$$\tau_{ij}=-2\mu_t\widetilde{S}_{ij}+\frac{1}{3}\tau_{kk}\delta_{ij}$$

$$\frac{\partial\rho\widetilde{Y}_s}{\partial t}+\frac{\partial}{\partial x_j}(\rho\widetilde{u}_j\widetilde{Y}_s)=\frac{\partial}{\partial x_j}\left(\frac{\mu}{S_{Cs}}\frac{\partial\widetilde{Y}_s}{\partial x_j}\right)\boxed{-\widetilde{w}_s-w_{S,s}}-\frac{\partial g_{Sj,s}}{\partial x_j}$$

$$\frac{\partial\rho\widetilde{h}}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho\widetilde{u}_j\widetilde{h}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Pr}}\frac{\partial\widetilde{h}}{\partial x_j}\right)-\frac{\partial q_{Sj}}{\partial x_j}$$

The filtered reaction rate
and
the SGS reaction rate

$$g_{Sj,s}=\frac{\mu_t}{Sc_{t,s}}\frac{\partial\widetilde{Y}_s}{\partial X_j}\qquad q_{Sj}=\frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial\widetilde{T}}{\partial x_j}$$

ASSCM SGS Combustion Model

$$\frac{\partial\rho\widetilde{Y}_s}{\partial t}+\frac{\partial}{\partial x_j}(\rho\widetilde{u}_j\widetilde{Y}_s)=\frac{\partial}{\partial x_j}\left(\frac{\mu}{S_{Cs}}\frac{\partial\widetilde{Y}_s}{\partial x_j}\right)-\boxed{\widetilde{w}_s}-\boxed{w_{S,s}}-\frac{\partial g_{Sj,s}}{\partial x_j}$$

The filtered reaction rate

$$\widetilde{w}_s=\rho^2\widetilde{K}\widetilde{Y}_{OX}\widetilde{Y}_{Fu}$$

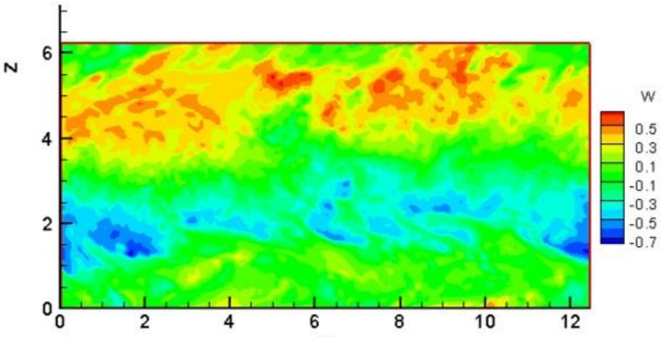
The SGS reaction rate

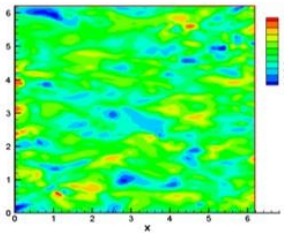
$$w_{S,s}=\rho^2[K(\widetilde{Y_{OX}Y_{FU}}-\widetilde{Y}_{OX}\widetilde{Y}_{Fu})+Y_{OX}(\widetilde{KY_{Fu}}-\widetilde{K}\widetilde{Y}_{Fu})+Y_{Fu}(\widetilde{KY_{OX}}-\widetilde{K}\widetilde{Y}_{OX})]$$

$$(\widetilde{KY_{OX}}-\widetilde{K}\widetilde{Y}_{OX})=C_{K,Y_{OX}}L_S^2\frac{\partial\widetilde{K}}{\partial x_j}\frac{\partial\widetilde{Y}_{OX}}{\partial x_j}$$

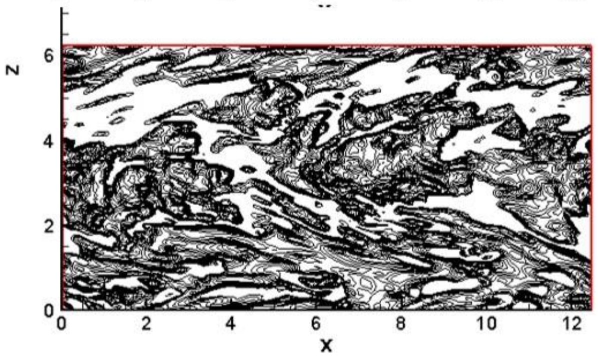
The constant C is 0.005

The DNS Instantaneous Results (1)



