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Numerical investigation of methanol bluff-body flame using variants of RANS turbulence models with Conditional Moment Closure Model

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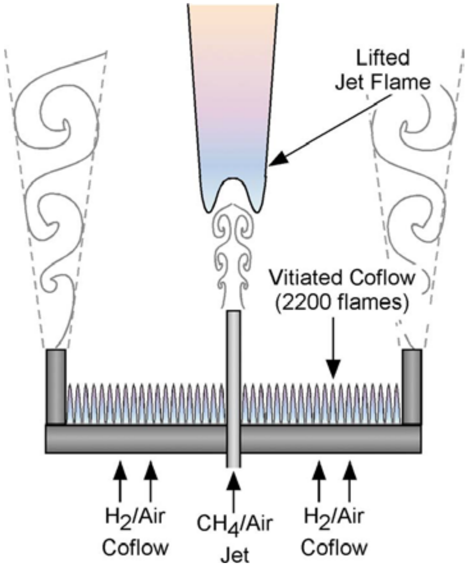
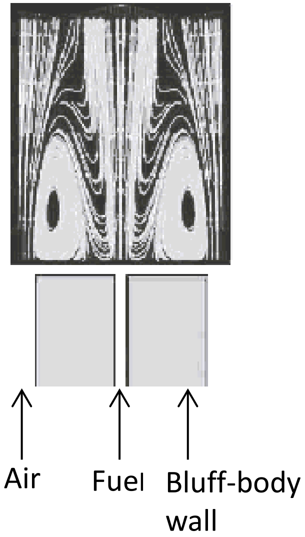
Introduction

- Turbulence chemistry interaction cannot be neglected
- Basic combustion model : inaccurate prediction
- Need : Advanced combustion models {e.g. Conditional moment closure (CMC) model}



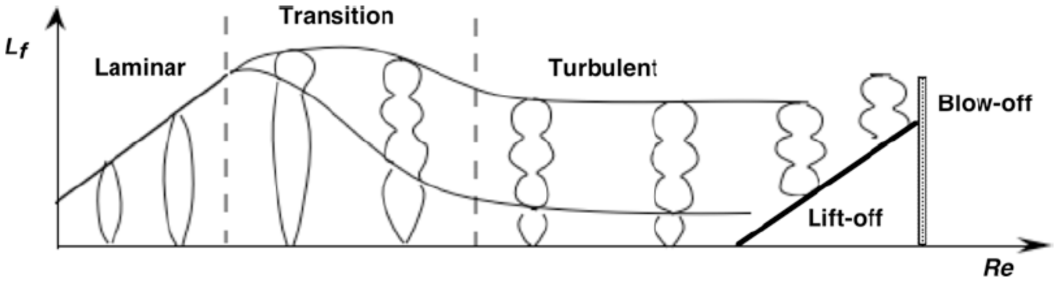
Schematic of a lifted flame burner

[Cabra et al. Combust. Flame (2005)]



Schematic of a bluff-body burner

[Dally et al. Combust. Flame (1998)]



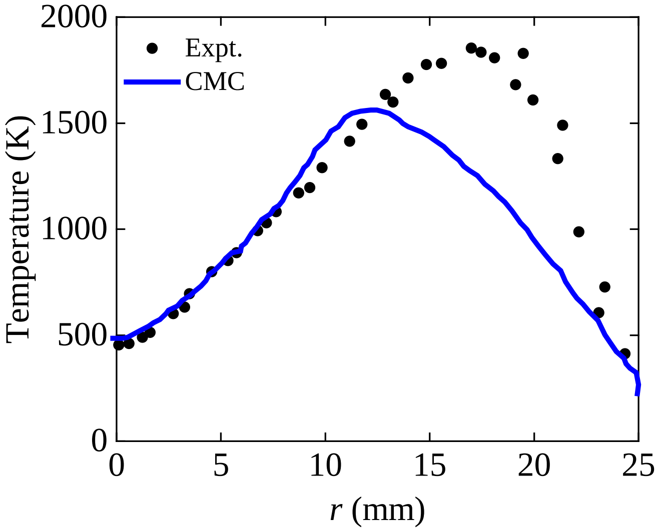
Flame length as a function of jet Reynolds number

[Hottel and Hawthrone Symp. Combust. Flame and Explosion Phenomena (1949)]

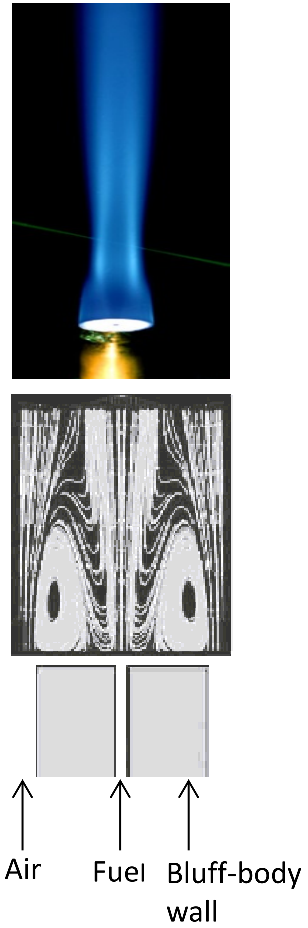
Objective/Motivation

- Study Methanol bluff-body flame
- Underprediction of unconditional quantities by the CMC model when used with *k*-*ε* turbulence model

  (Kim et al. Combust. Flame (2002))
- Need : CMC model and superior turbulence model

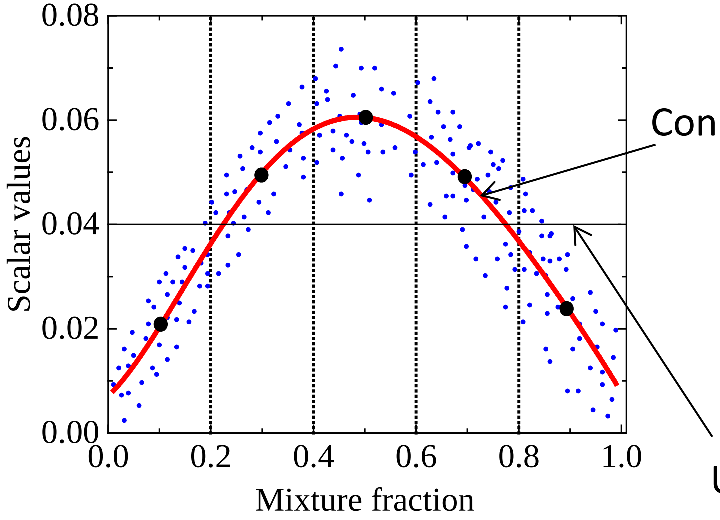


Comparison of predicted unconditional mean temperature with measurements
(Kim et al. Combust. Flame (2002))



