Multiphysics Multiscale Simulations of Entrained Flow Gasification

Mayank Kumar, Cheng Zhang, Ahmed Ghoniem

Presenter: Mayank Kumar

Reacting Gas Dynamics Computational Lab, MIT

NETL Workshop on Multiphase Flow Science, Pittsburgh

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MASDAR INSTITUTE
OF SCIENCE AND TECHNOLOGY
معهد مصدر
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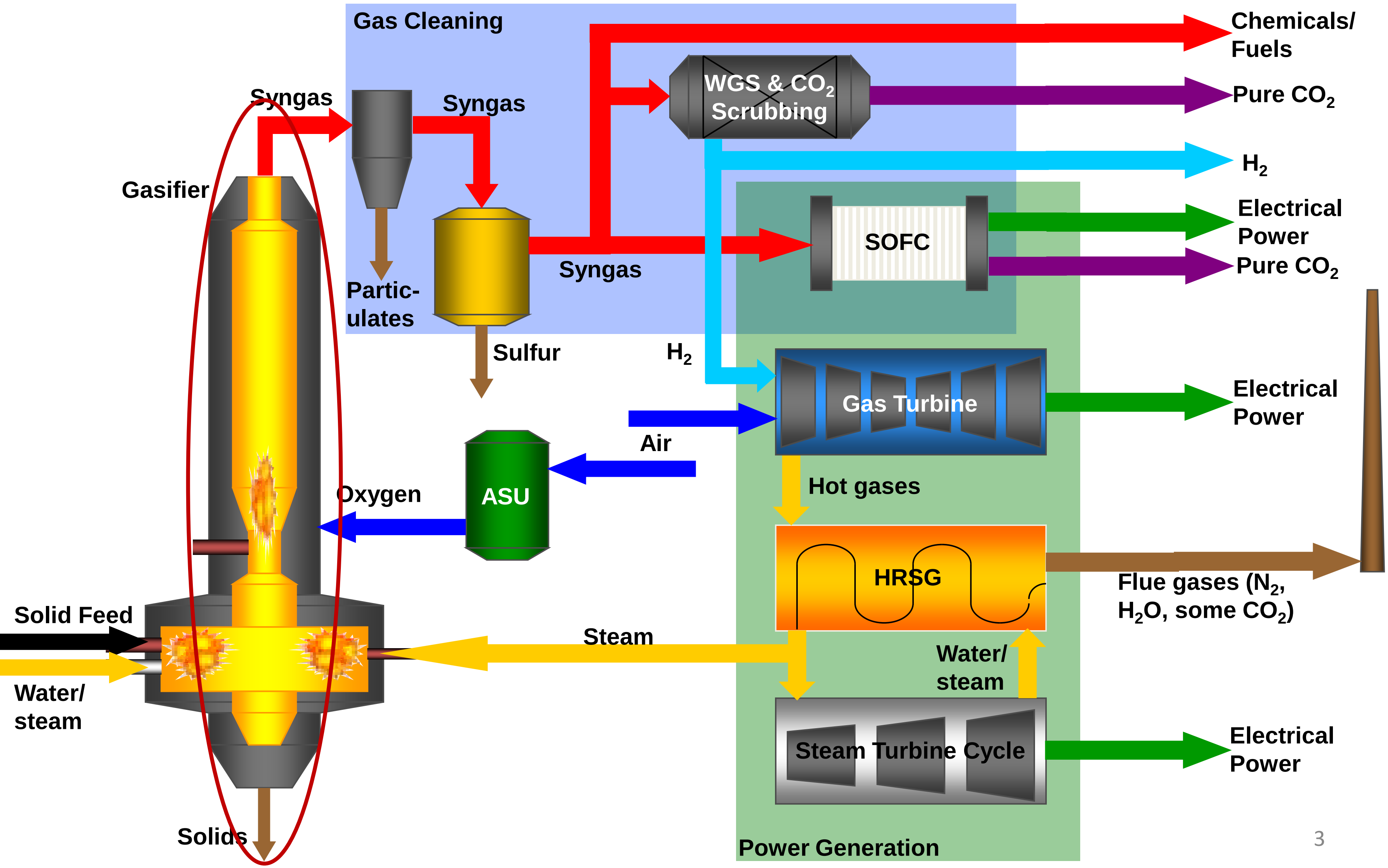
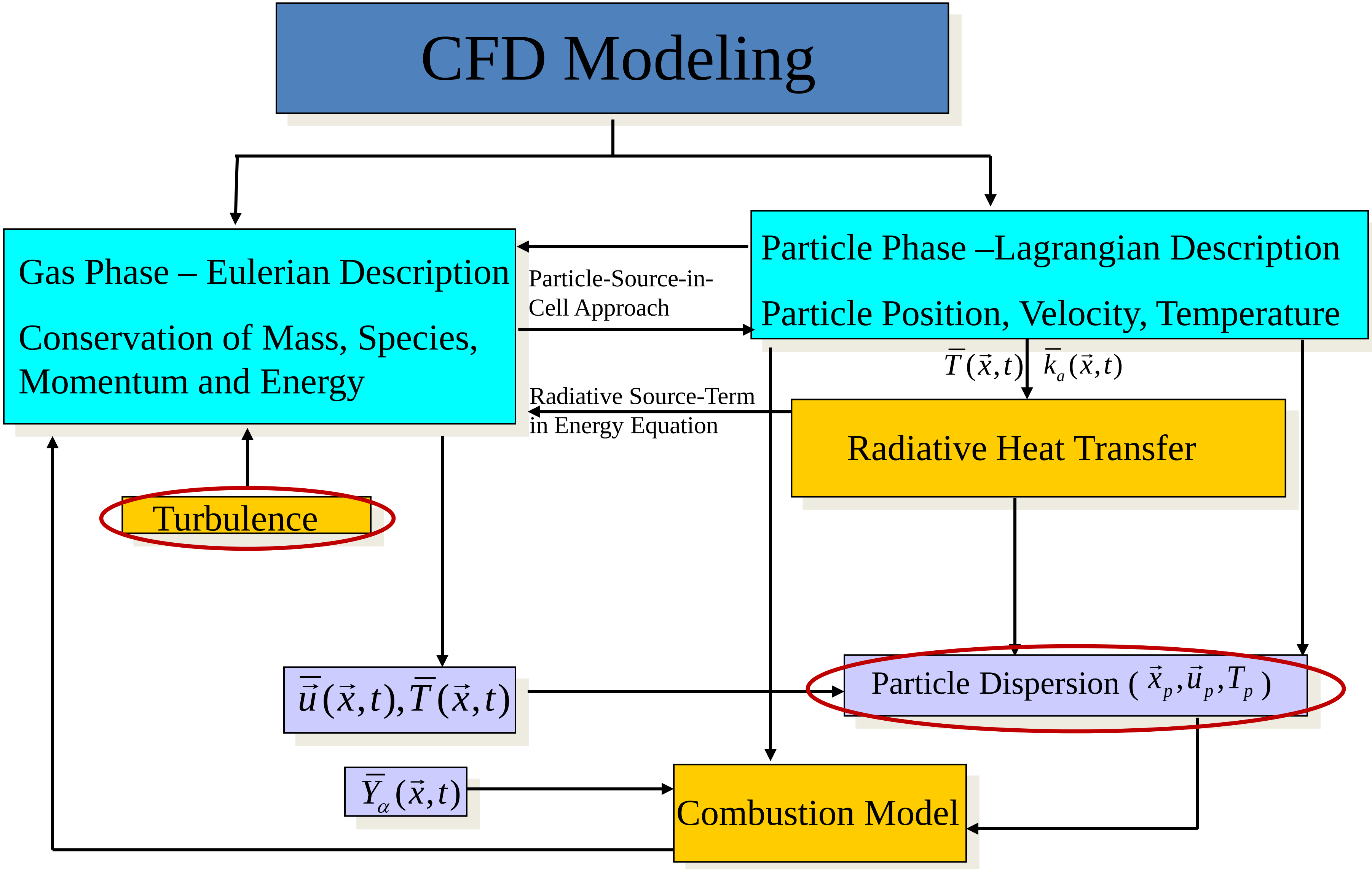
MITei MIT Energy Initiative

Outline

- Model setup
- Sample results : MHI gasifier
- Flow solver validation studies
- Particle turbulent dispersion model validation
- Revisit MHI gasifier : Pilot and Research Scale

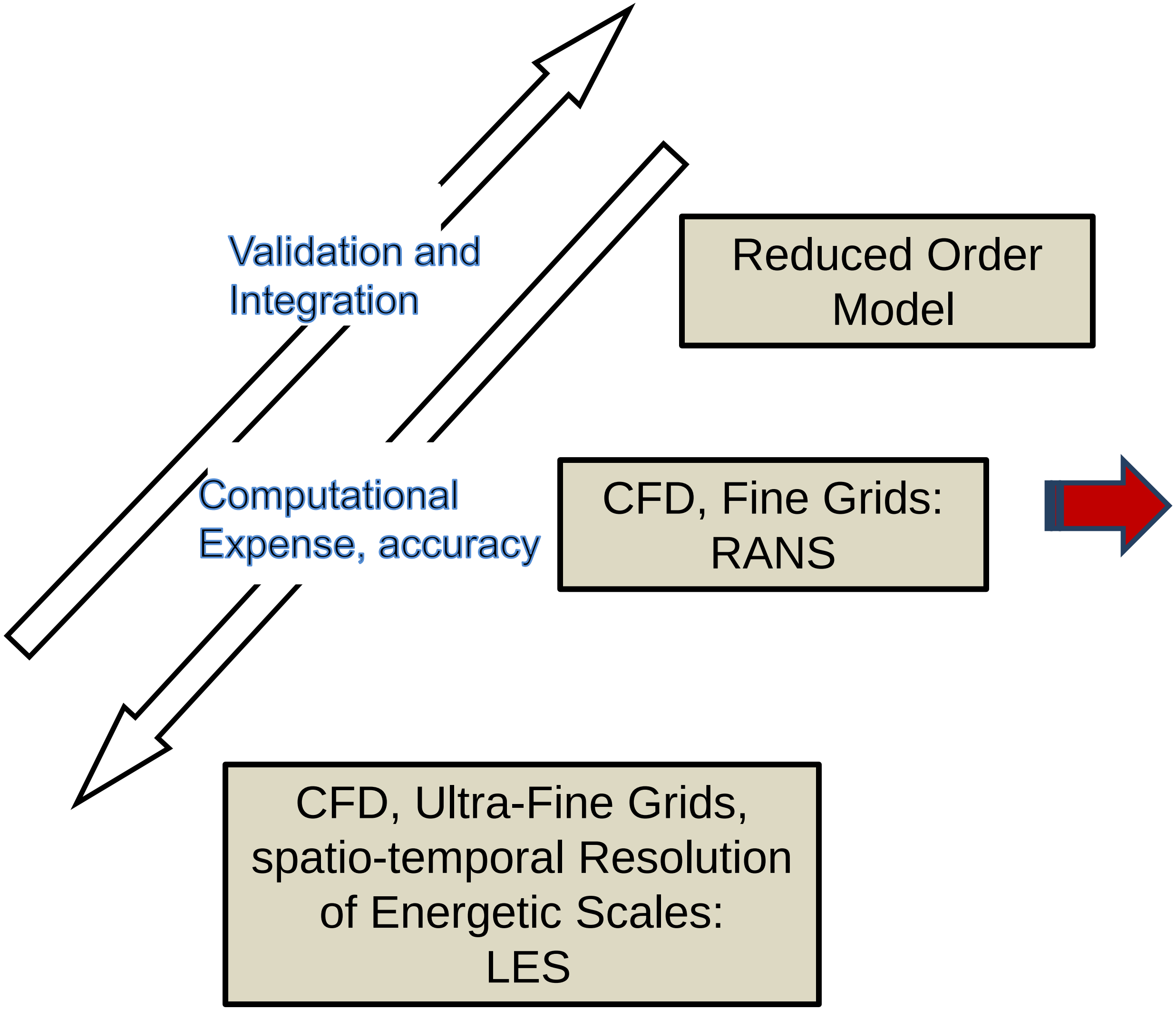
Gasifier Integrated in Polygeneration/IGCC





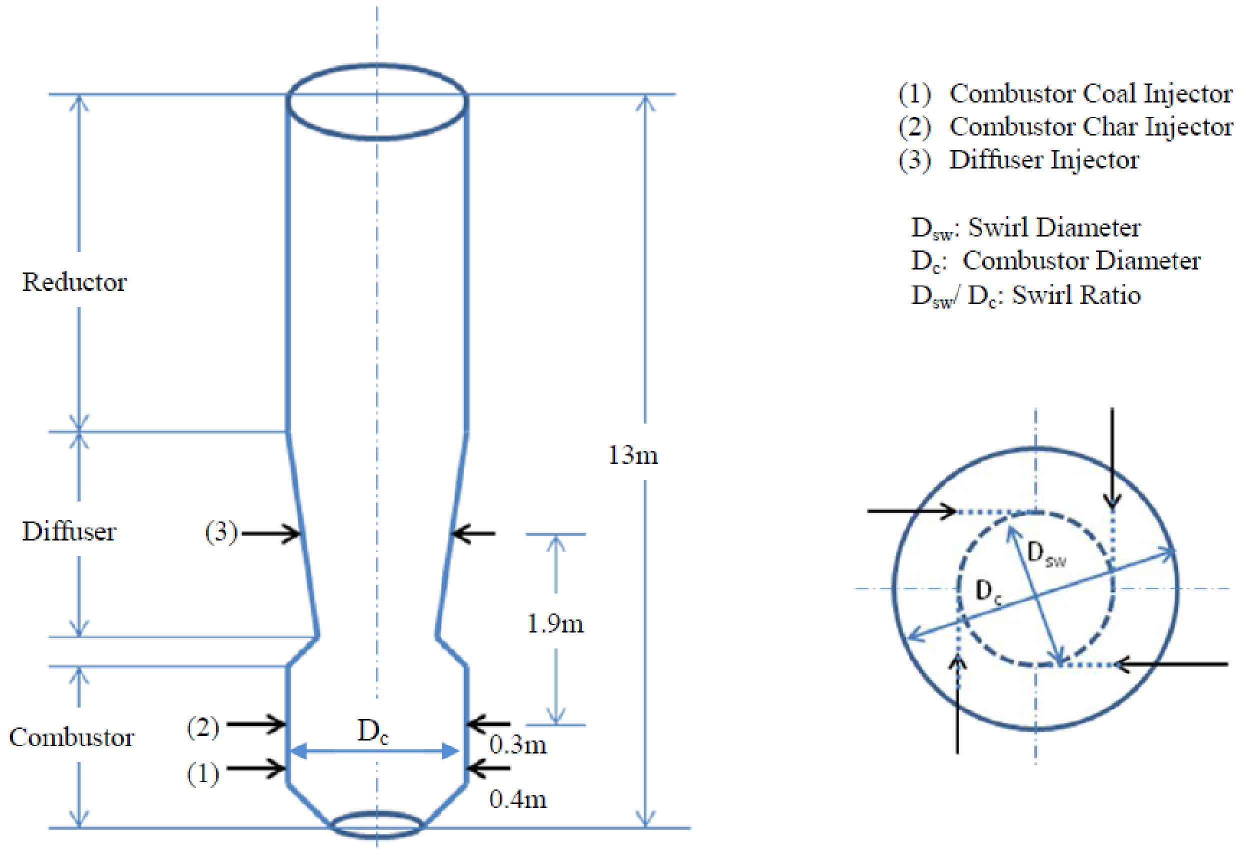
CFD Modeling
Gas Phase – Eulerian Description
Conservation of Mass, Species, Momentum and Energy
Particle-Source-in-Cell Approach
Particle Phase –Lagrangian Description
Particle Position, Velocity, Temperature
$\overline{T}(\vec{x},t)$ $\overline{k}_a(\vec{x},t)$
Radiative Source-Term in Energy Equation
Radiative Heat Transfer
Turbulence
$\overline{\vec{u}}(\vec{x},t), \overline{T}(\vec{x},t)$
Particle Dispersion ($\vec{x}_p, \vec{u}_p, T_p$)
$\overline{Y}_\alpha(\vec{x},t)$
Combustion Model