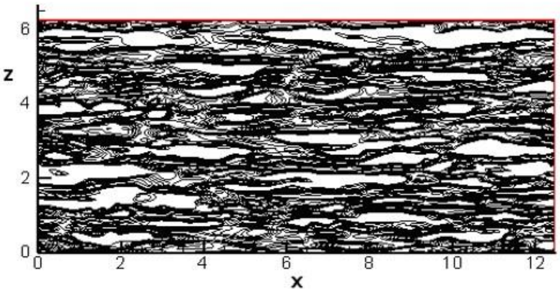


Instantaneous Longitudinal Velocity (case 8)



Instantaneous Concentration Fluctuation (case 8)

The DNS Instantaneous Results (2)



Instantaneous Concentration Fluctuation (case 5)

- **In cases without scalar-velocity interaction, the velocity is rather independent of the scalar, and the scalar transportation does not affect the velocity field. Typically the velocity/scalar field is full of the strip structures.**
- **In the interaction cases (case 8), The buoyancy term is a moderate two-way coupling between the velocity and the scalar transportation. The buoyancy force is in the y direction, but the transportation induced by it can be seen in the longitudinal (z) direction.**

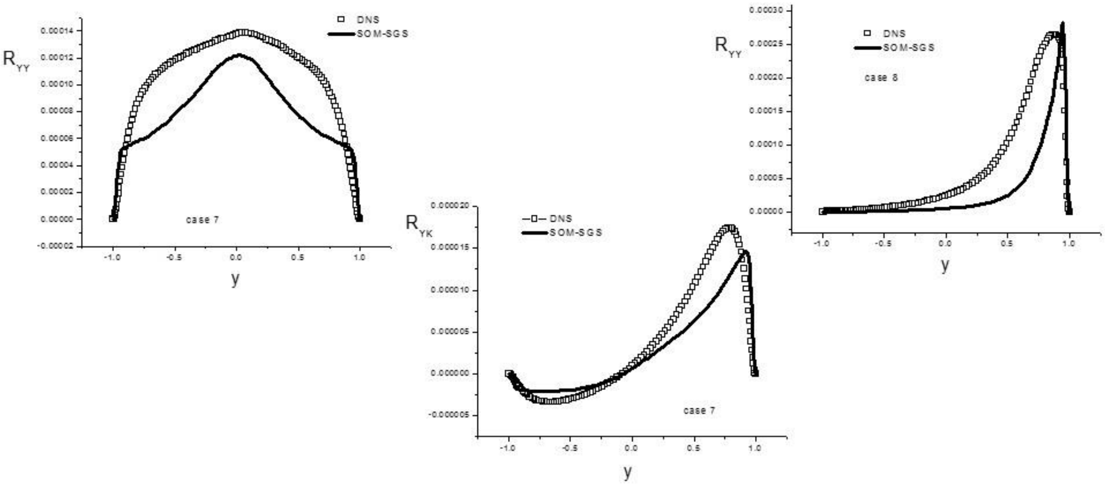
The DNS Verification (1)

The ASSCM model is generally given as:

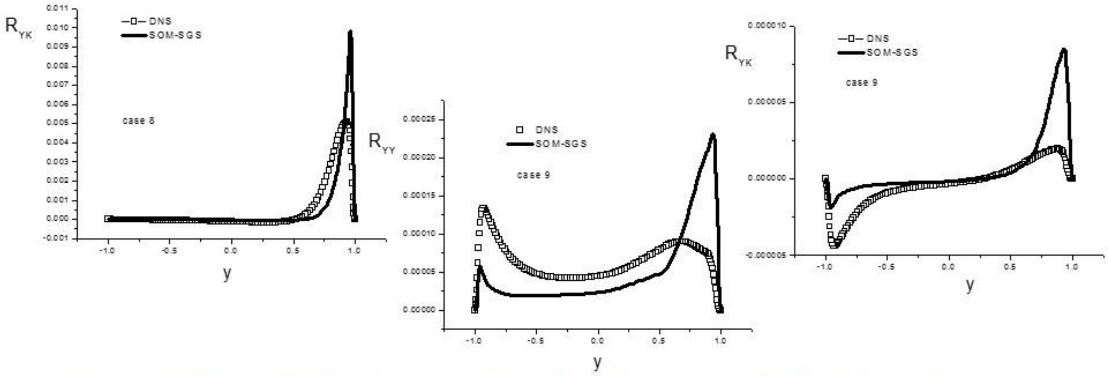
$$R_{\Phi\Psi} = \widetilde{\Phi\Psi} - \tilde{\Phi}\tilde{\Psi} = C_{\Phi,\Psi} L_S^2 \frac{\partial\tilde{\Phi}}{\partial x_j}\frac{\partial\tilde{\Psi}}{\partial x_j}$$