Schematic of a bluff-body burner
[Dally et al. Combust. Flame (1998)]

Conditional moment closure model



Conditional Average

Unconditional Average

Mixture Fraction: $$\xi = \frac{\dot{m}_f}{\dot{m}_f + \dot{m}_o}$$

Conditional mean mass fraction:

[Klimenko and Bilger Prog. Energy Comb. Sci .(1999)]

$$Q_\alpha(\eta, x_i, t) = \left\langle Y_\alpha(x_i,t) \middle| \xi(x_i,t) = \eta \right\rangle$$

$$0 \le \eta \le 1$$

$$\underbrace{\frac{\partial Q_\alpha}{\partial t}}_{\text{I}} + \underbrace{\langle u_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i}}_{\text{II}} + \underbrace{\frac{1}{\langle \rho | \eta \rangle P(\eta)} \frac{\partial}{\partial x_i} \left(\langle \rho | \eta \rangle \langle u_i' y_\alpha' | \eta \rangle P(\eta) \right)}_{\text{III}} = \underbrace{\frac{1}{2} \langle \chi | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2}}_{\text{IV}} + \underbrace{\frac{\langle \omega_\alpha | \eta \rangle}{\langle \rho | \eta \rangle}}_{\text{V}}$$

Conditional velocity (Linear model):

[Kuznetsov and Sabel'nikov Turbulence and Combust. (1990)]

$$\langle u_i | \eta \rangle = \langle \tilde{u}_i \rangle + \frac{\langle u'' \xi'' \rangle}{\langle \xi''^2 \rangle} \left(\eta - \tilde{\xi} \right)$$

Conditional moment closure model (contd.)

Conditional scalar dissipation rate (AMC model):
[Peters Prog. Energy Comb. Sci. (1984)]

$$\langle \chi | \eta \rangle = \langle \chi | \eta = 0.5 \rangle \exp[-2(erf^{-1}(2\eta - 1))^2]$$

$$\langle \chi | \eta = 0.5 \rangle = \tilde{\chi} \Big/ \int_0^1 \exp[-2(erf^{-1}(2\eta - 1)^2]\tilde{P}(\eta) d\eta$$

Conditional flux (gradient diffusion hypothesis):

$$\langle u_i' Y_\alpha' | \eta \rangle = -D_t \frac{\partial Q_\alpha}{\partial x_i}$$

Chemical source term:

$$\langle \omega_\alpha (Y_\alpha, T) | \eta \rangle = \omega_\alpha (Q_\alpha, Q_T)$$

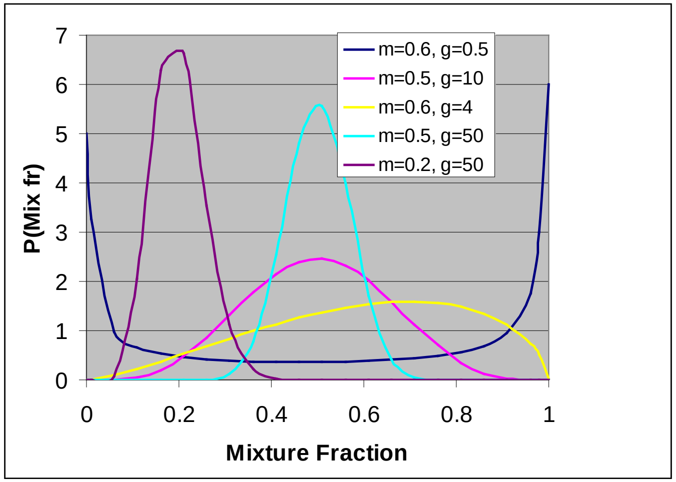
Conditional radiation heat loss:

$$\langle S_R | \eta \rangle = 4\sigma \sum_\alpha p_\alpha \times \kappa_\alpha \left(Q_T^4 - T_0^4 \right)$$

Steffan-Boltzmann constant $\sigma = 5.669\times10^{-8}$ W/m^2 K^4 , p_α is partial pressure, κ_α is Planck's mean absorption coefficient of species α, T_0 is room temperature

Conditional moment closure model (contd.)

β-PDF : $\tilde{P}(\eta) = \dfrac{\eta^{\alpha-1}(1-\eta)^{(\beta-1)}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha+\beta)$ $\alpha = \tilde{\xi}\gamma;\ \beta = (1-\tilde{\xi})\gamma;\ \gamma = \dfrac{\tilde{\xi}(1-\tilde{\xi})}{\tilde{\xi}^{\prime\prime 2}} - 1$



ξ = 0; pure air

ξ = 1; pure fuel

$$\int_0^1 \tilde{P}(\eta)d\eta = 1; \quad \tilde{\phi} = \int_0^1 \langle \phi \,|\, \eta \rangle \tilde{P}(\eta)d\eta$$

Mean mixture fraction :

$$\tilde{\rho}\frac{\partial \tilde{\xi}}{\partial t} + \tilde{\rho}\tilde{v}\cdot\nabla\tilde{\xi} = -\nabla\cdot\left\{\tilde{\rho}(-D_t\nabla\tilde{\xi})\right\}$$

Variance of mixture fraction :

$$\tilde{\rho}\frac{\partial \tilde{\xi}^{\prime\prime 2}}{\partial t} + \tilde{\rho}\tilde{v}\cdot\nabla\tilde{\xi}^{\prime\prime 2} = -\nabla\cdot\left\{\tilde{\rho}(-D_t\nabla\tilde{\xi}^{\prime\prime 2})\right\} + 2\tilde{\rho}D_t(\nabla\tilde{\xi})^2 - \tilde{\rho}\tilde{\chi}$$