CFD modeling……in perspective



- Testing utility and limits of applicability of a commercial CFD solver
- With improved submodels incorporated via UDFs

RANS modeling: Two-stage Entrained Flow Coal Gasifier

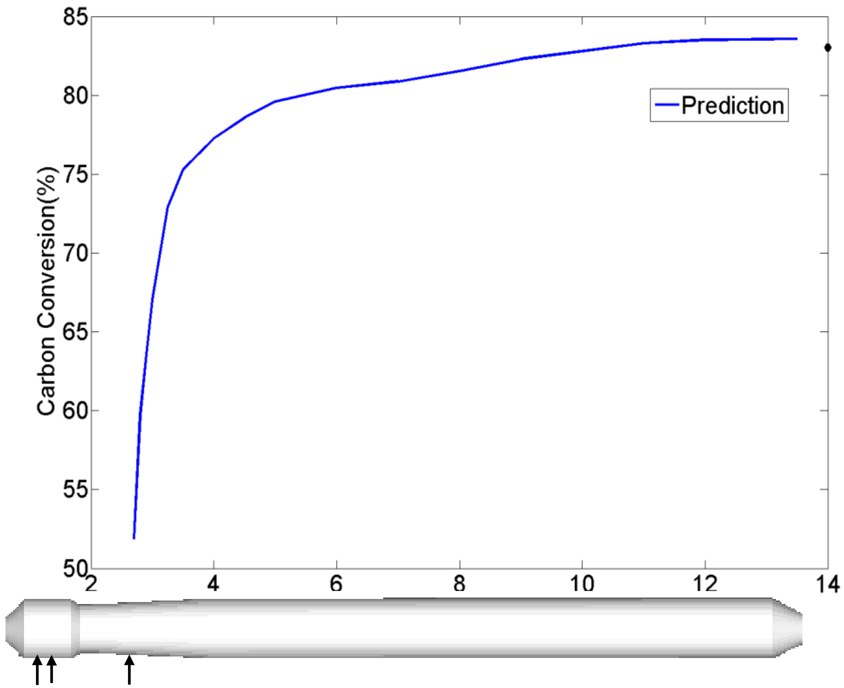


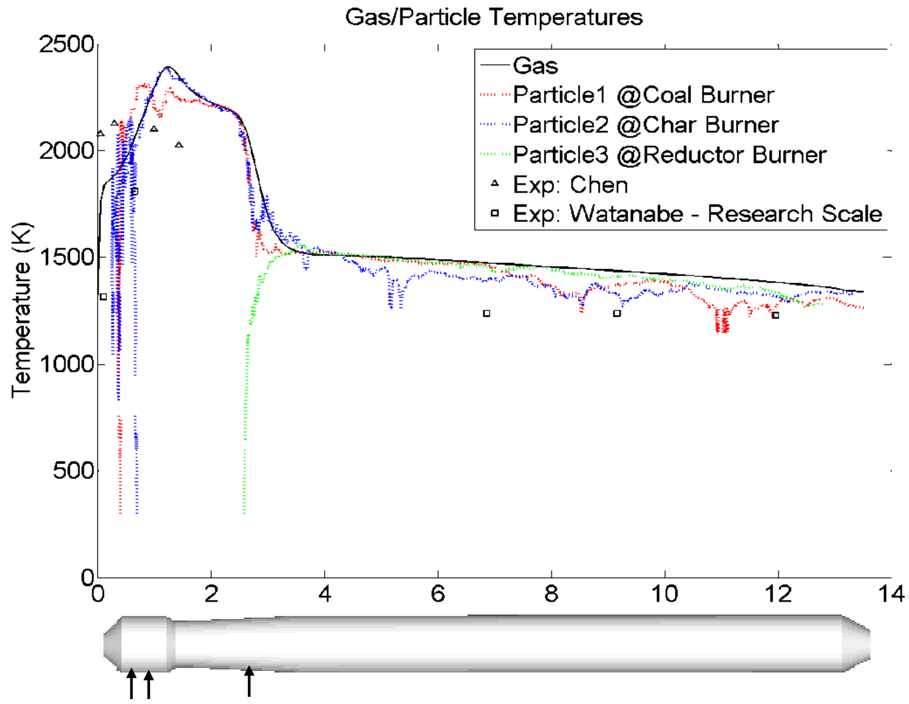
Schematic view of the gasifier

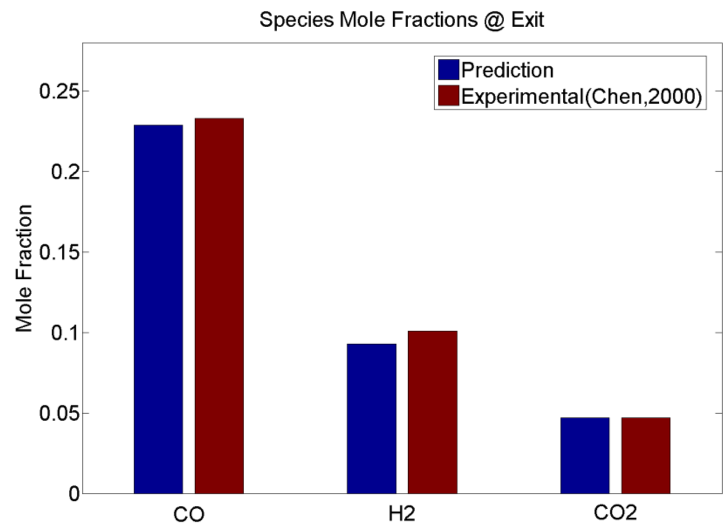
- Mitsubishi Heavy Industries design
- Air-blown, dry coal feed
- 200 tons/day pilot scale

Chen et al., Chem Eng. Sci, 55, pp.3861-3874 (2000).

Sample Results



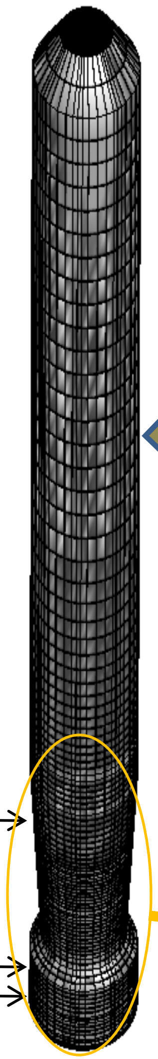




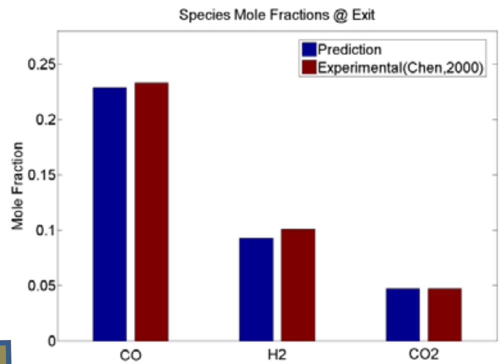
- Species and conversion are in good agreement with experimental data
- Discrepancy in temperature prediction

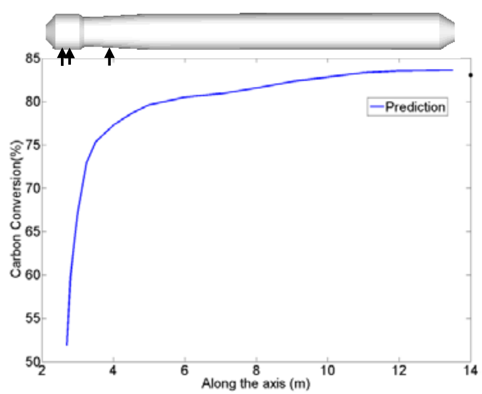
Validation studies

Use canonical cases in literature to validate the basic constituent models



Two-stage, air blown, dry feed, MHI design

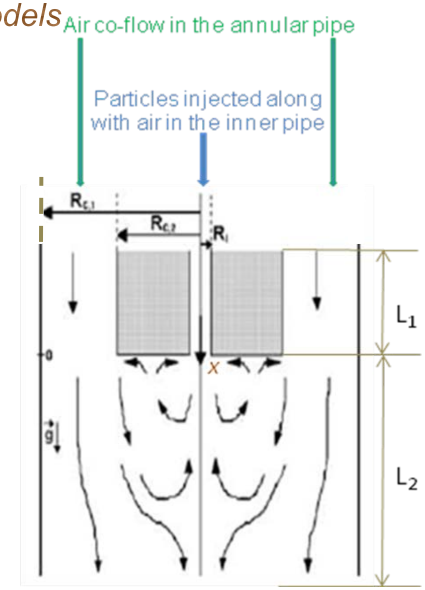




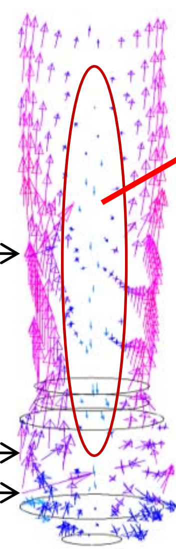
Kumar et. al., Proc. ASME Intl. Mech. Eng. Cong. & Expo, Florida, 2009.

An Extensive and "Modular" validation approach needed

Is validation of the integrated model SUFFICIENT?



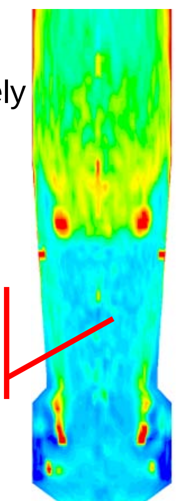
Two-phase bluff body flow



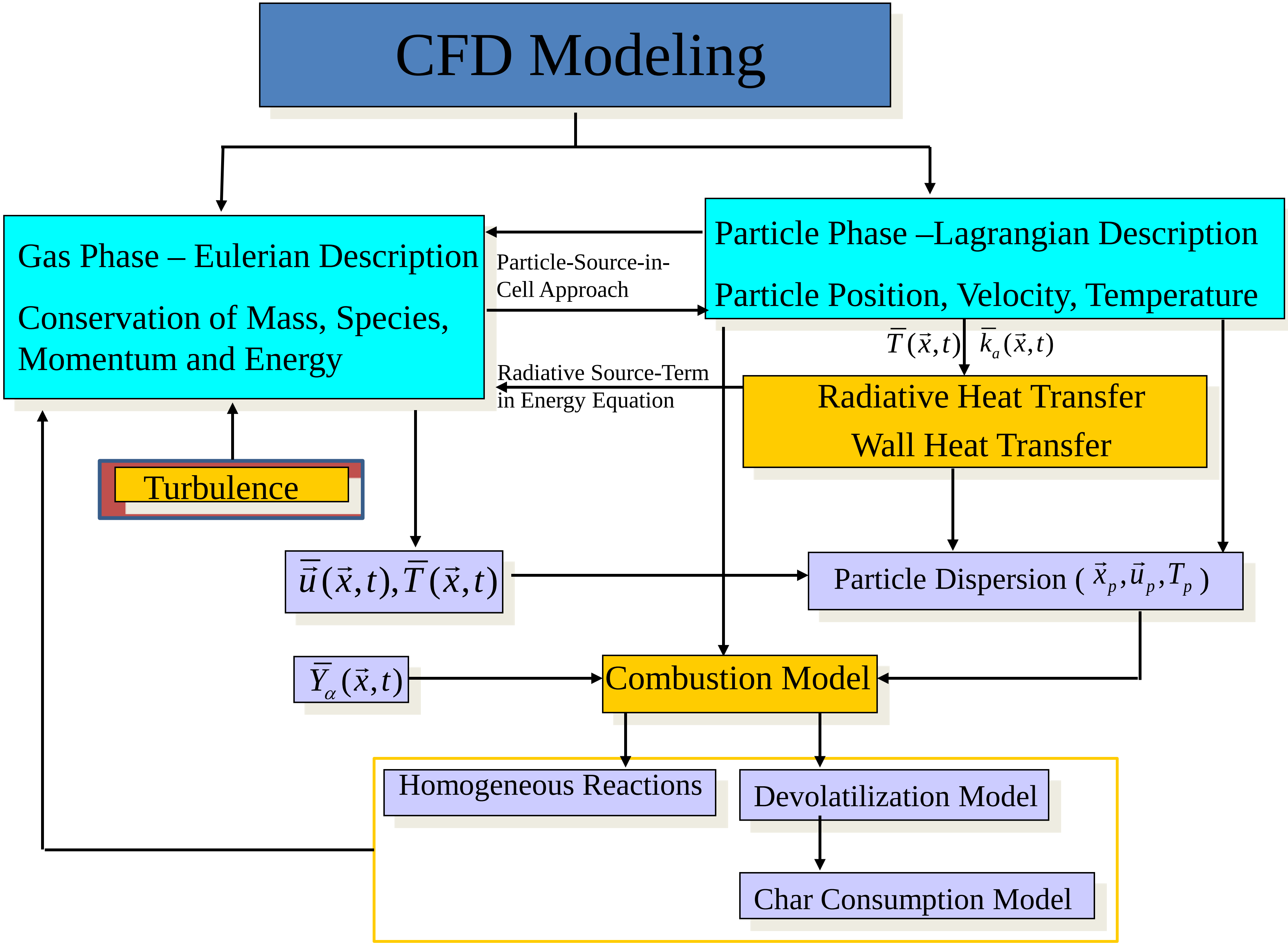
Velocity Vectors

Which turbulence model can accurately predict the recirculation zone ?

Is char distribution accurately predicted by the turbulent particle dispersion model?