Directly from instantaneous DNS database

From the filter-averaged DNS database



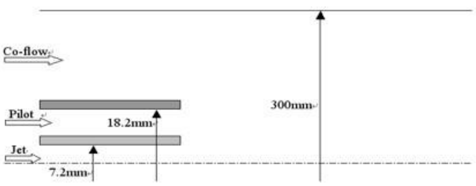
DNS Verification (2)

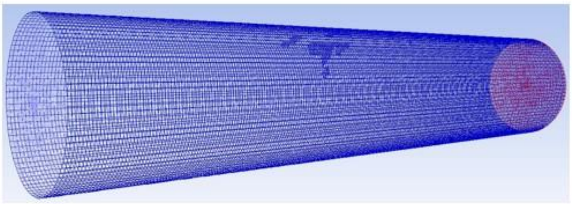


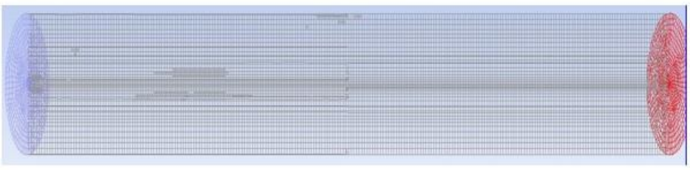
- **The model results has the same trend as the exact solution. For all 3 cases, the R_{YY} value remains in the same range, while the R_{KY} value changes significantly**
- **There are maximum errors of about 30%, 50% and even over 100%...**
- **Though these cases are not ideal examples for real reaction flow, they give a theoretical understanding of the model. In some regions, the ASSCM combustion model is close to the exact solution, so further validation should be carried out.**

LES Validation - Gas Jet Flame (Flame D)