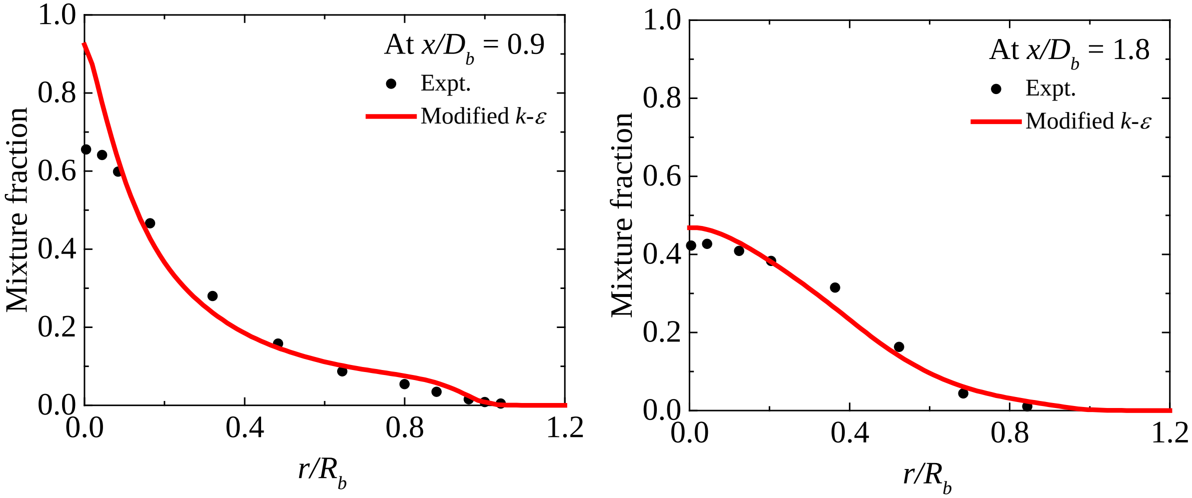
Initial validation of CMC model

- Test case

  CH_4/H_2 bluff-body flame

Initial boundary conditions

	Jet	Coflow
V (m/s)	118	40
T (K)	298	298
Y_{O_2}	0	0.23
Y_{N_2}	0	0.77
Y_{CH_4}	0.89	0
Y_{H_2}	0.11	0
ξ_{st}	0.05	

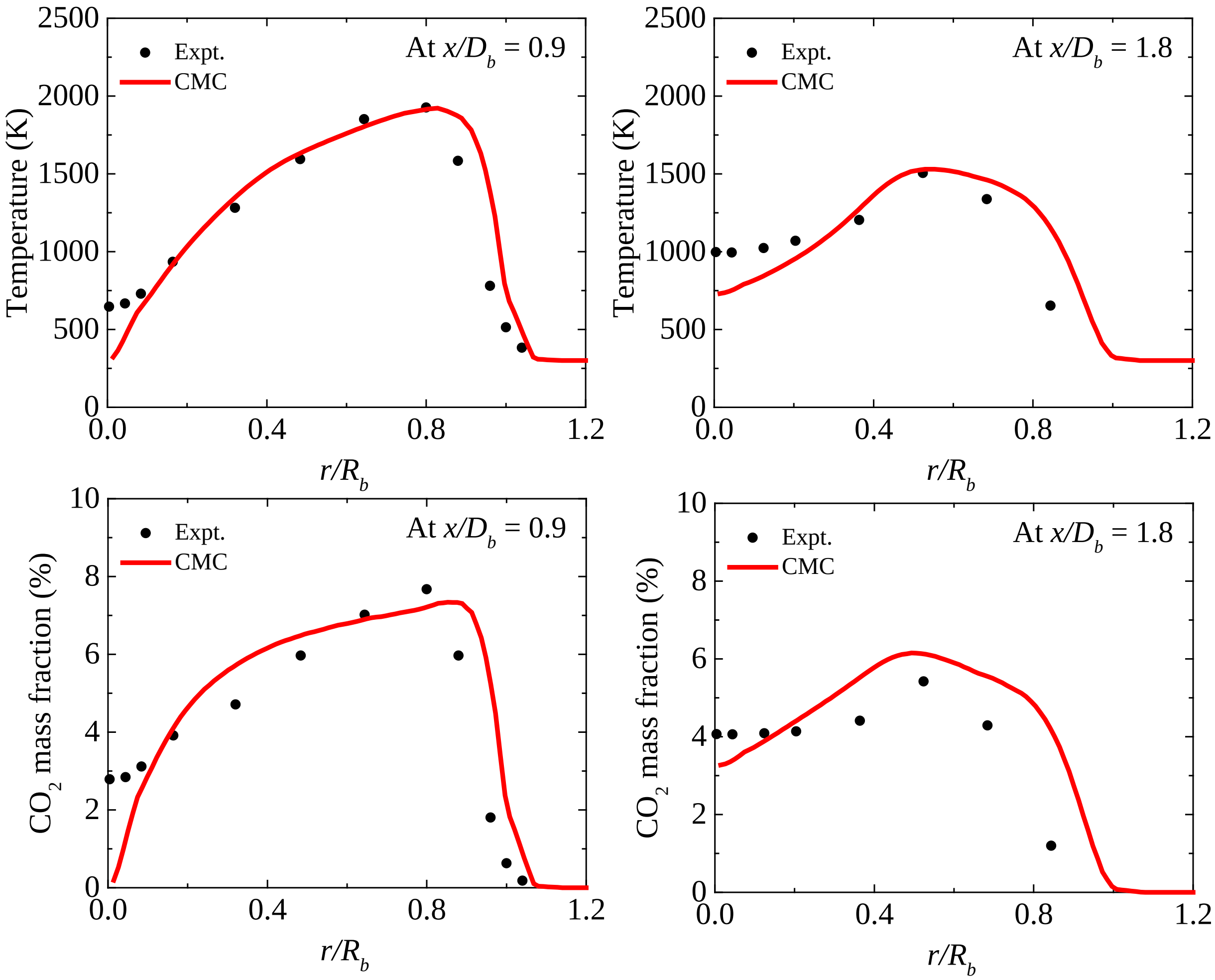


Comparison of predicted mean mixture fraction with measurements

Note:

- Predicted mean mixture fraction are in good agreement with the experimental data at both the axial locations

Initial validation of CMC model (contd.)

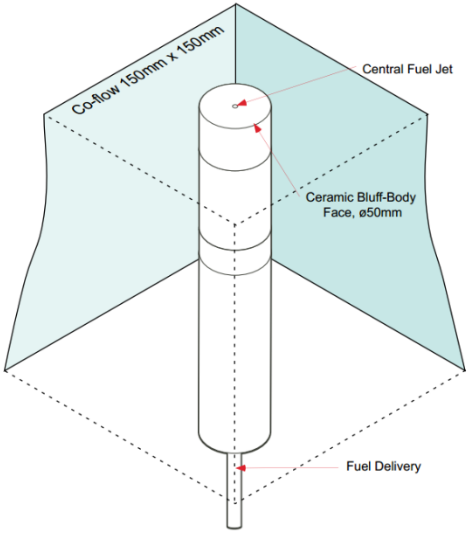


Note:

- Predicted temperature and CO_2 mass fraction agree very well with the experimental data at both the axial locations

Comparison of predicted unconditional mean temperature and CO_2 mass fraction with measurements

Methanol bluff-body flame



Schematic of the bluff-body burner [Dally et al. Combust. Flame (1998)]