Char Concentration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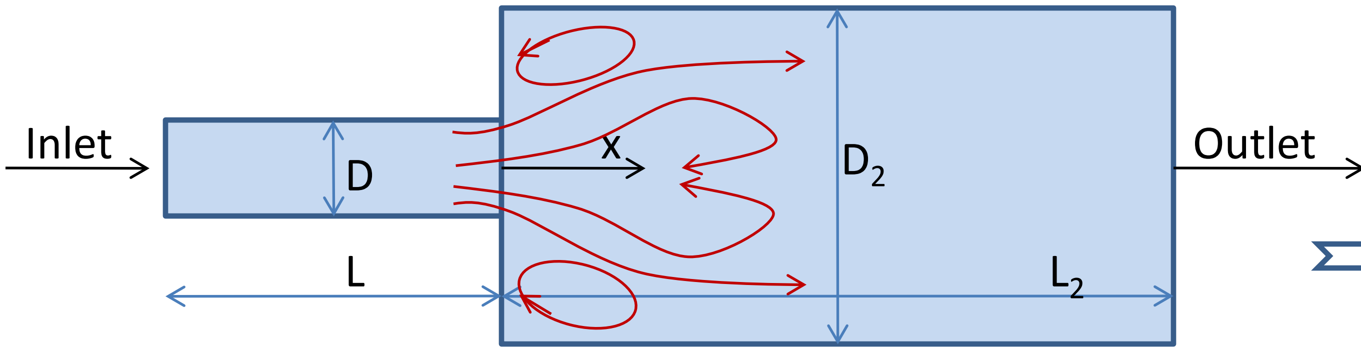
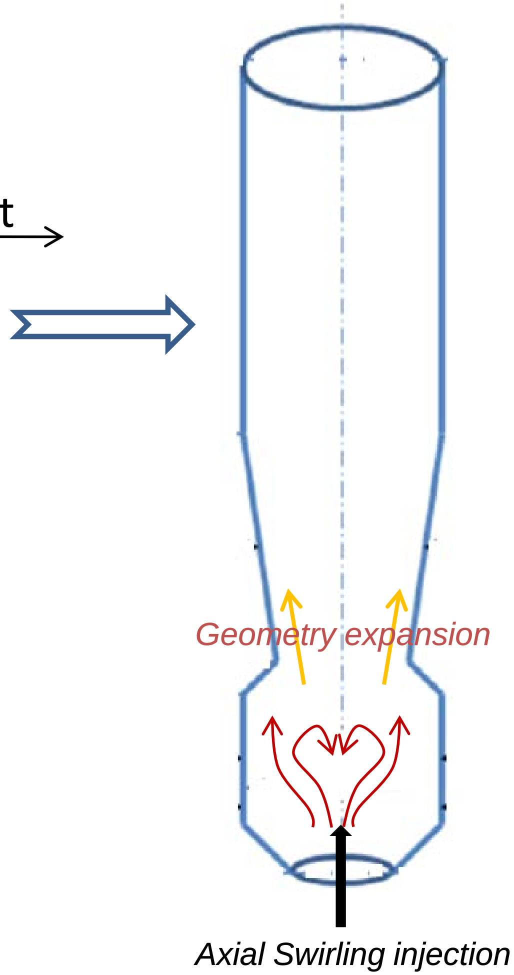
Combustion Model
Homogeneous Reactions
Devolatilization Model
Char Consumption Model

Sudden Axisymmetric Expansion Test Case





D = 5.078 cm
L = 2D

D_2 = 1.94D
L_2 = 11.8D
Re = 30000

Velocity data at section x = -2D is used for velocity-inlet boundary condition.
Turbulent intensity is specified as 10% at inlet.

800k grid points, denser near all the walls and also in the mixing layer.
For LES, a further refined mesh of 1.7 million points was also used.

RANS : k-ε vs k-ω turbulence model

k-ε Model Equations:

$$\frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G - \rho\varepsilon + S_k$$

$$\frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_1 G - C_2\rho\frac{\varepsilon^2}{k} + S_\varepsilon$$

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

k-ω Model Equations:

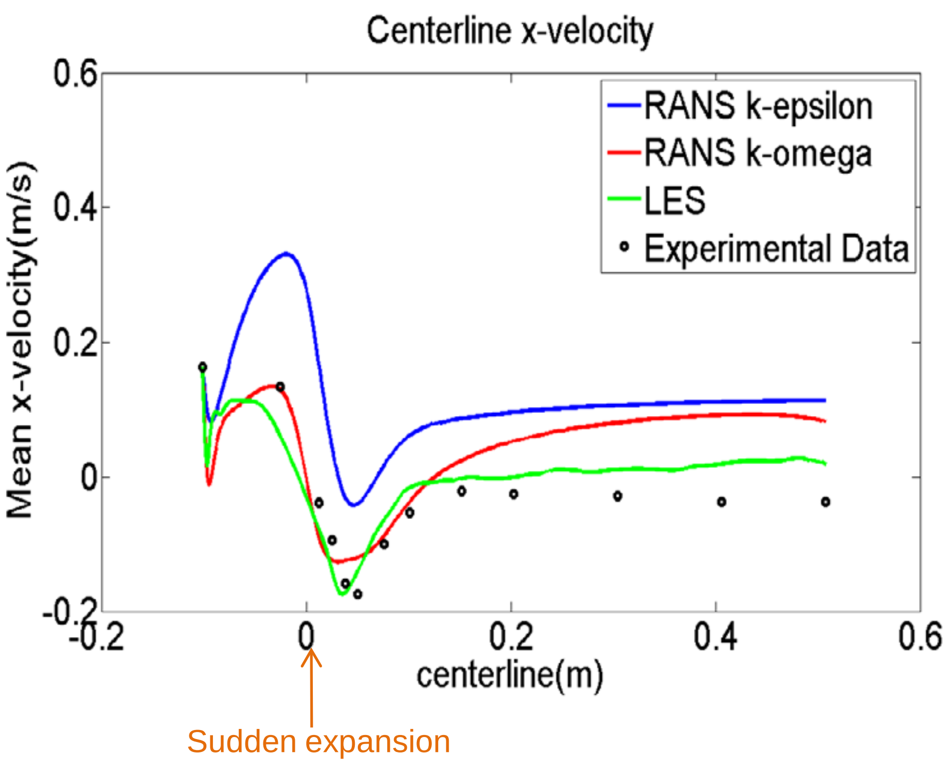
$$\frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\Gamma_k \frac{\partial k}{\partial x_j}\right] + G_k - Y_k + S_k$$

$$\frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\Gamma_\omega \frac{\partial \varepsilon}{\partial x_j}\right] + G_\omega - Y_\omega + S_\omega$$

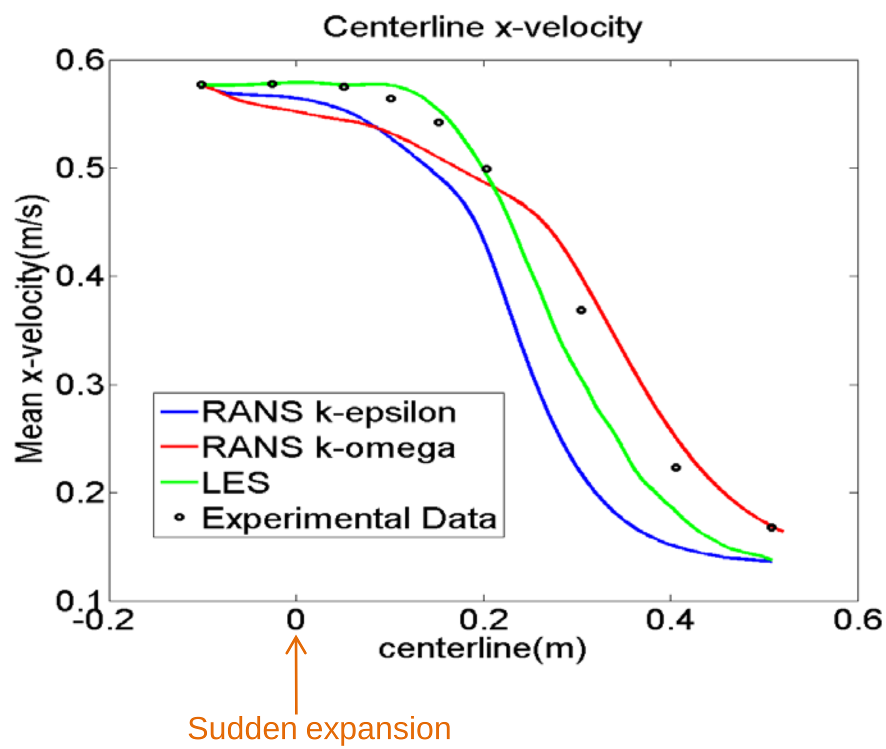
- ω, the specific dissipation rate can be thought of as a ratio of k and ε
- k-ω model is reported to be better for swirling and shearing flows.

Sudden Expansion Test Case: Results

Swirling flow

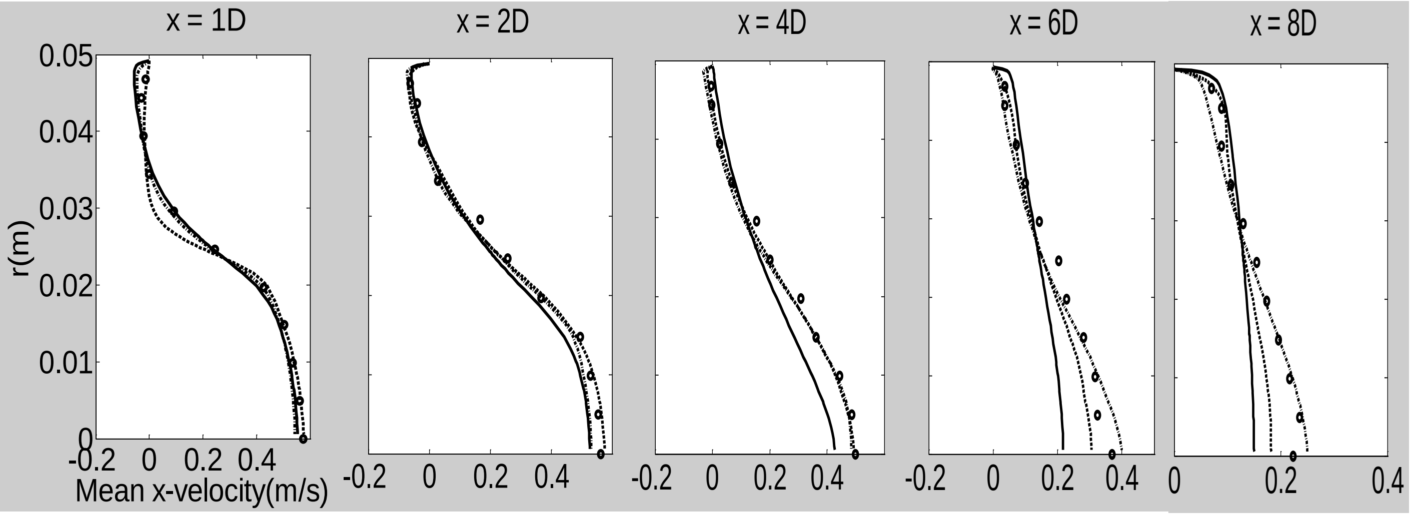


Non-swirling flow

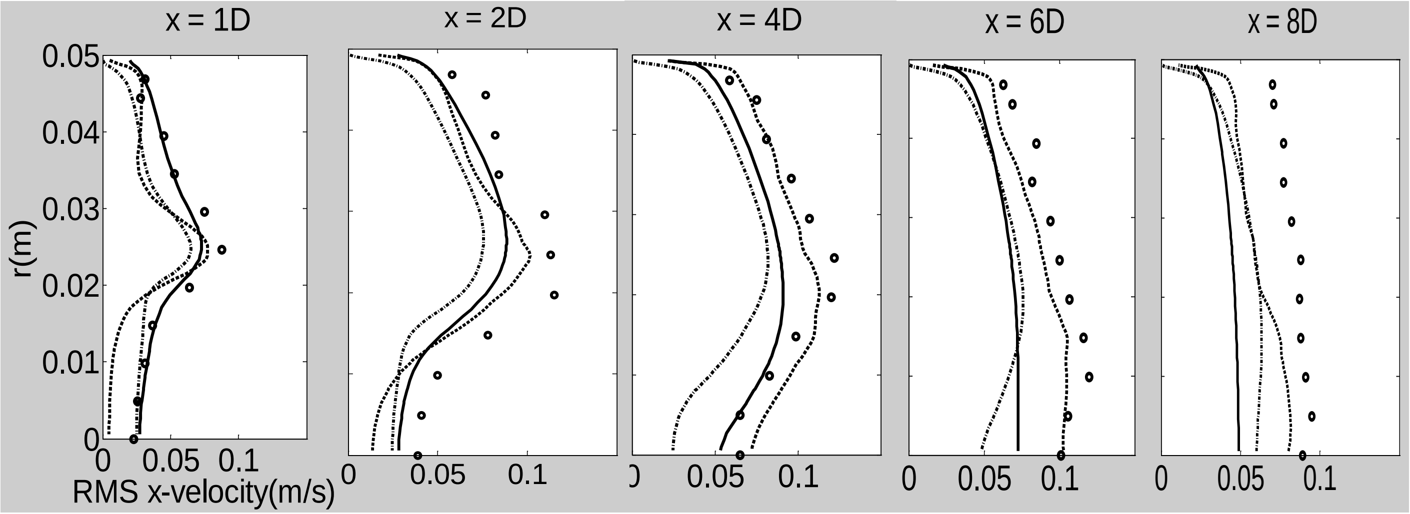


- LES provides best predictions of x-velocity along centerline, k-ω model also predicts well.

Sudden Expansion Test Case: *Non-swirling* flow



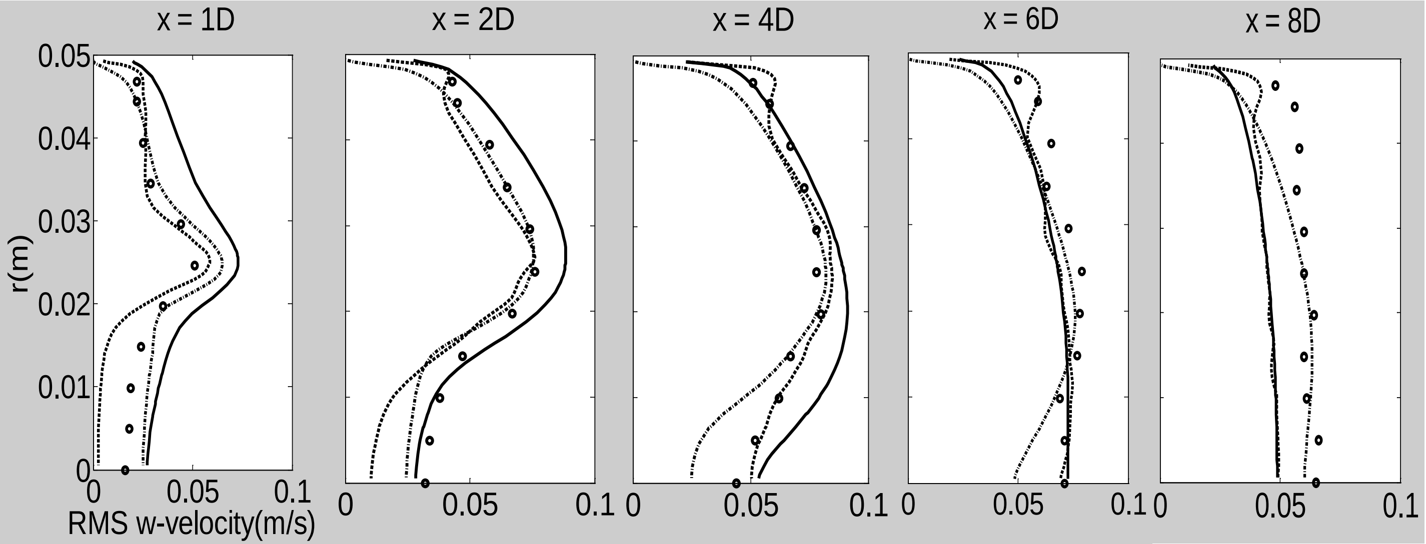
Mean x-velocities, non-swirl case. Solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments



RMS x-velocities, non-swirl case. Solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

- LES and RANS k-ω are more accurate than RANS k-ε .