Jet flame structure and the simulation mesh





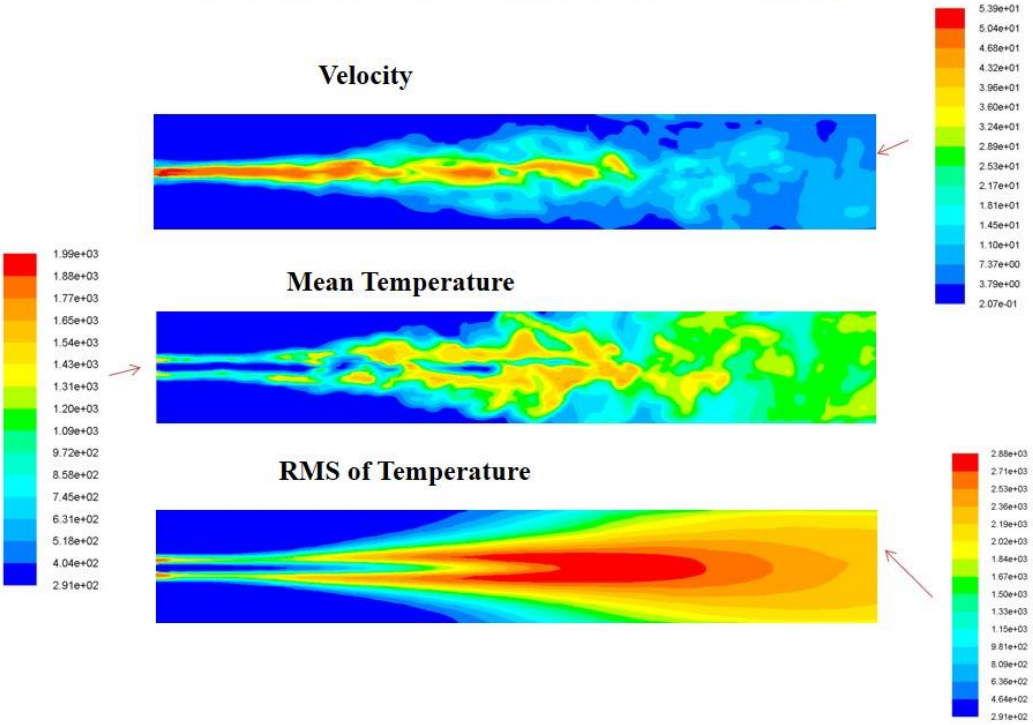


Central section of the simulation mesh

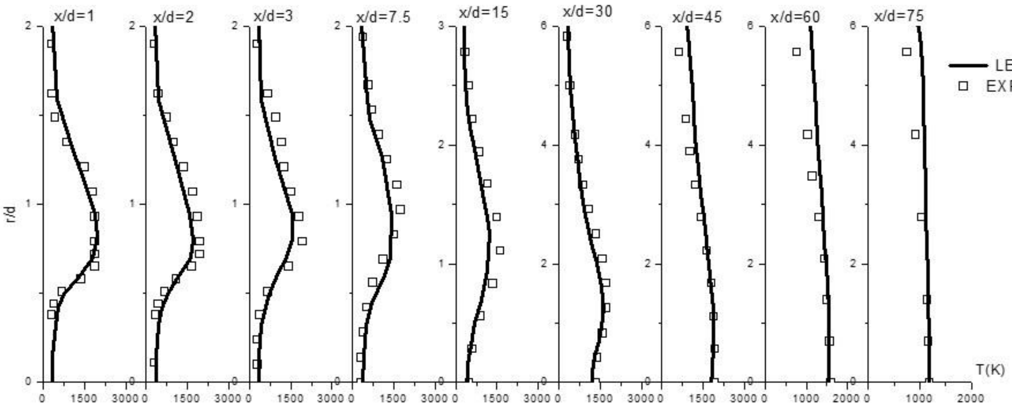
- **The methane-air reaction kinetics :**

$$w_{fu} = 2.119\times10^{11} Y_{ox}^{1.3} Y_{fu}^{0.2} \exp(-2.027\times10^{8} / RT)$$

Instantaneous Contours for Flame D



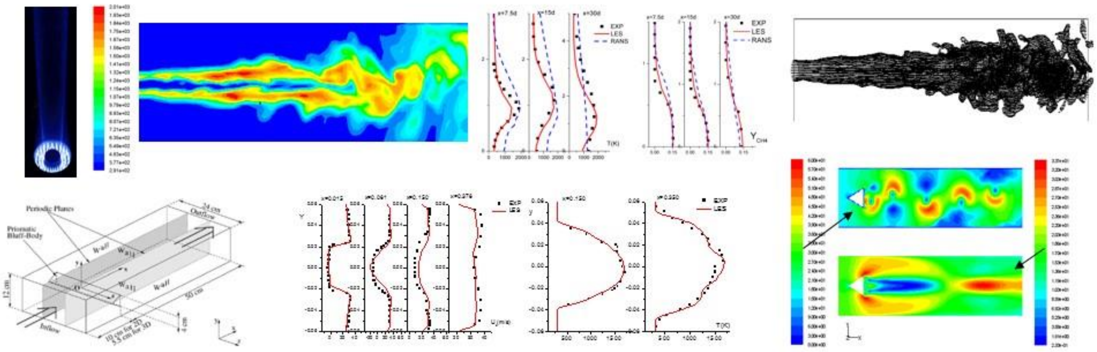
The Average Temperature



The error is less than 5%

ASSCM SGS model validaiton

- **We have proposed *the algebraic sub-grid turbulent combustion model (ASSCM)* and used it in premixed combustion and a partly-diffusion flame. The statistical results were close to measurements.**
- **Here, we applied it for *two-phase* combustion cases.**