Diameters (mm)	
Jet	Bluff-body
3.6	50

Initial boundary conditions

	Jet	Coflow
V (m/s)	80	40
T (K)	373	300
Y_{O_2}	0	0.23
Y_{N_2}	0	0.77
Y_{CH_3OH}	1	0
ξ_{st}	0.135	

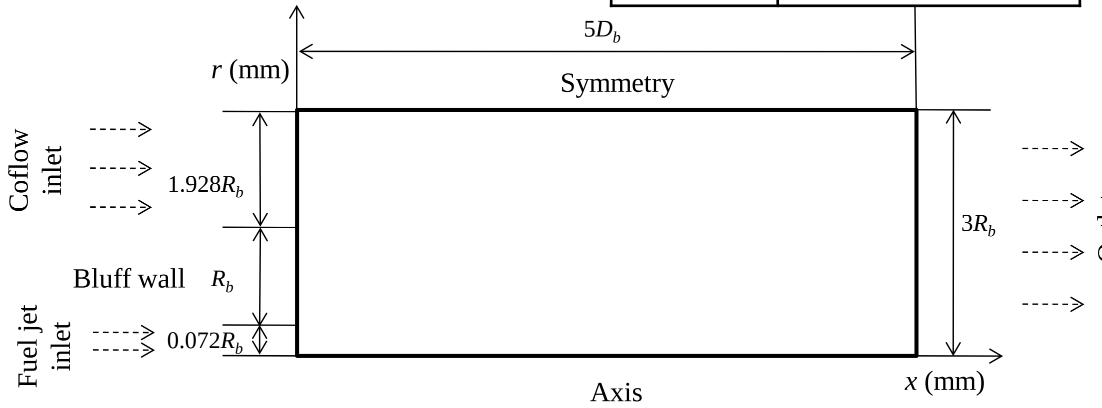
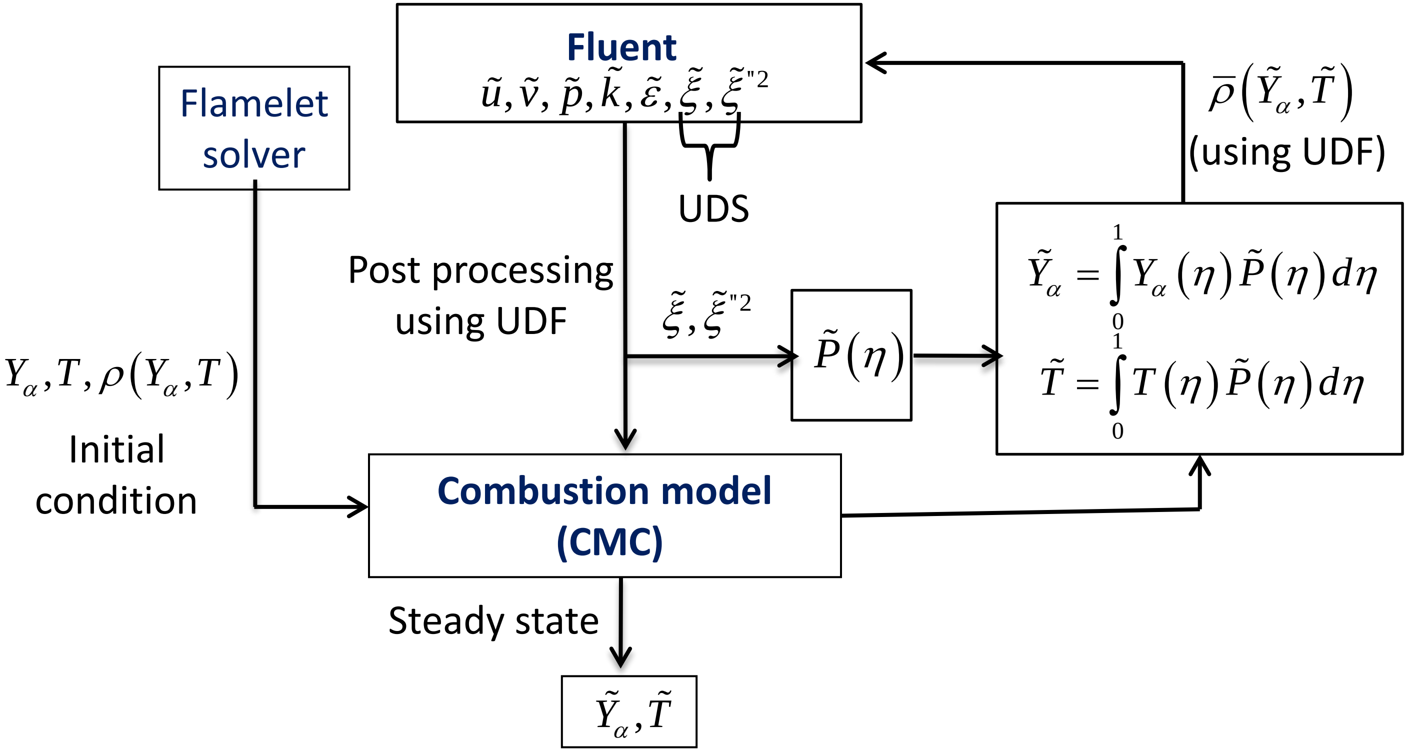


Diagram of computational details

Fluent-CMC coupling



Fluent

$\tilde{u},\tilde{v},\tilde{p},\tilde{k},\tilde{\varepsilon},\underbrace{\tilde{\xi},\tilde{\xi}''^2}_{\text{UDS}}$

Flamelet solver

$Y_\alpha, T, \rho(Y_\alpha, T)$

Initial condition

Post processing using UDF

$\tilde{\xi},\tilde{\xi}''^2$

$\tilde{P}(\eta)$

$$\tilde{Y}_\alpha = \int_0^1 Y_\alpha(\eta)\tilde{P}(\eta)\,d\eta$$

$$\tilde{T} = \int_0^1 T(\eta)\tilde{P}(\eta)\,d\eta$$

$\bar{\rho}(\tilde{Y}_\alpha,\tilde{T})$

(using UDF)

Combustion model (CMC)

Steady state

$\tilde{Y}_\alpha,\tilde{T}$

Coupling flow chart

User defined scalars (UDS):

Mean mixture fraction, Variance of mixture fraction

Macros used in Fluent :

DEFINE_DUFFISIVITY

(to specify turbulent diffusivity of UDS)