Sudden Expansion Test Case: *Non-swirling* flow



RMS tangential velocities, non-swirl case. Solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

Calculating fluctuation velocities in RANS:

$$u'^2 + v'^2 + w'^2 = 2k$$

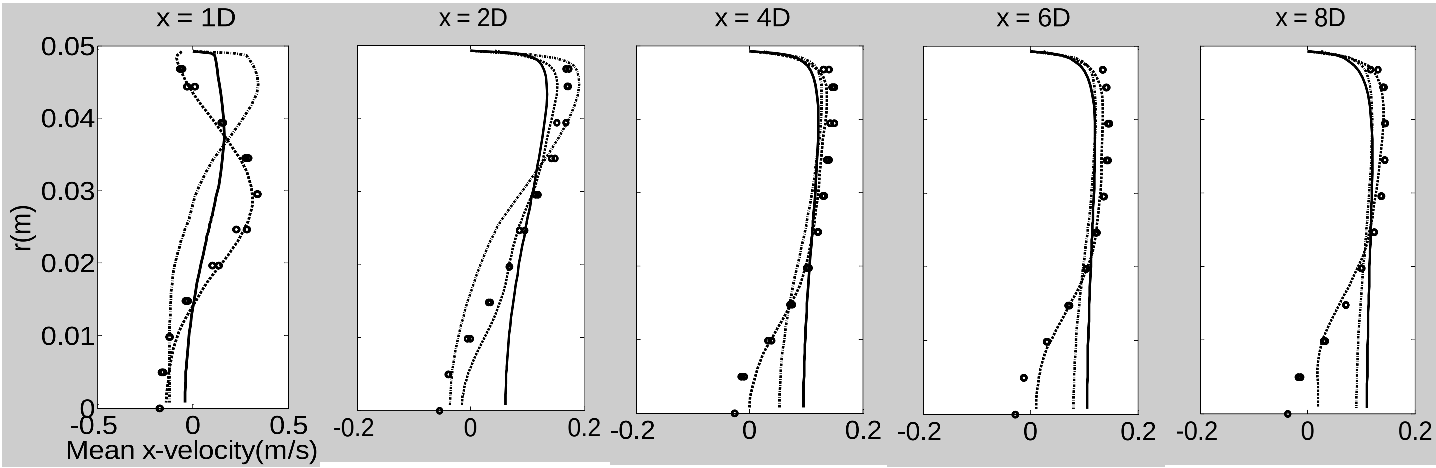
k is the turbulent kinetic energy, solved for in RANS

$$\Rightarrow u' = v' = w' = \sqrt{2k/3}$$

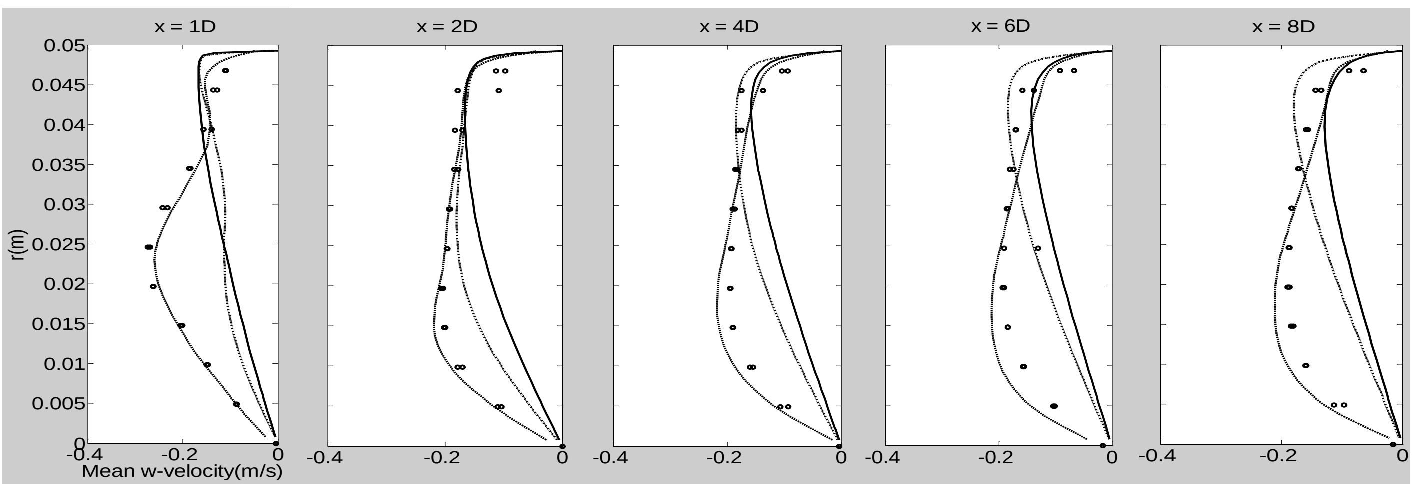
Assuming isotropic turbulence

- Accurate prediction of the turbulent kinetic energy, *k*, also leads to accurate prediction of the particle trajectories via the particle turbulent dispersion model.
- RANS prediction of rms values is also acceptable.

Sudden Expansion Test Case: *Swirling* flow



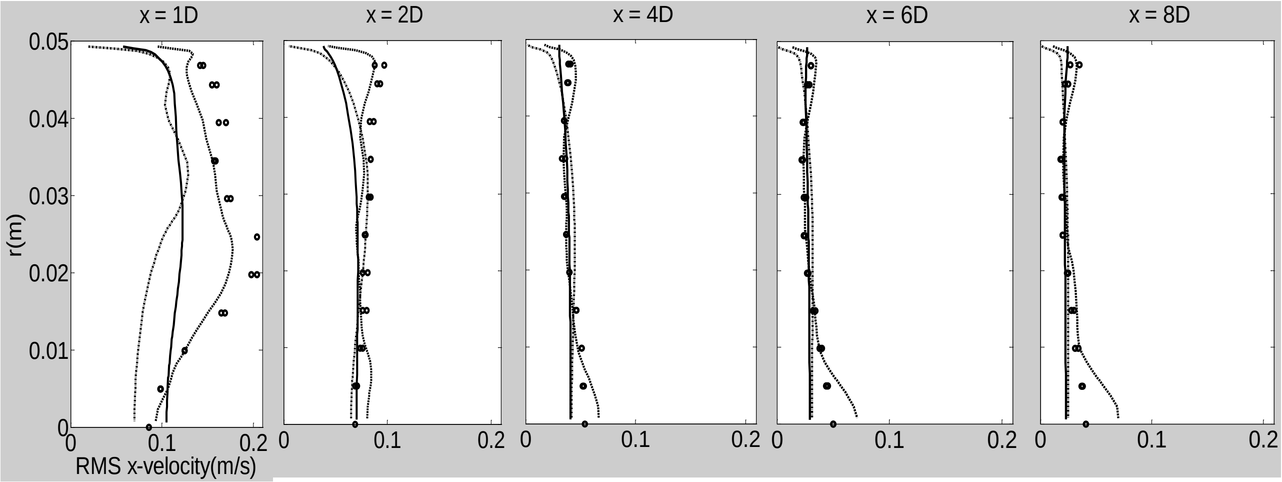
Mean x-velocities, swirl case. solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments



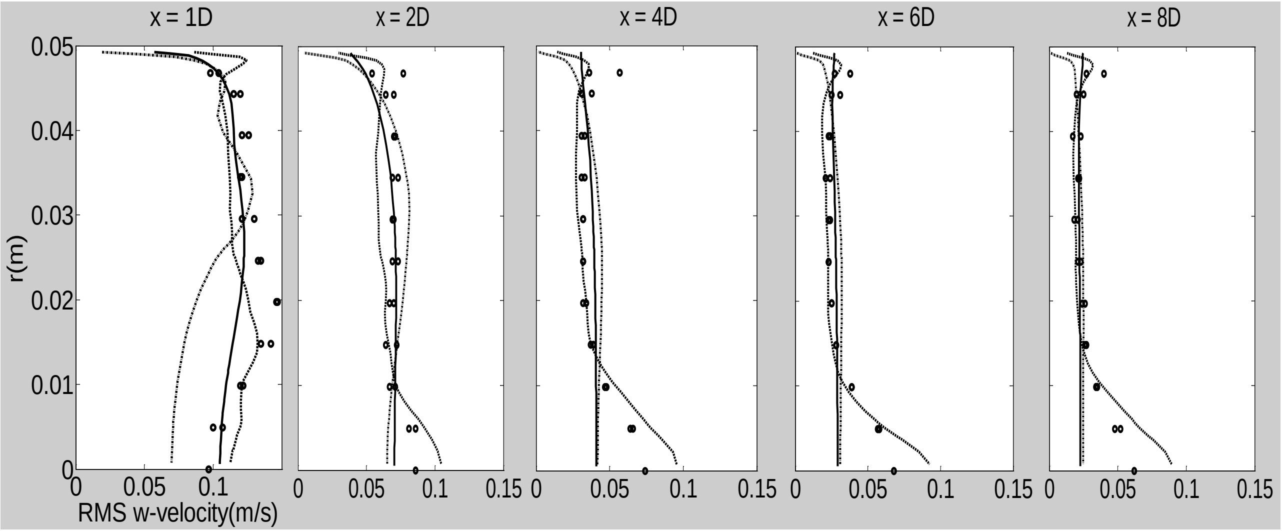
Mean tangential velocities, swirl case. solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

- LES is accurate, but the RANS k-ε model does not seem to predict the swirling flow well, the k-ω model performs slightly better.
- Swirl number is high (*S*=0.6) in this case. Sommerfield et. al (1992) predicted mean flow field well with k-ε model with moderate swirl number (*S*=0.47) in a sudden expansion geometry.

Sudden Expansion Test Case: *Swirling* flow



RMS x-velocities, swirl case. Solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments



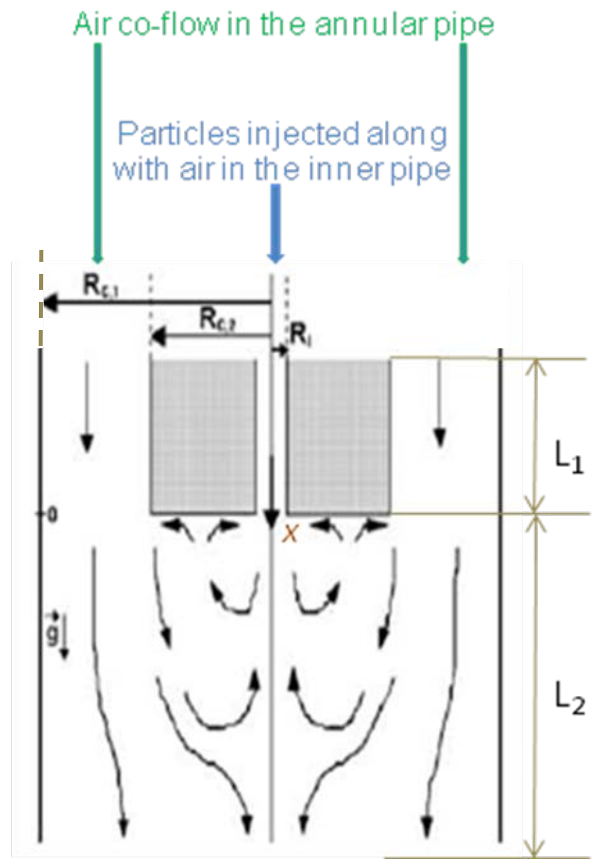
RMS tangential-velocities, swirl case. Solid line: k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

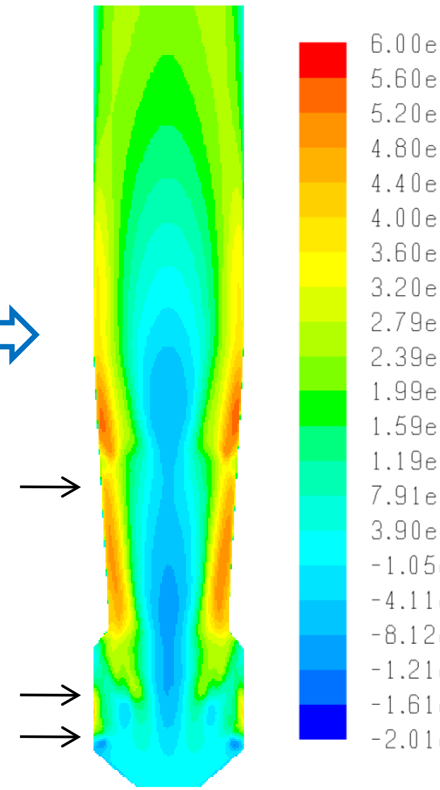
➢ In gasifiers with high swirl numbers (S~0.6), standard k-ε model may lead to inaccurate prediction of flow field.