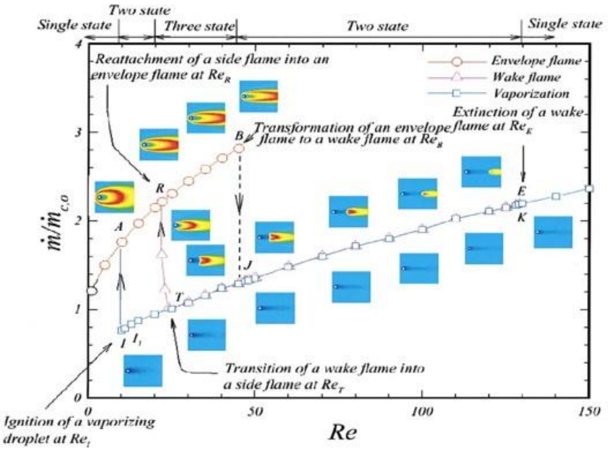


F. Wang, L. X. Zhou, C. X. Xu, Large-Eddy Simulation of Premixed Combustion and Validation of an algebraic second order moment RANS Combustion Model, Journal of Propulsion Technology, 2008, 29(1): 33-36
F. Wang, L. X. Zhou, C. X. Xu, Large-eddy simulation of correlation moments in turbulent combustion and validation of the RANS-SOM combustion model, Fuel, 2006, 85(9): 1242-1247

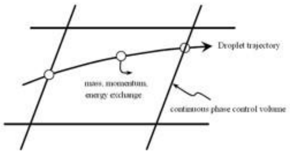
Content

- **Numerical simulation on**
  - **gas combustion : An algebraic sub-grid scale turbulent combustion model**
  - **spray flames : An droplet burning model**

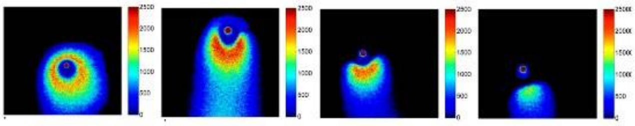
Full Status two phase combustion model



There is single droplet burning in combustion chamber and spray flames
Need to be modeling

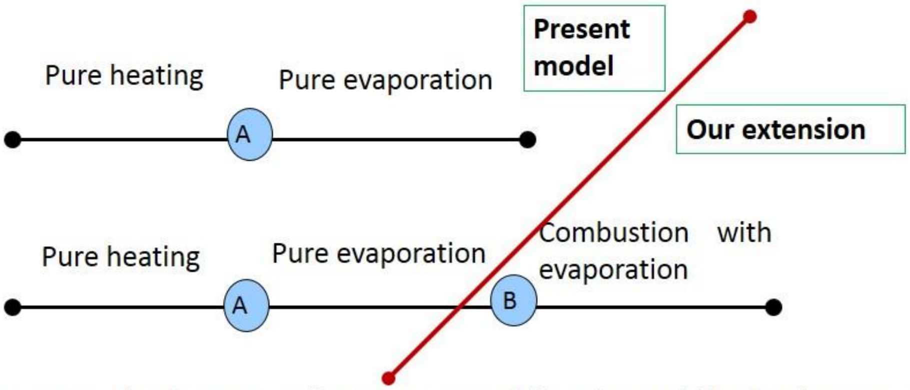


H H Chiu, AIAA 95-2427, A new droplet model for spray combustion, 1995



X. Mercier, M. Orain, F. Grisch, Appl. Phys. B 88, 151–160 (2007)

The full status droplet combustion model (1)



The upper one is the general treatment of droplet, while the lower one is our new model;

The critical point B is from the droplet ignition studies; and the correlation of the droplet combustion with evaporation state is from single droplet combustion studies.

The full status droplet combustion model (2)

- For the criterion for point B, three judgments are used:
  1. The droplet diameter is bigger than 0.001mm;
  2. The ambient temperature is higher than 1200 K;
  3. The evaporation time is longer than the ignition time.

- The ignition delay time function is:

$$\tau_i = A\exp\left(\frac{E}{RT_\infty}\right)C_{oxygen}^{-0.5}C_{methanol}^{-0.1}$$

- The evaporation time is defined as: $\tau_e = d_{d0}^2 / k_e$

- As for the burning correlation, the traditional D^2 law is taken, here the K_c is 0.7 mm^2/s.