DEFINE_ADJUST

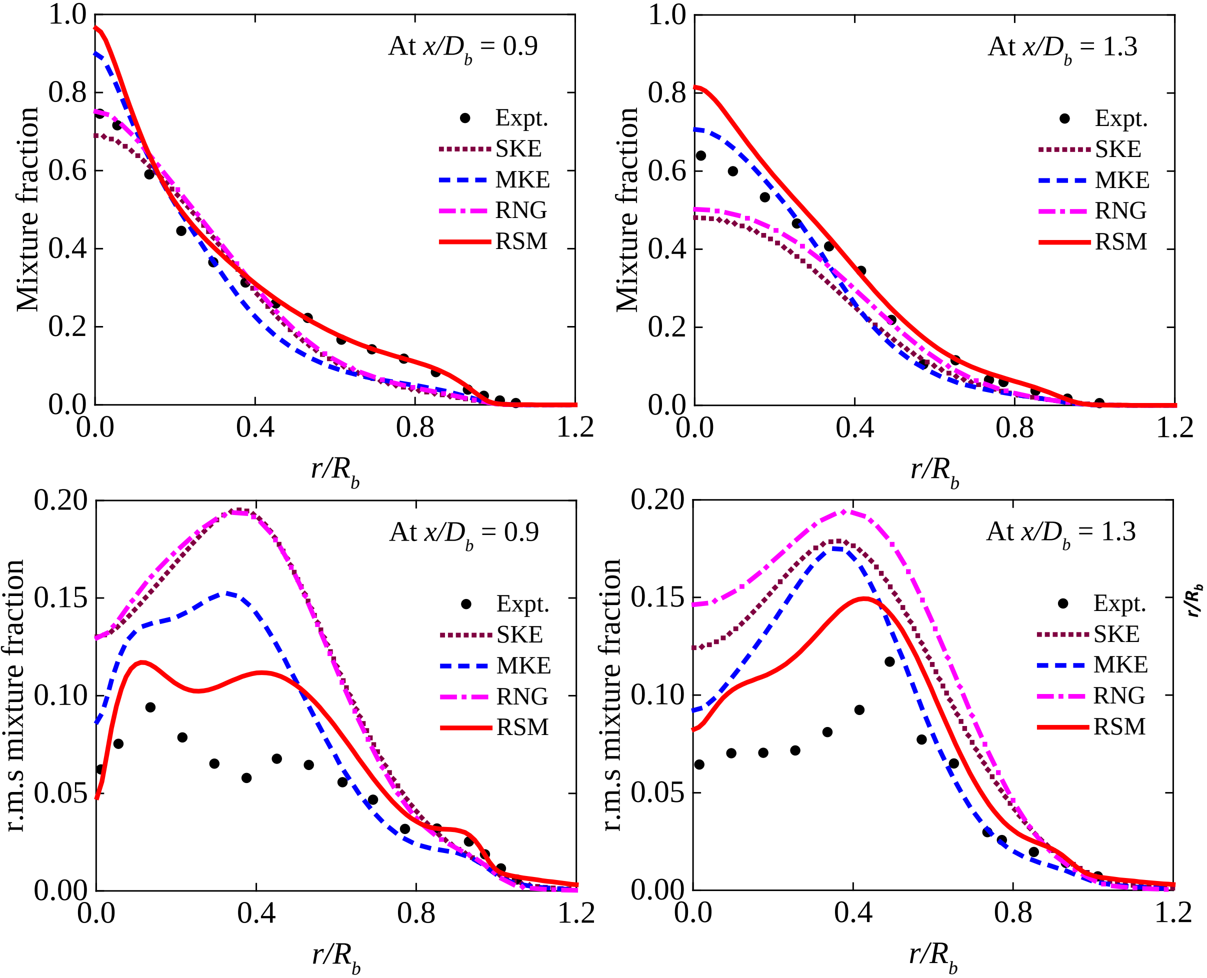
(for post processing)

DEFINE_PROPERTY

(for supplying density from CMC)

Fluent	**CMC**
Number of grids	Number of grids
Axial : 457	Axial : 65
Radial : 258	Radial : 35