Two-phase bluff body flow case

R_1 = 0.01 m
$R_{c,1}$ = 0.15m
$R_{c,2}$ = 0.075m
Re ≈ 73000
L_1= 0.1 m
L_2 = 0.8 m

$$\frac{\overline{U_l}}{\overline{U_C}} = 0.84$$

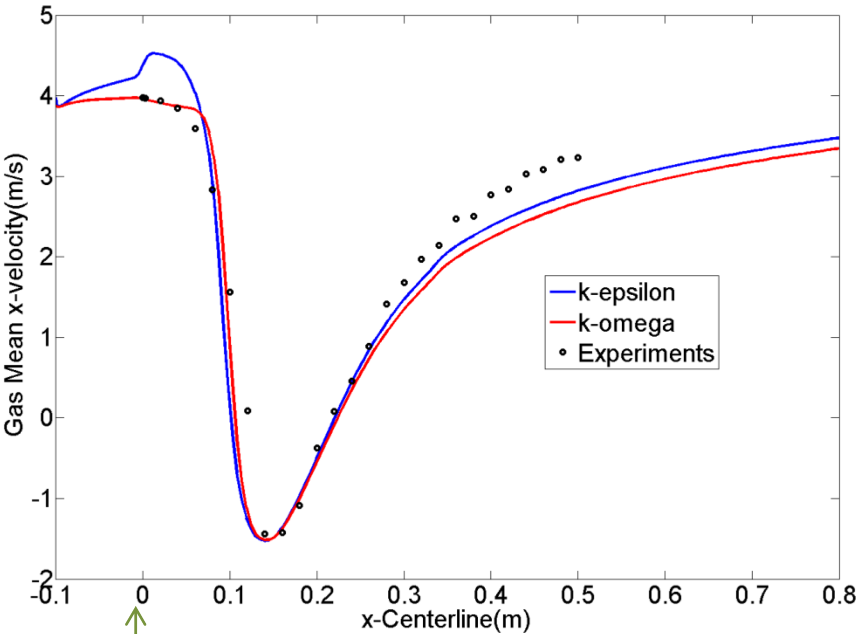




Contours of x-velocity

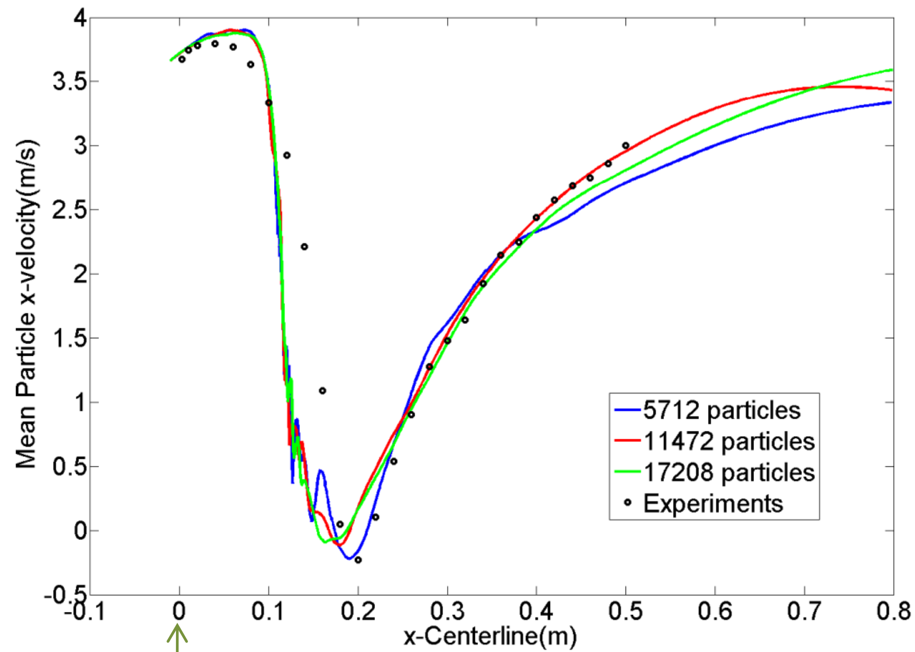
- length of the simulation domain downstream of bluff body : 0.8 m
- particle phase: glass beads
- particles are injected with air in the inner pipe. Only air is fed into the co-flow.
- The case is used for validation of flow solver and the particle turbulent dispersion model.

Bluff Body Test Case: Results



Gas mean x-velocities. Solid line: RANS k-ε , symbols: experiments

expansion

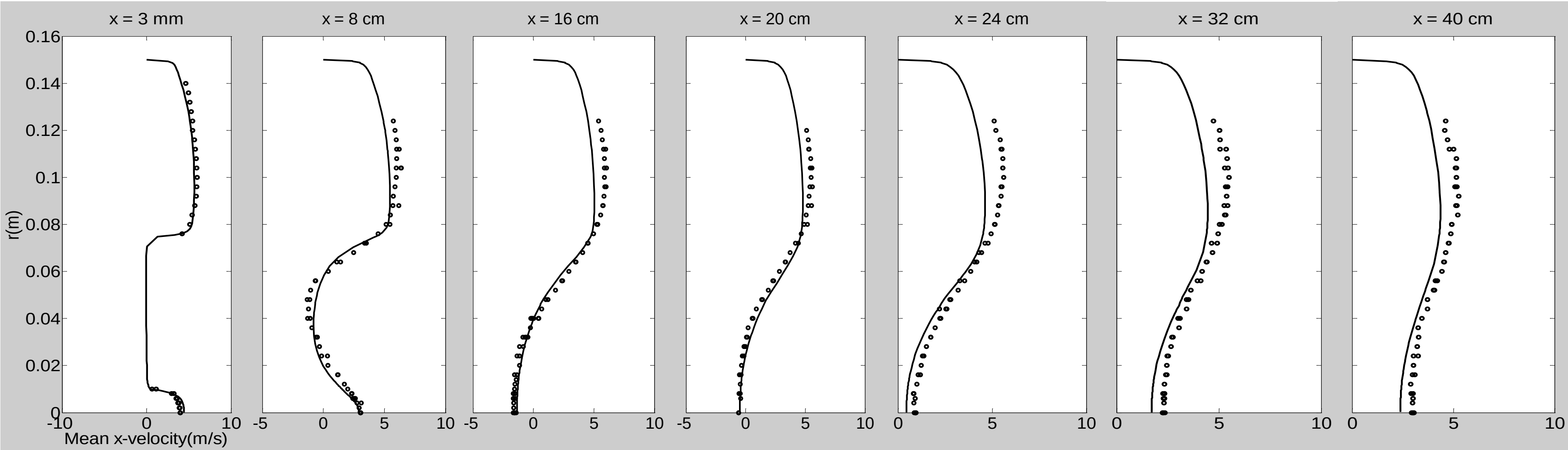


Particle mean x-velocities. Solid line: predictions, symbols: experiments

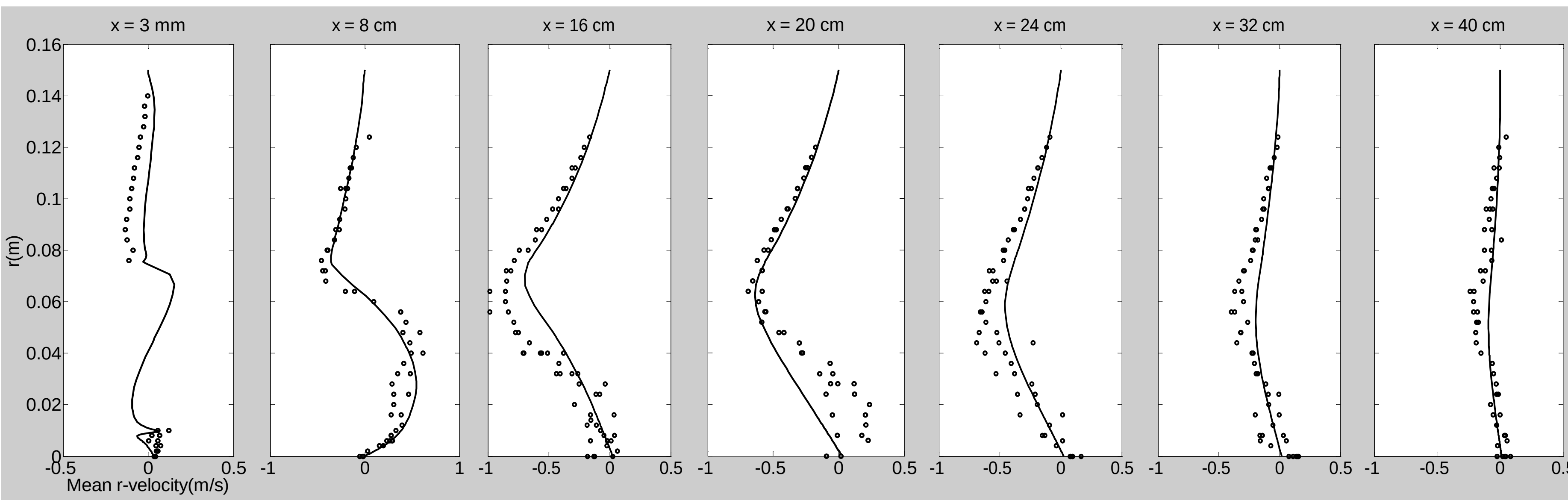
expansion

- Gas mean x-velocity is predicted well along the centerline by the RANS standard k-ε model.
- Particle mean x-velocities are also reasonably predicted. Though the centerline x-velocity is underpredicted just downstream of the bluff body, predictions are good farther downstream; the radial variations are also well predicted as shown later.

Bluff Body Test Case: *Gas Phase* Results



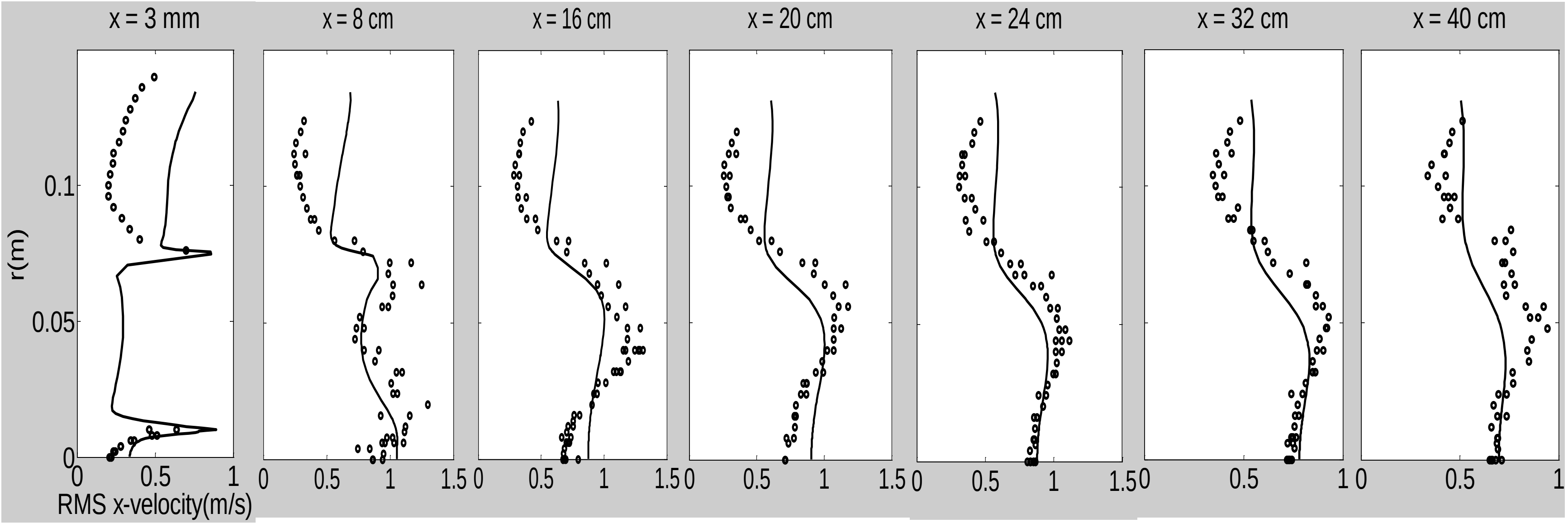
Gas mean x-velocities. Solid line: RANS k-ε , symbols: experiments



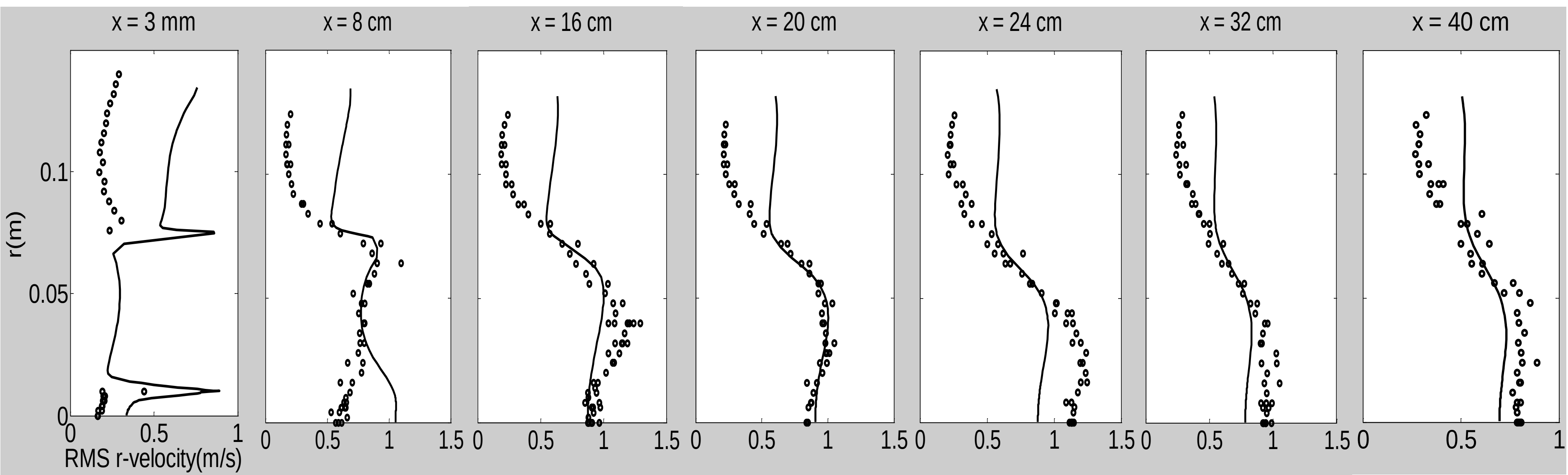
Gas mean radial-velocities. Solid line: RANS k-ε , symbols: experiments

- The radial variations of both axial and radial velocities are well predicted.