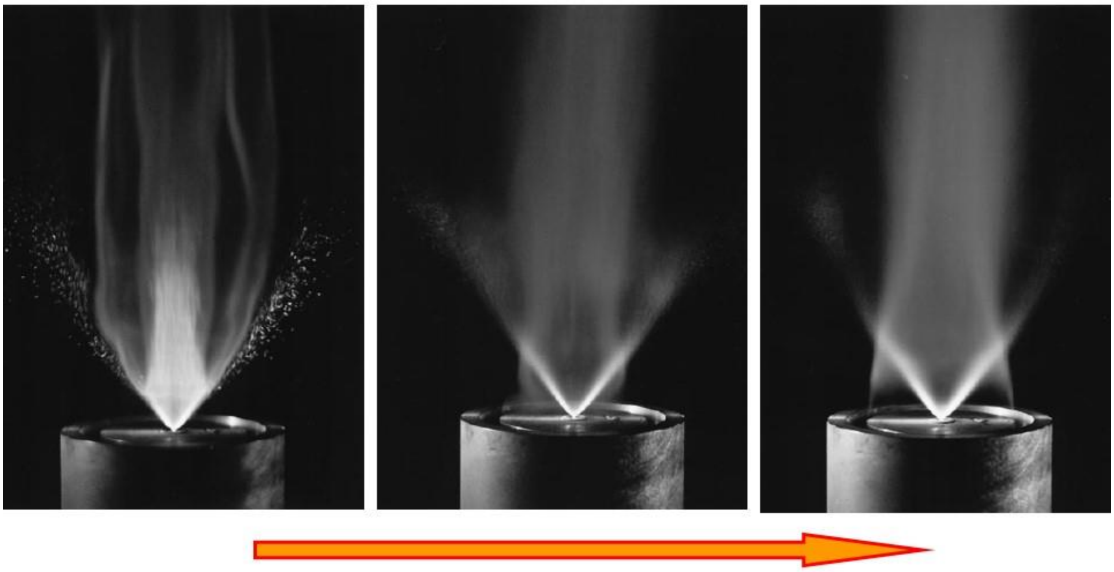
$$k_c = -d(d_d^2)/dt$$

$$\frac{dT_d}{dt} = \frac{NuCp_g}{3\Pr_g Cp_l}\left(\frac{\overline{T_g} - T_d}{\tau_d}\right) + \frac{h_{fg}}{Cp_l}\frac{m_d}{m_d}$$

$$m_d = \frac{dm_d}{dt} = -\frac{m_d}{3Sc_g\tau_d}(Sh + Sh^{st})\ln(1+B)$$

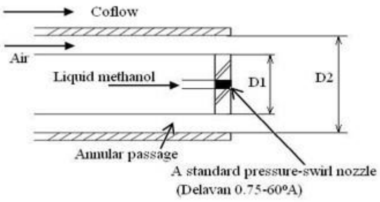
After burning:

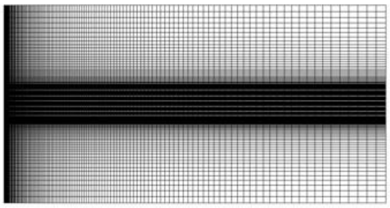
$$\frac{d(d_p)}{dt} = \frac{4k_\infty}{\rho_p C_{p,\infty} d_p}(1 + 0.23\sqrt{\mathrm{Re}_d})\ln[1 + \frac{C_{p,\infty}(T_\infty - T_p)}{h_{fg}}]$$

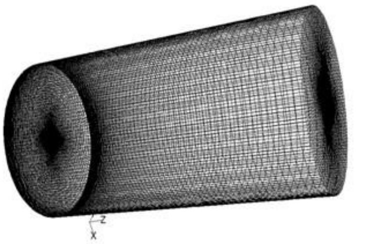


More air, more gas mixture combustion preferential

J. A. Friedman, M. Renksizbulut, Investigating a methanol spray flame Interacting with an annular air jet using phase-doppler interferometry and planar laser-induced fluorescence, Combustion and Flame, 117:661 ¨ C684, 1999