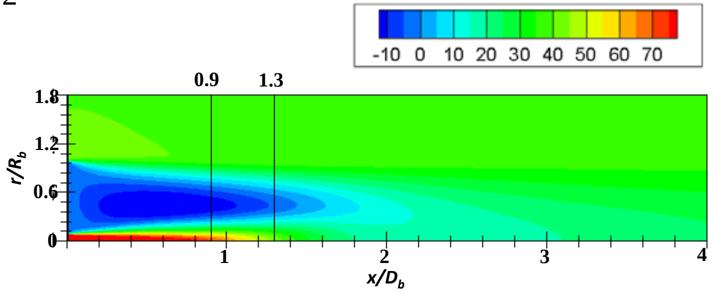
Results



SKE : $C_{\varepsilon1}$ -1.44
$C_{\varepsilon2}$ -1.92

MKE : $C_{\varepsilon1}$ -1.6
$C_{\varepsilon2}$ -1.92

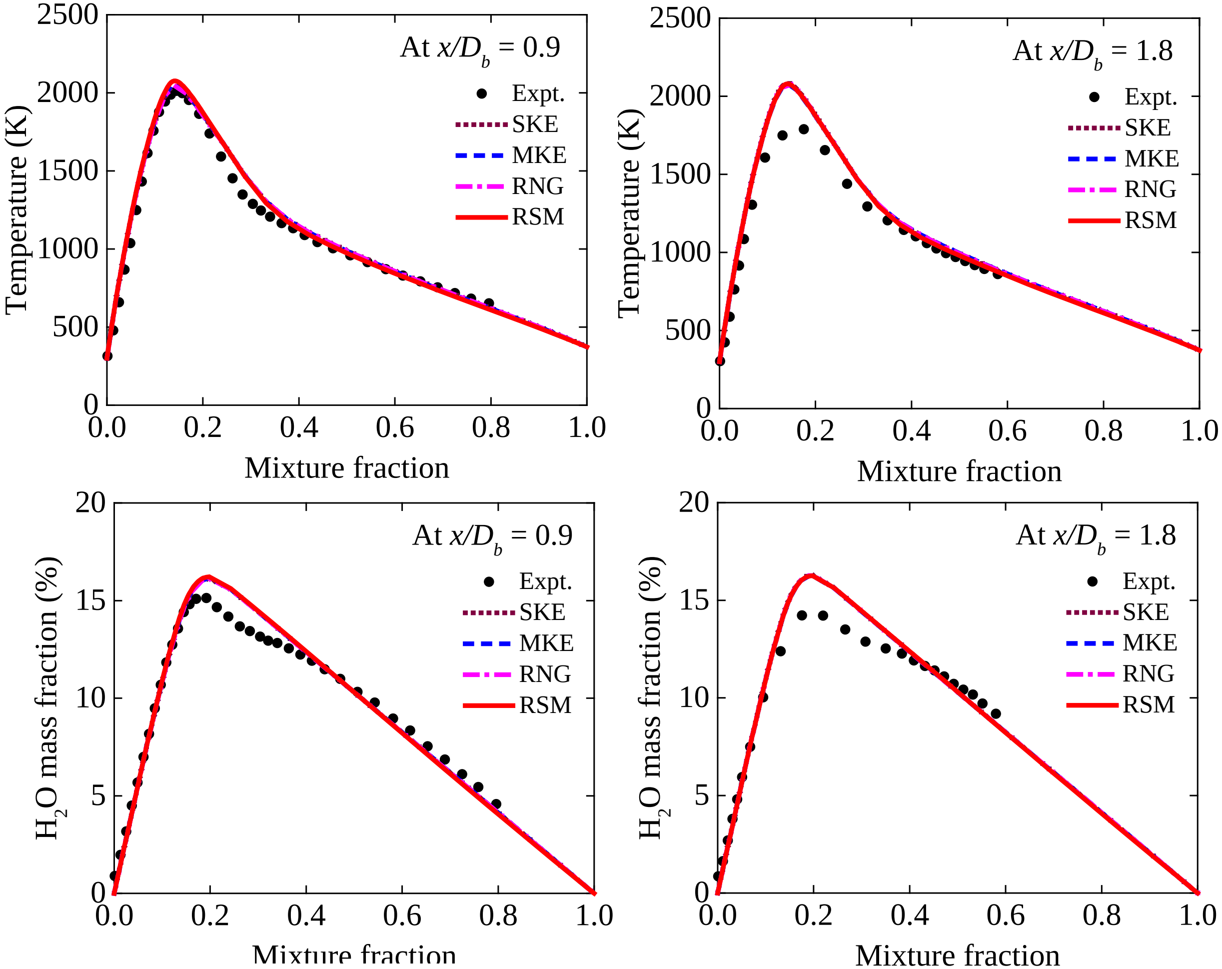
[Sreedhara and Huh Combust. Flame (2005)]



***u*-velocity (m/s) contour indicating the flow structure over a bluff-body**

Comparison of predicted mean mixture fraction and r.m.s mixture fraction with measurements

Results (contd.)

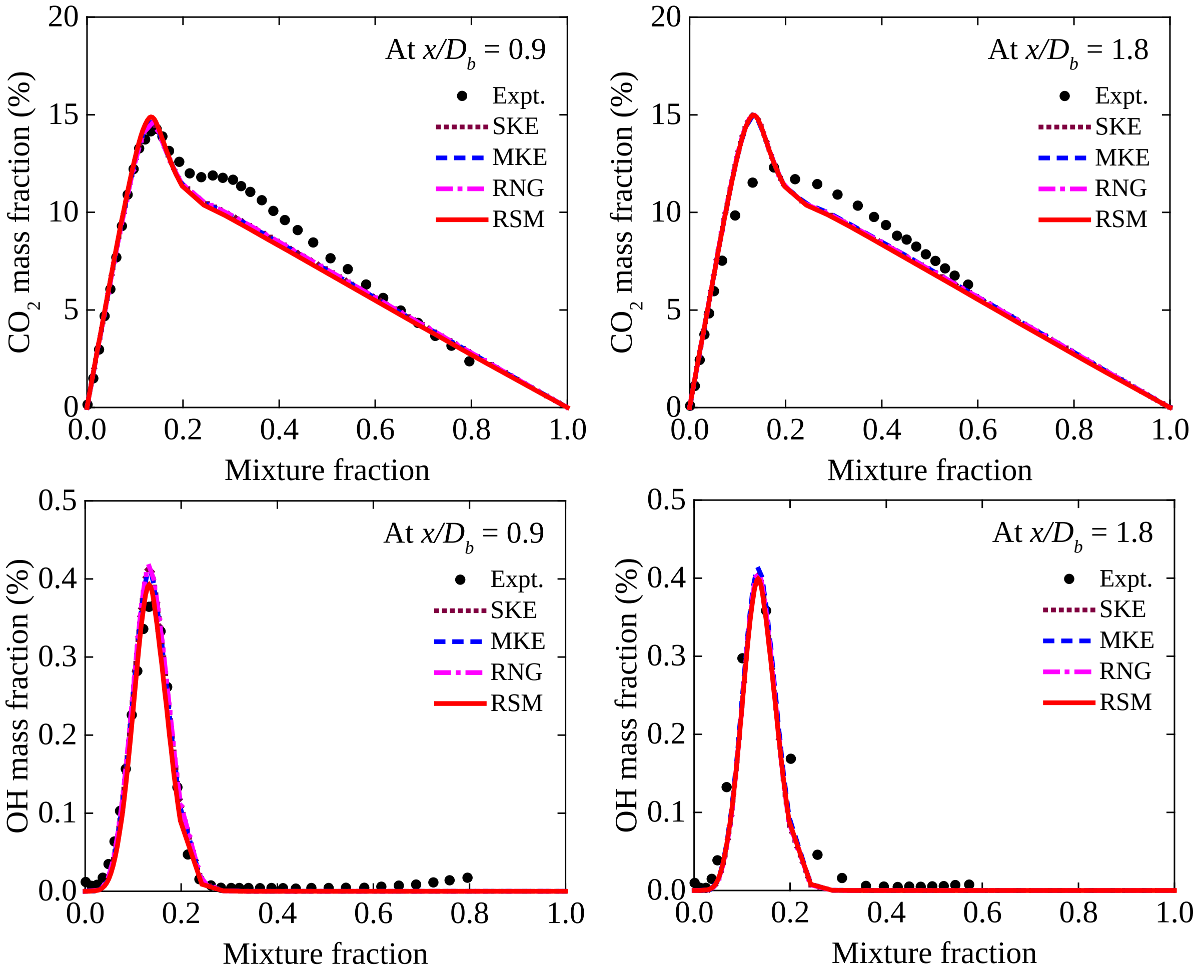


Comparison of predicted conditional mean temperature and H_2O mass fraction with measurements

Note:

- ❖ Stoichiometric mixture fraction is 0.135
- ❖ Predicted conditional statistics agree well with the experimental data

Results (contd.)