Bluff Body Test Case: *Gas Phase* Results

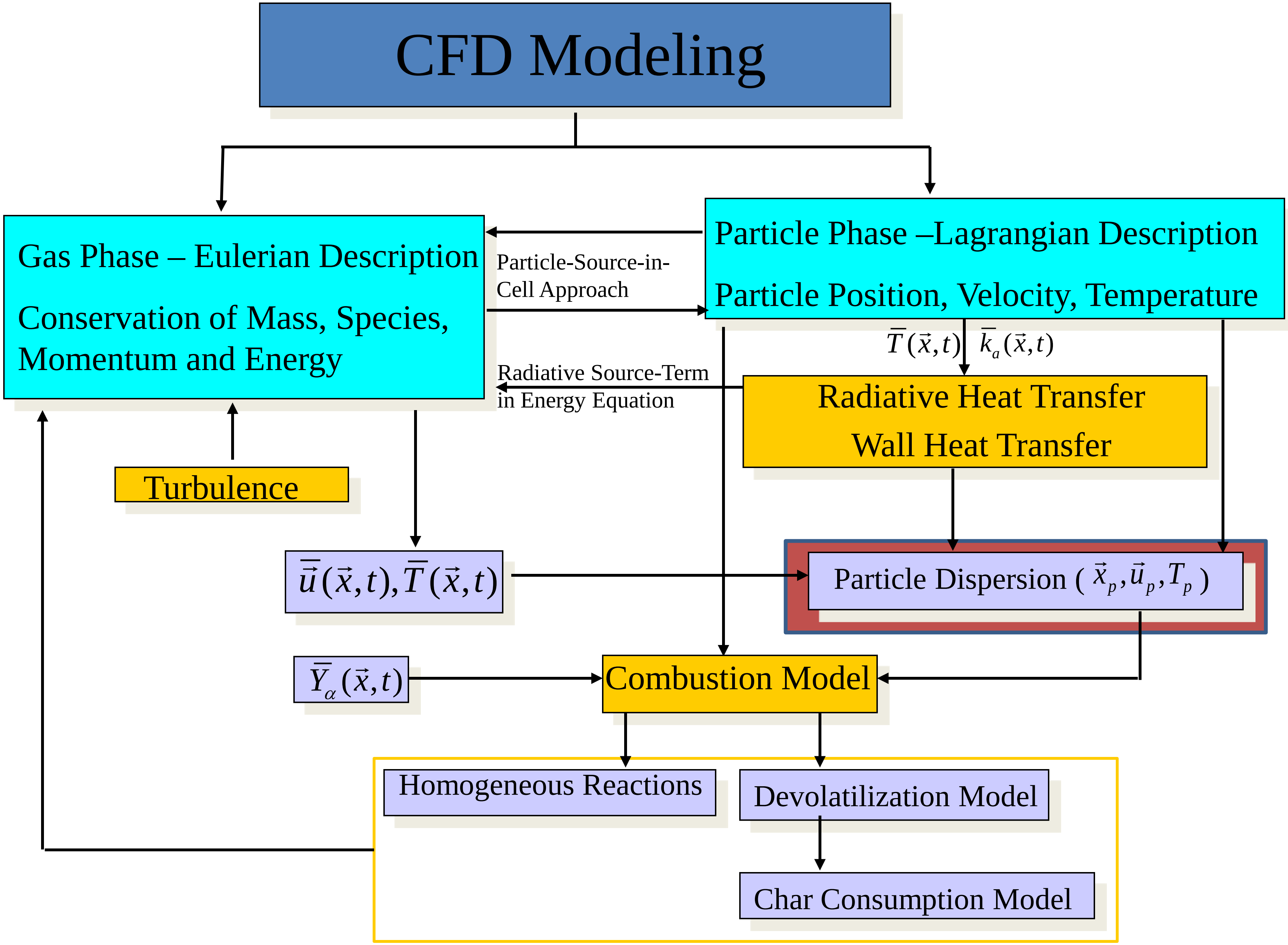


Gas rms x-velocities. Solid line: RANS k-ε , symbols: experiments



Gas rms radial-velocities. Solid line: RANS k-ε , symbols: experiments

- The prediction of rms values is reasonable. There is some overprediction outside of the second shear layer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Particle Turbulent Dispersion Model

$$\frac{du_p}{dt} = C_D \frac{\rho}{\rho_p d_p} \left| u - u_p \right| \left(u - u_p \right) + F_x$$

: particle momentum equation

- Fluid turbulence model affects the particle trajectory calculation via the drag force term: the gas velocity *u* in the drag force has a mean and fluctuating component:

$$u = \overline{u} + u'$$

- The fluid fluctuation velocity is sampled using a normal distribution from the mean turbulent kinetic energy field:

$$u' = \varsigma \sqrt{\overline{u'^2}} = \varsigma \sqrt{2k/3}$$

- The particle is assumed to interact with a succession of fluid phase eddies during its trajectory and the particle-eddy interaction time is taken to be the smaller of the eddy-traverse time, T_{cross}, and the eddy lifetime, T_e

$$T_e = C_L \frac{k}{\varepsilon}$$

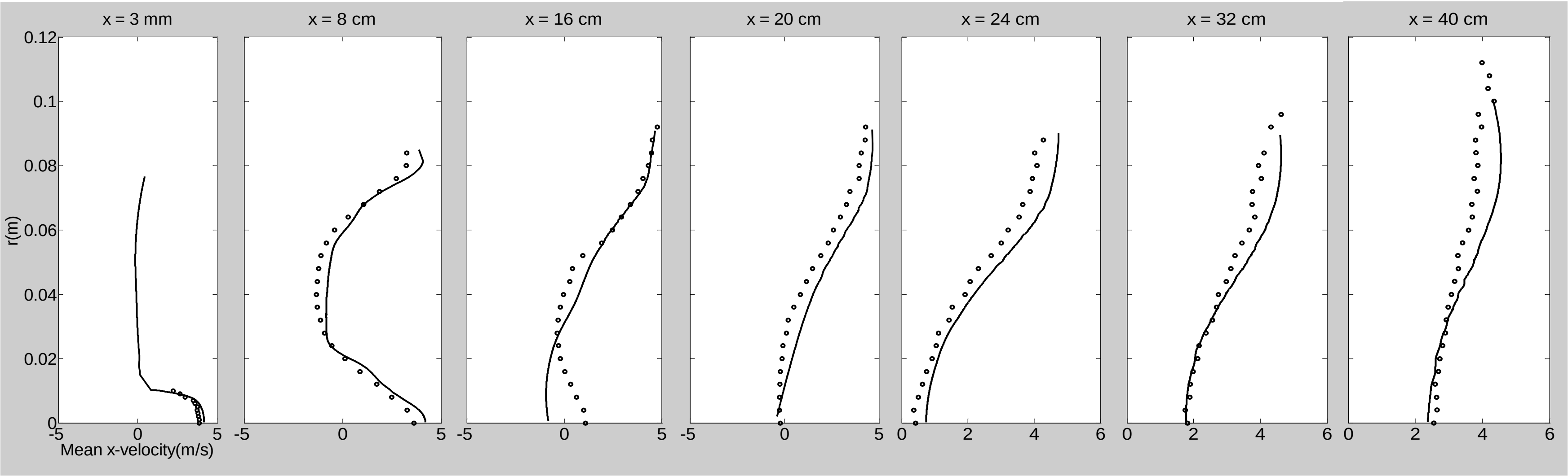
C_L not ‘well-known’

$$T_{cross} = \tau \ln \left[1 - \left(\frac{L_e}{\tau \left| u - u_p \right|} \right) \right], \quad L_e = C_{Le} \frac{k^{1.5}}{\varepsilon}$$

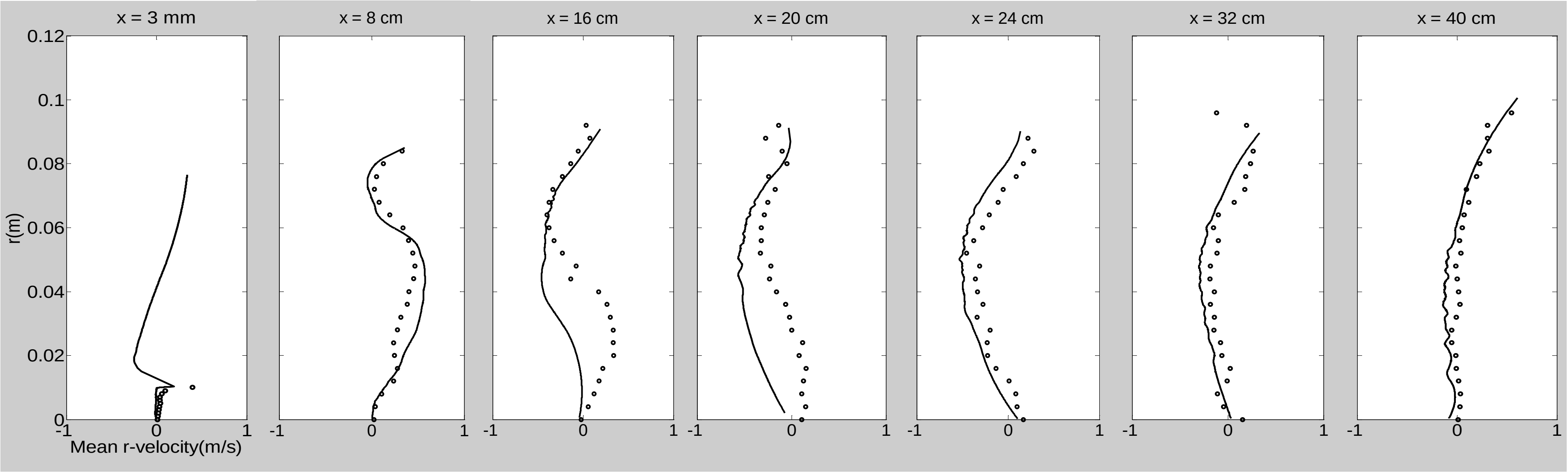
$$\tau = \frac{\rho_p d_p^2}{18\mu}$$

- By tracking a large number of representative particles, the effect of ‘random’ dispersion of particles by turbuelnce is taken into account.

Bluff Body Test Case: *Particle Phase* Results



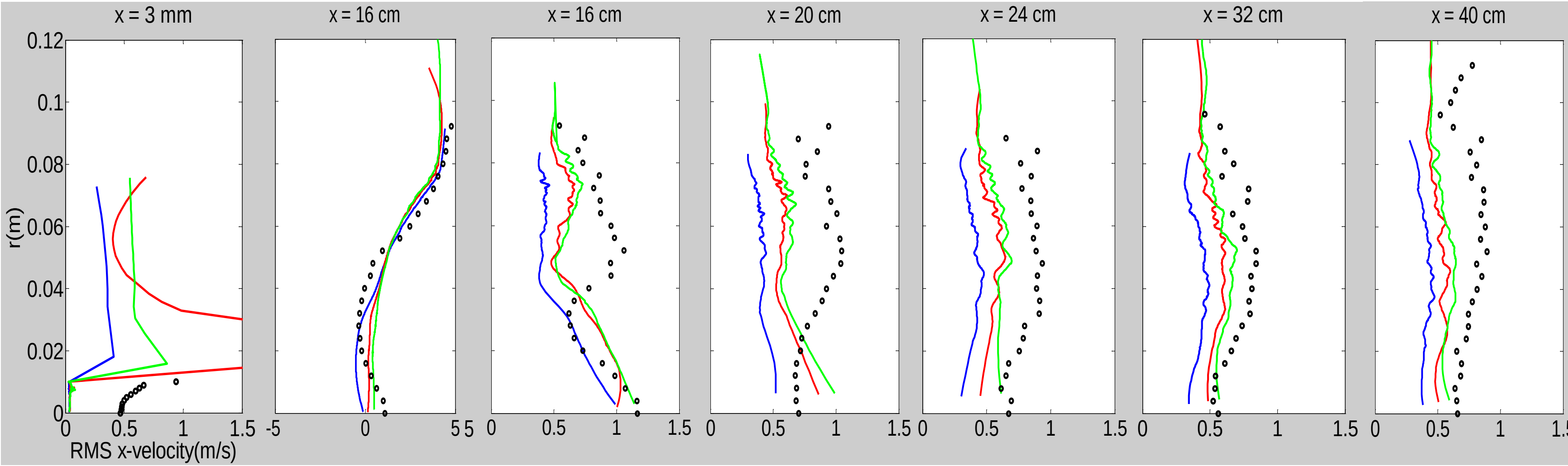
Particle mean x-velocities. Solid line: RANS k-ε , symbols: experiments



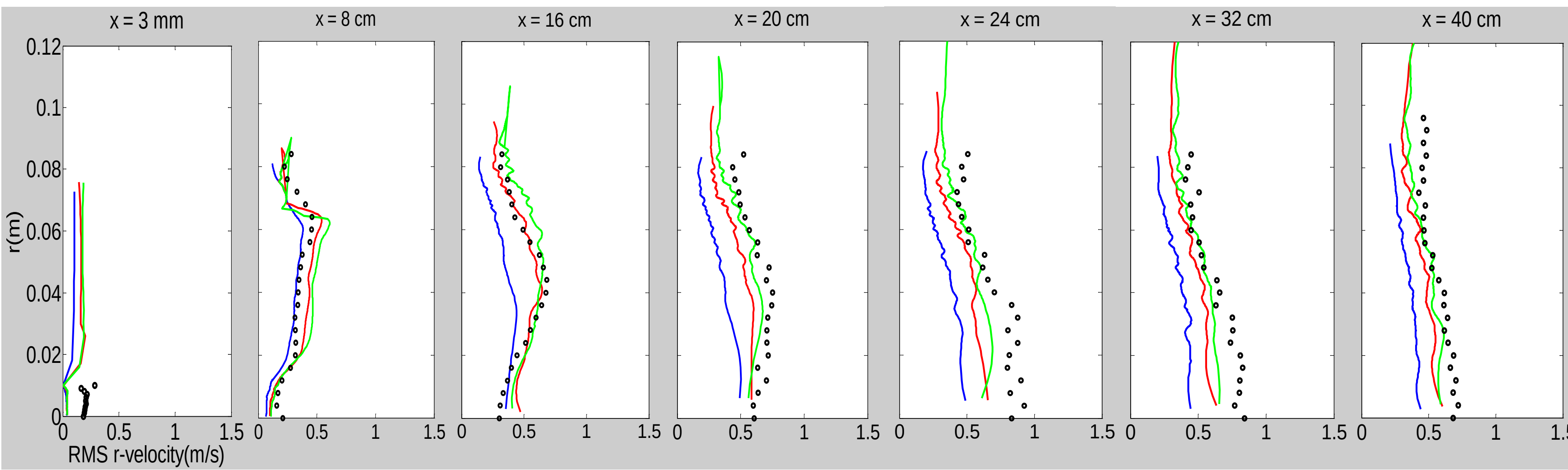
Particle mean radial-velocities. Solid line: RANS k-ε , symbols: experiments

- The mean velocities are predicted reasonably well, except for a couple of sections within the recirculation zone

Bluff Body Test Case: *Particle Phase* Results



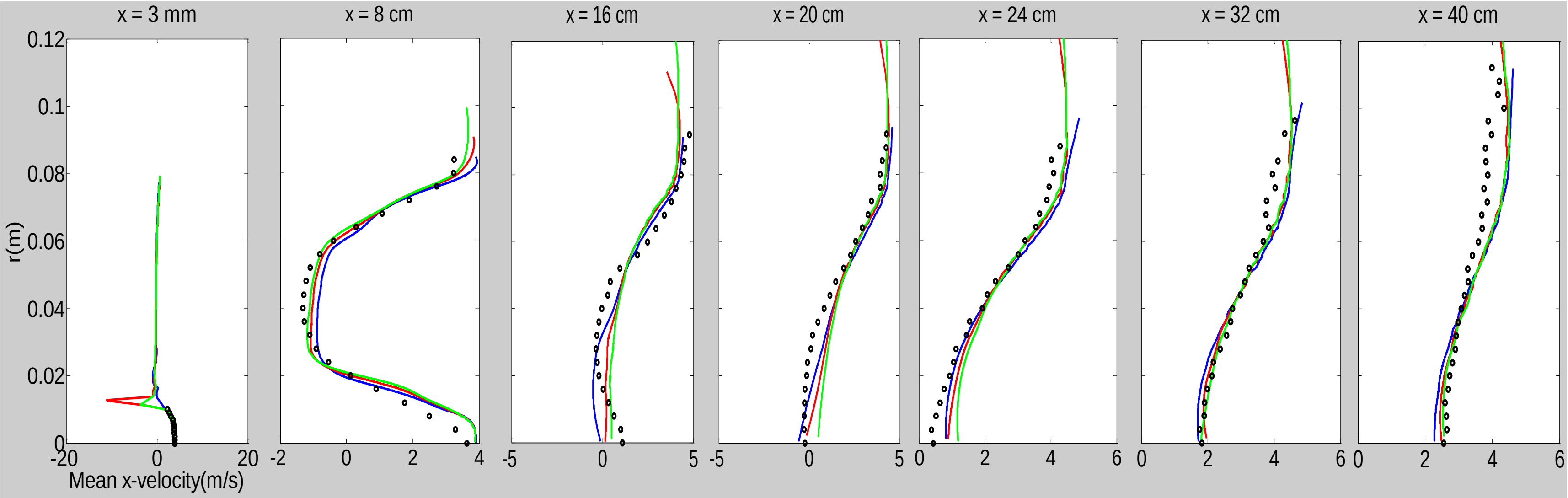
Particle rms x-velocities. RANS k-ε. Blue line: $C_L = 0.15$, Red line: $C_L = 0.4$, Green line: $C_L = 0.6$, , symbols: experiments



Particle rms radial-velocities. RANS k-ε. Blue line: $C_L = 0.15$, Red line: $C_L = 0.4$, Green line: $C_L = 0.6$, , symbols: experiments

- The rms values are affected by the value of C_L. $C_L = 0.6$ leads to good agreement.