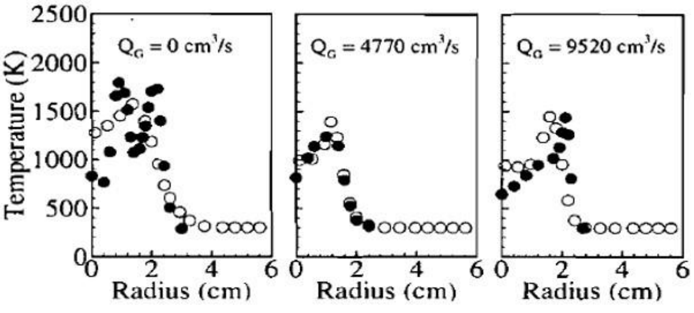




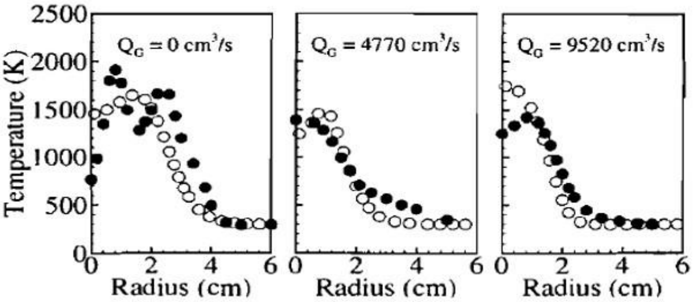


LES in gas phase;
ASSCM turbulent combustion model;

$$w_{fu} = 1.799\times10^{10}\rho^{2}Y_{CH_3OH}^{0.25}Y_{O_2}^{1.5}\exp(\frac{-1.256\times10^{8}}{RT})$$