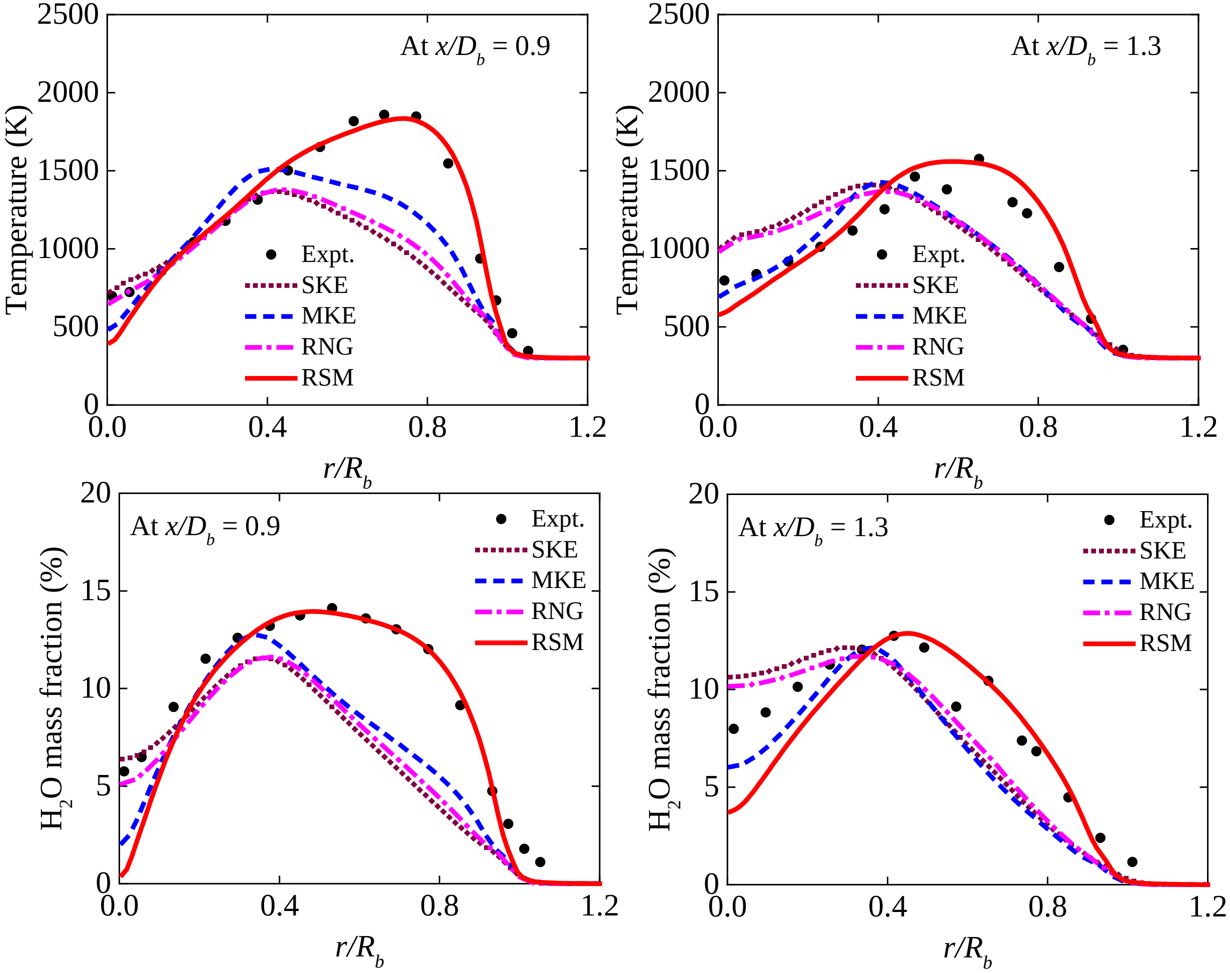


Note

- ❖ Accuracy of prediction of conditional quantities show a least dependency on turbulence models

Comparison of predicted conditional mean CO_2 and OH mass fractions with measurements

Results (contd.)

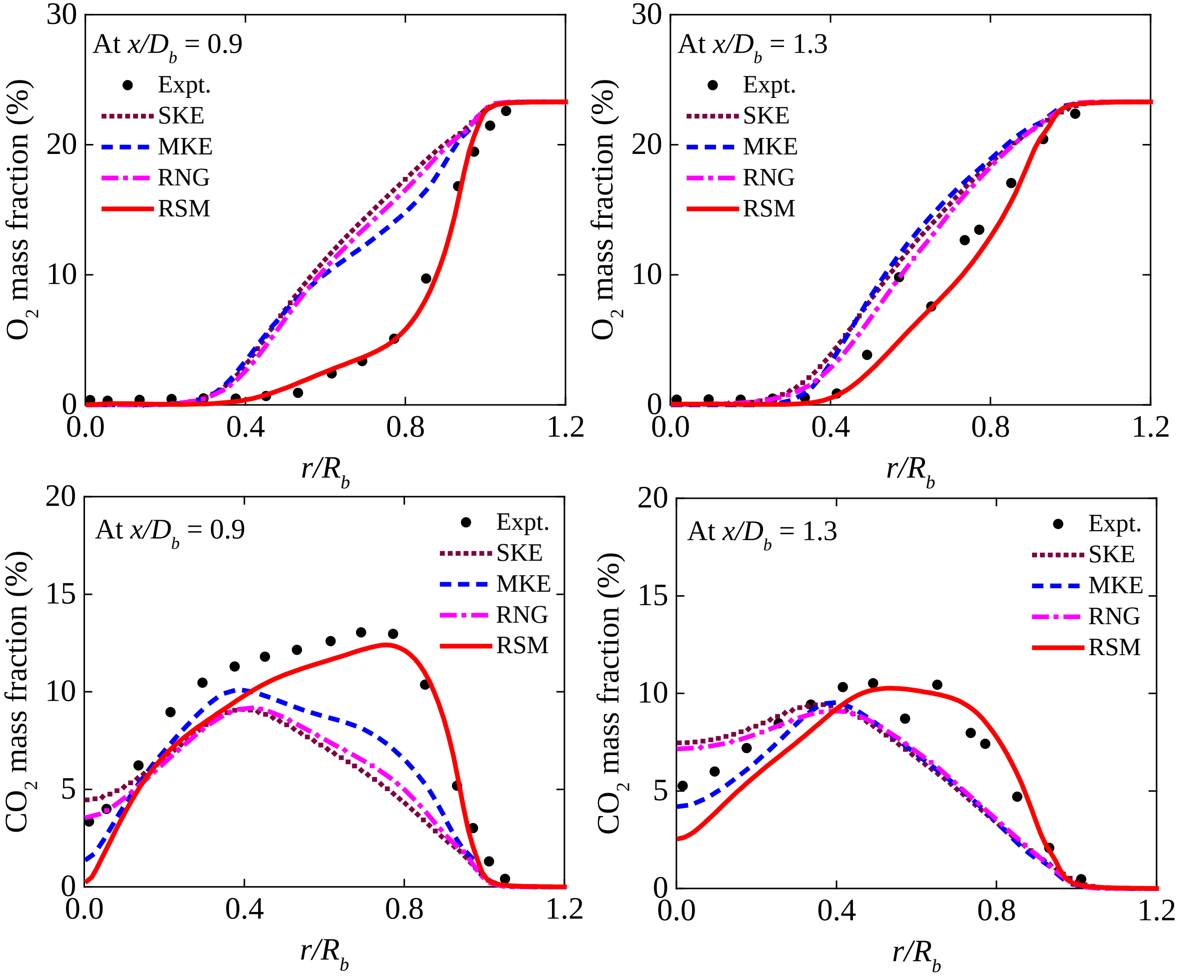


Comparison of predicted unconditional mean temperature and H_2O mass fractions with measurements