Bluff Body Test Case: *Particle Phase* Results



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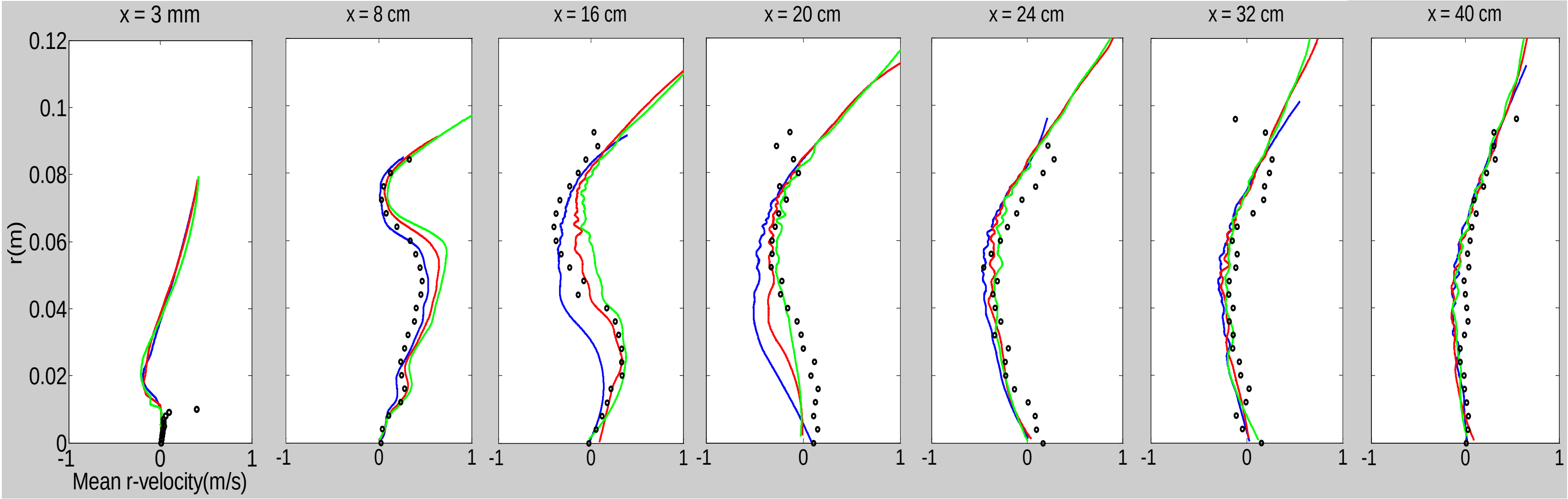
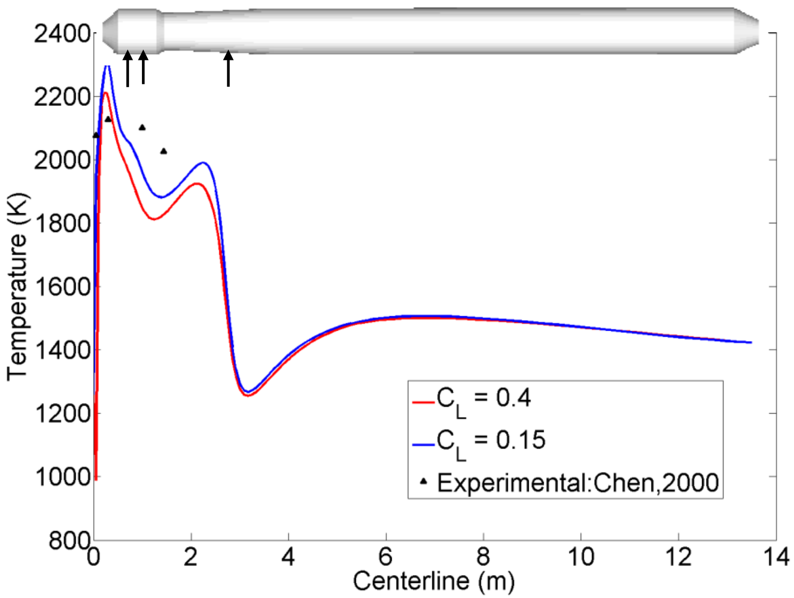
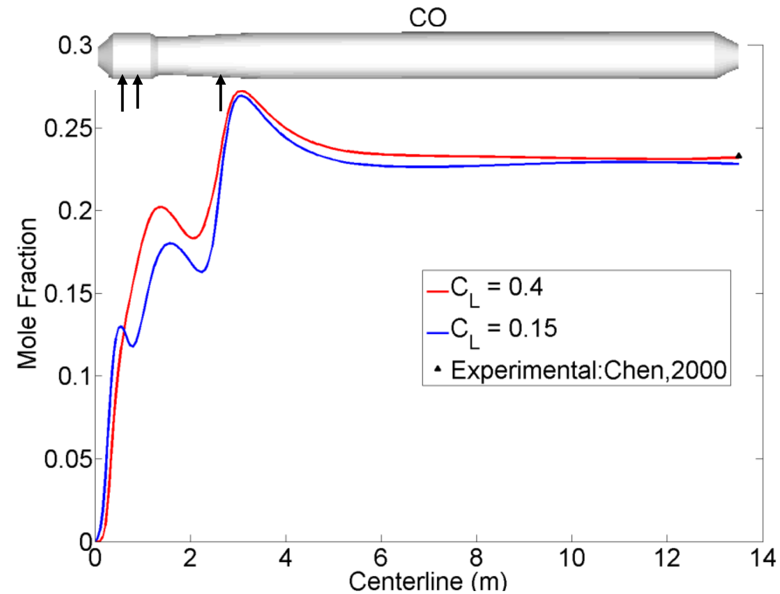
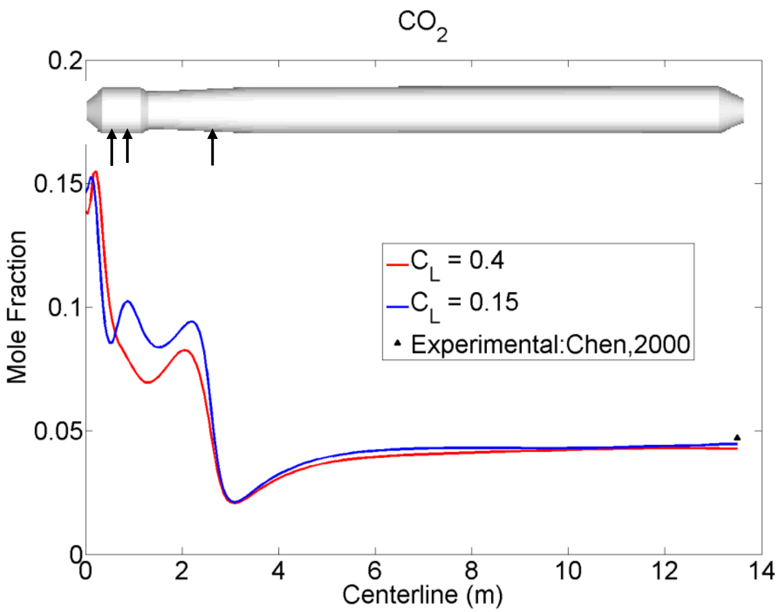


Particle mean r-velocities. RANS k-ε. Blue line: C_L = 0.15, Red line: C_L = 0.4, Green line: C_L = 0.6, , symbols: experiments

Particle Dispersion: Gasifier

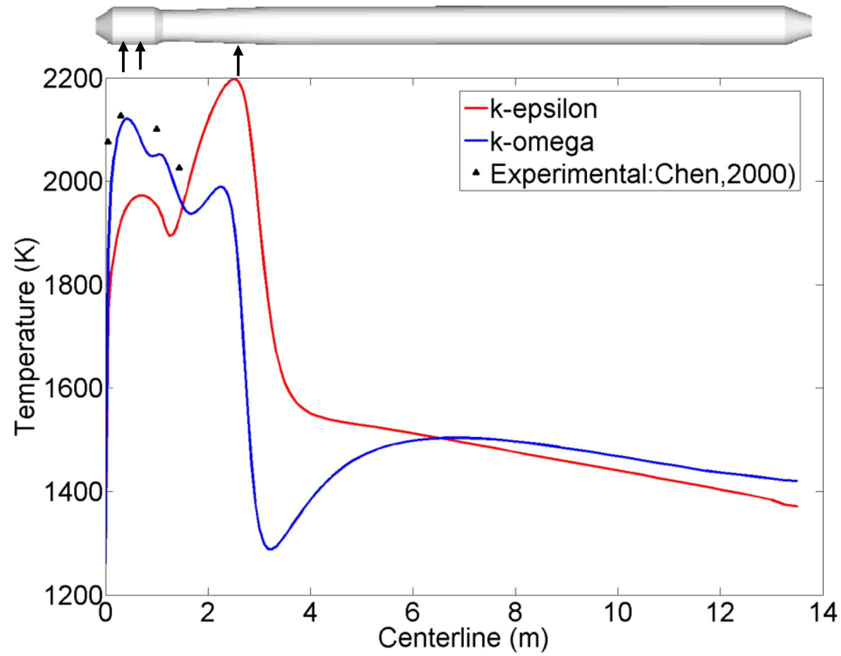


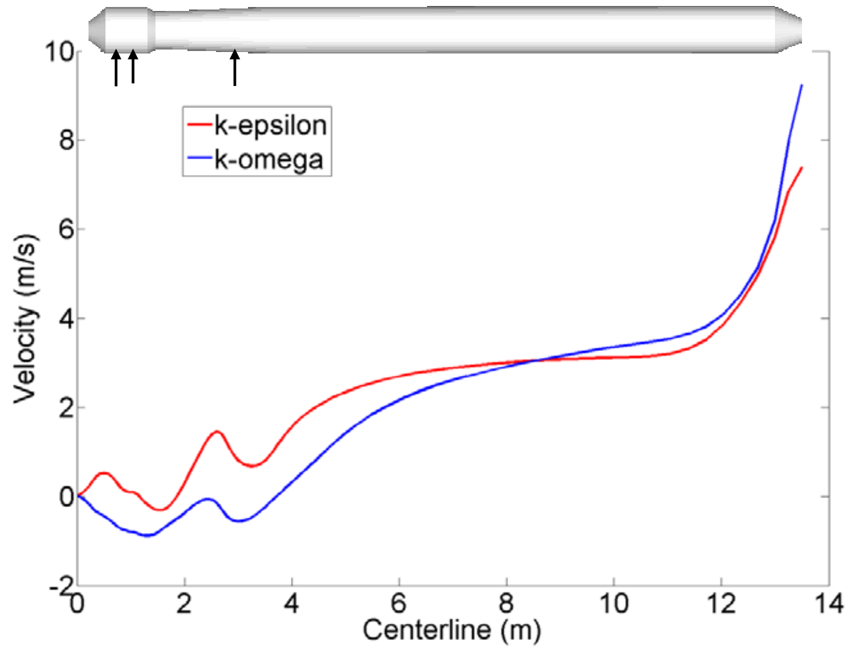


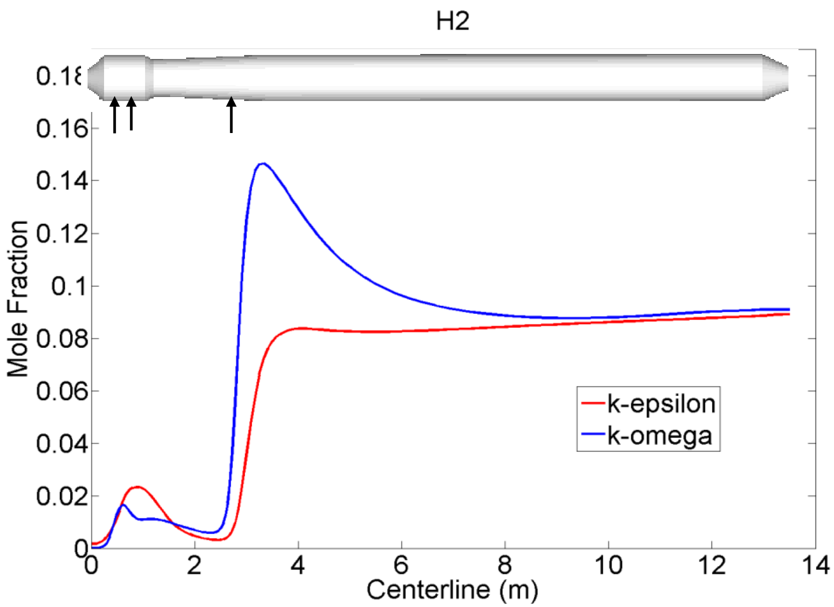


- Varying C produces noticeable changes in the combustor section.
- The equilibrium exit compositions are not affected
- k -ω turbulence model has been used.