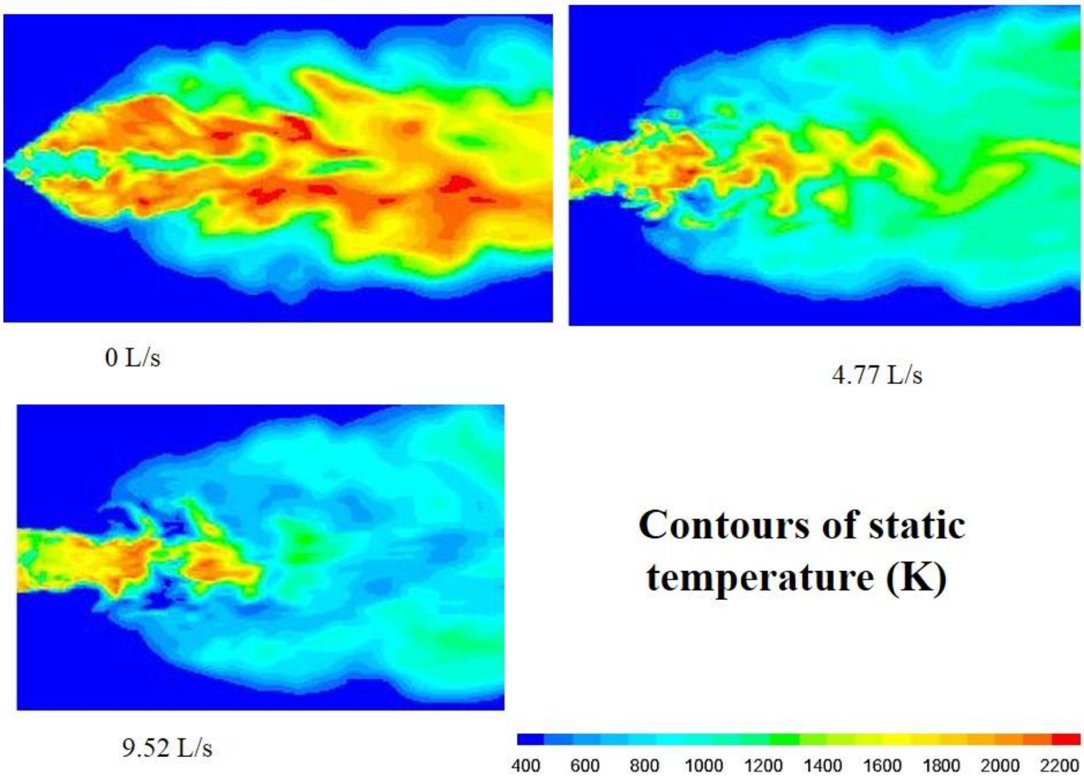


(a) $z = 2.5$ cm



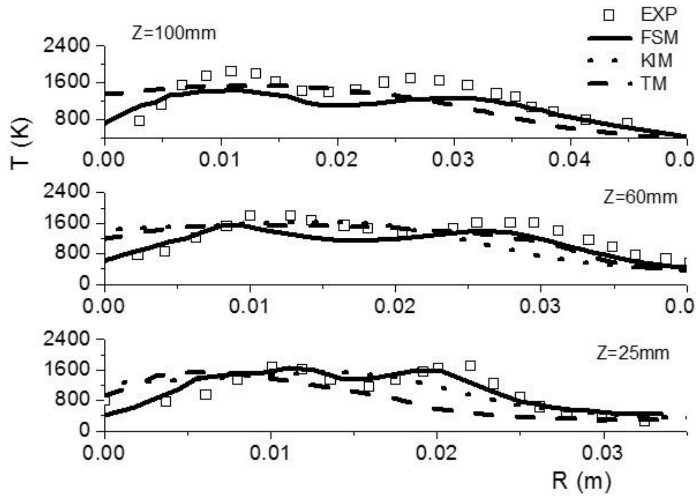
(b) $z = 8.0$ cm

W.T. Kim, K.Y. Huh and J.A. Friedman, and M. Renksizbulut. Numerical simulation of a steady hollow-cone methanol spray flame within an annular air jet. Combust. Sci. Technol. 171:119-139,2001



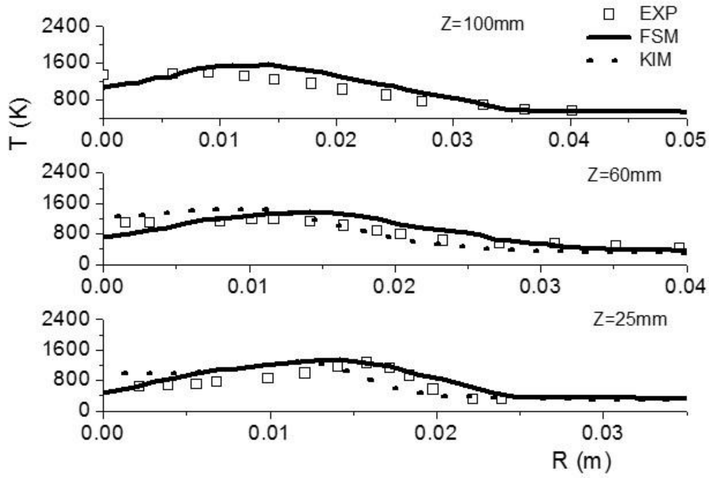
Contours of static temperature (K)

Temperature profiles (case 1)



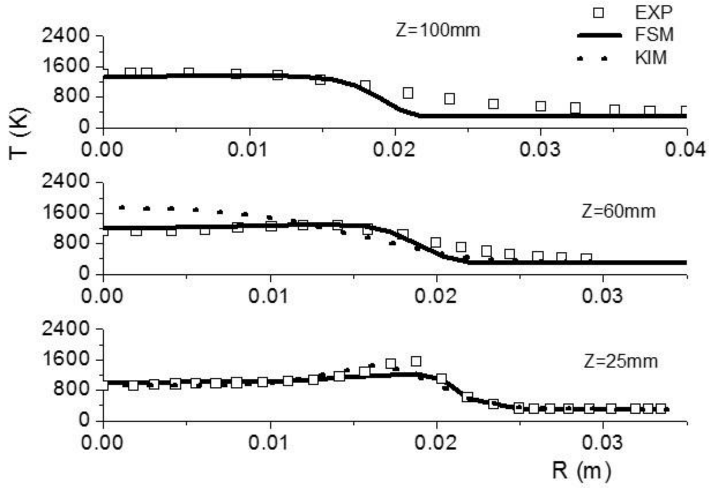
FSDCM - new model; Original – traditional model; ☐ - experimental data

Temperature profiles (case 2)



FSDCM - new model; □ - experimental data

Temperature profiles (case 3)



FSDCM - new model; □ - experimental data

Thank you!