Note:

- Inaccurate prediction of temperature and H_2O mass fraction by CMC model when coupled with SKE, MKE and RNG models
- CMC model shows an excellent agreement with the experimental data when used with **Reynolds stress model**

Results (contd.)

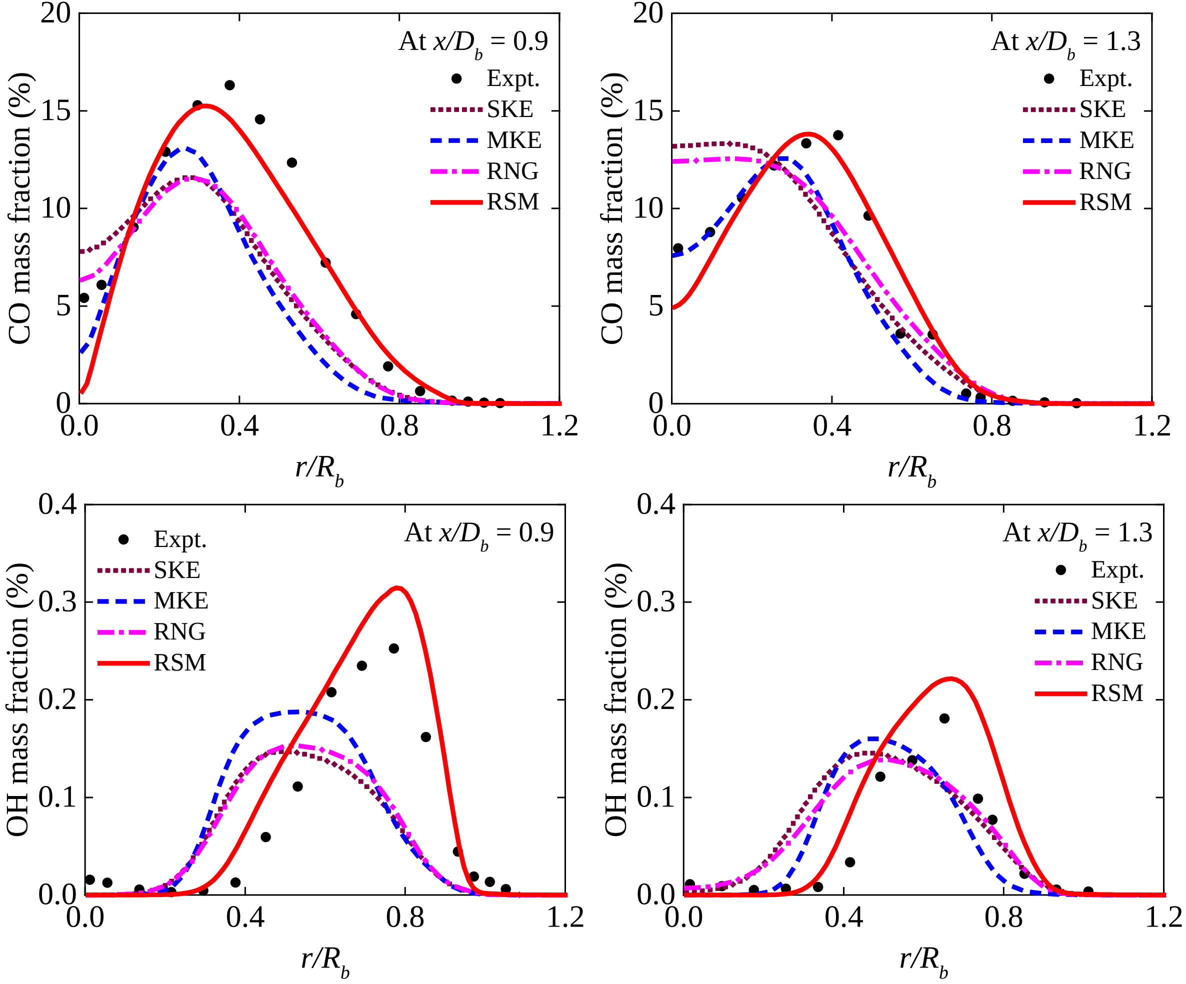


Comparison of predicted unconditional mean O_2 and CO_2 mass fractions with measurements

Note:

- ❖ CMC model shows superior predictions of O_2 and CO_2 mass fractions when used with Reynolds stress model
- ❖ All other turbulence models overpredict and underpredict O_2 and CO_2 mass fractions respectively

Results (contd.)



Note:

- ❖ Unconditional mean quantities show significant variations using four different turbulence models
- ❖ RSM performs better

Comparison of predicted unconditional mean CO and OH mass fractions with measurements

Results (contd.)

CPU time required for Fluent and CMC solvers

Models	Fluent (hours)	CMC (hours)	Fluent+ CMC (hours)
SKE	0.77	33.6	34.32
MKE	0.75	34.6	35.31
RNG	0.83	34.0	35.75
RSM	1.72	32.0	33.55

Note:

- Time taken to solve the flow with RSM model field was almost two times higher compared to that with other turbulence models.
- Total time (Fluent + CMC) taken for a complete cycle did not change significantly for different models.

Conclusions

- CMC model has been coupled with ANSYS Fluent software to assess the performance of different turbulence models.
- SKE and RNG models showed a significant underprediction of mean mixture fraction
- Mixture fraction profiles predicted by the Reynolds stress turbulence model showed an excellent agreement with the experimental data at all axial locations
- Accuracy of prediction of conditional quantities showed a least dependency on turbulence models
- CMC model showed an improved prediction of unconditional mean temperature and species mass fractions when coupled with the Reynolds stress turbulence models.
- Predictions of unconditional quantities depended upon accurate prediction of PDF of mixture fraction.
- The coupling of Fluent and CMC also provides an opportunity to perform LES-CMC simulations for solving turbulent flame problems.

THANK YOU