MHI Pilot Scale Gasifier: k-ω model



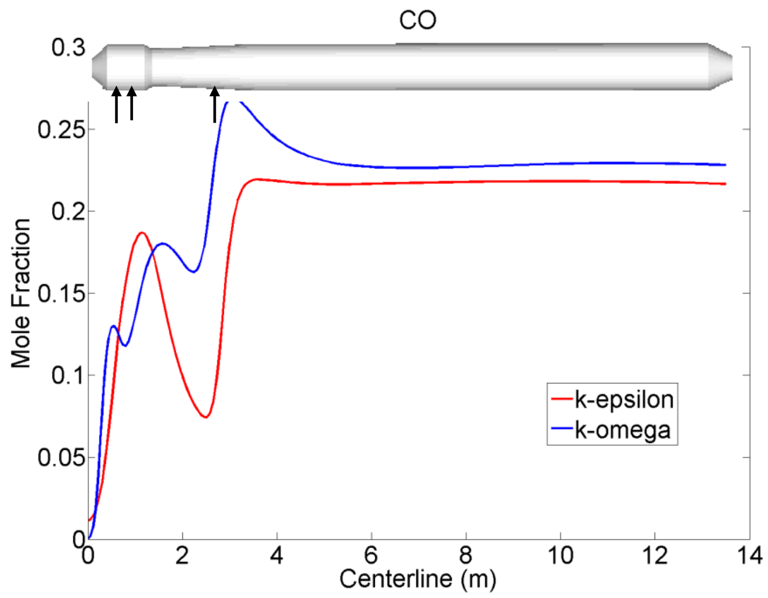


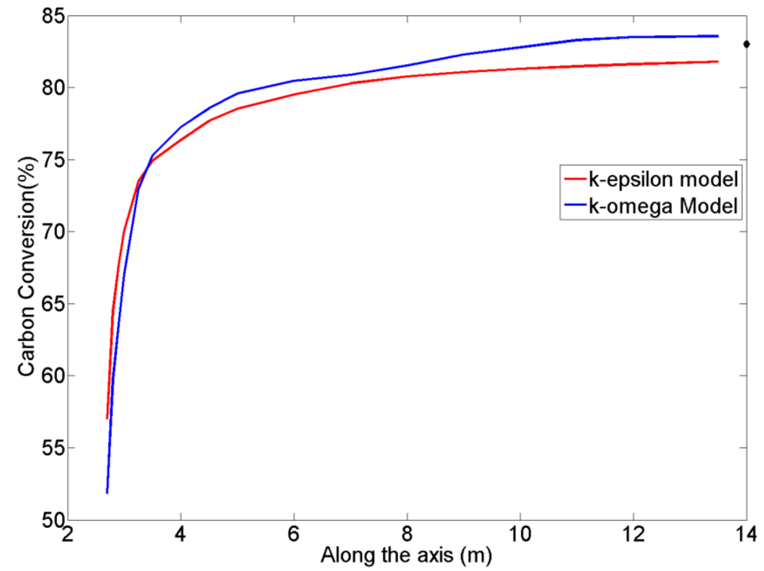


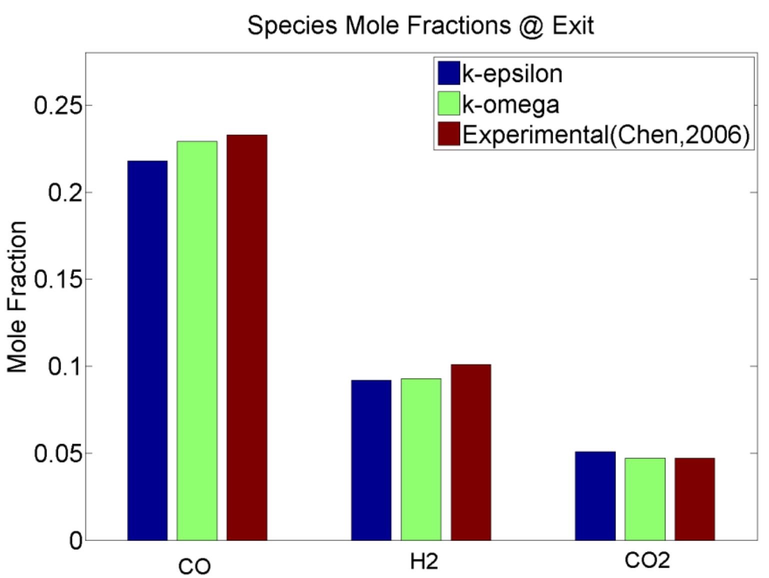
- Peaks are observed in the temperature and species profiles around the diffuser injection with the k-ω model.

- Final mol fractions are similar but there are variations in the profiles.

MHI Pilot Scale Gasifier: k-ω model

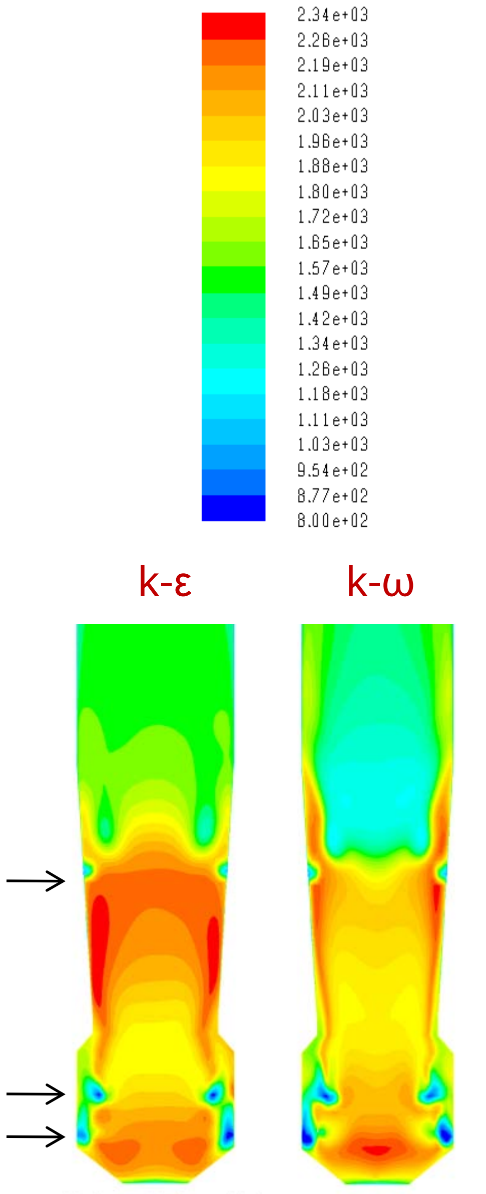




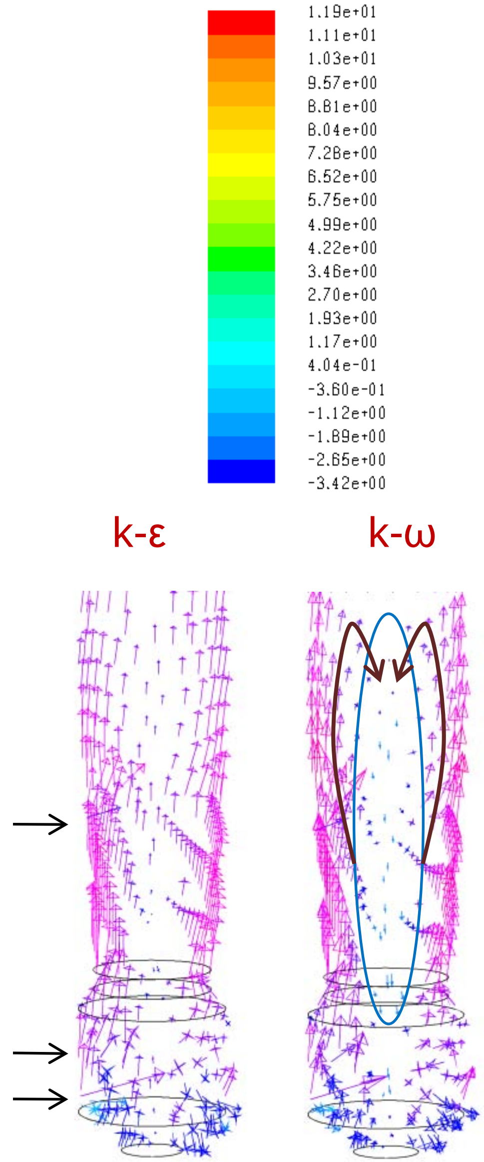


- Conversion slightly increases from 82% to 83.7% - exp value is 83%.

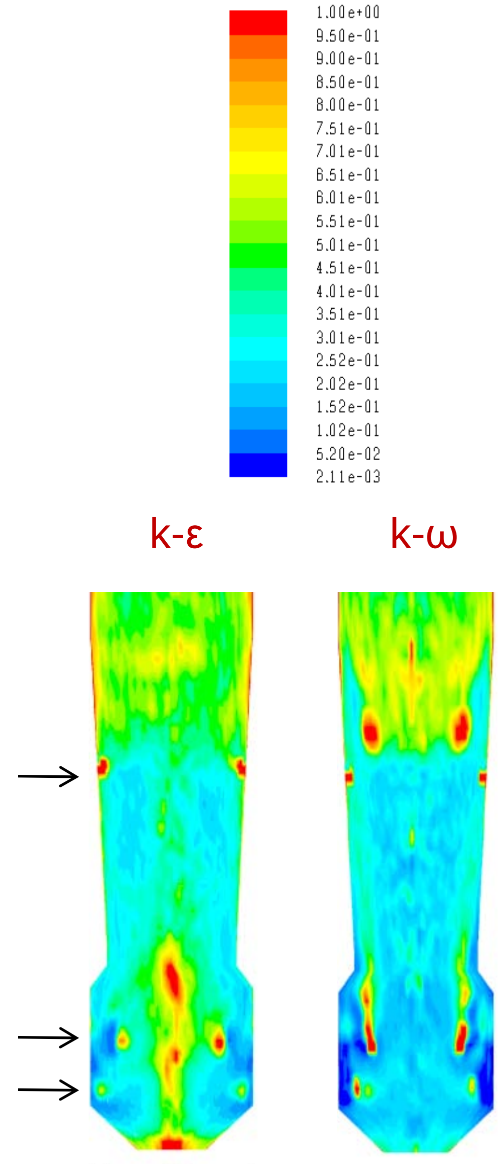
k-ε vs k-ω model



Temperature

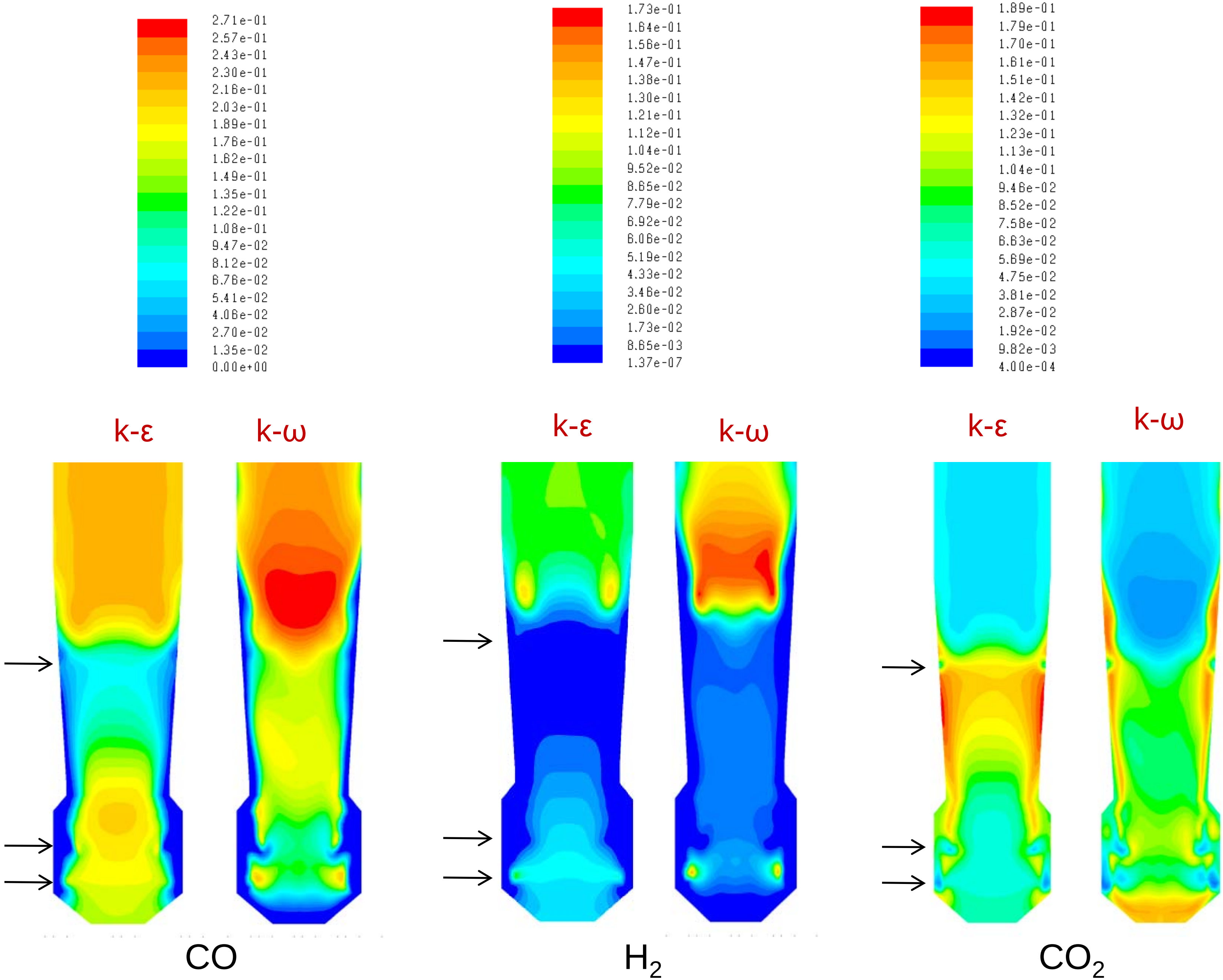


Velocity vectors

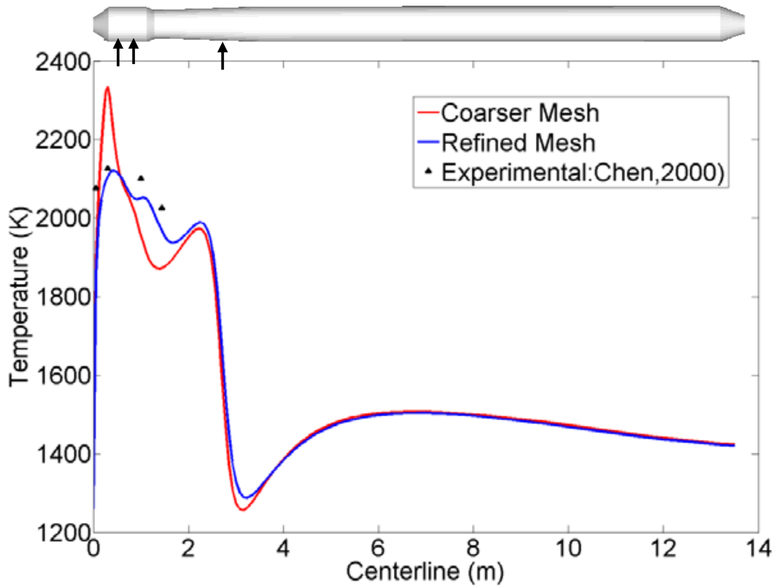


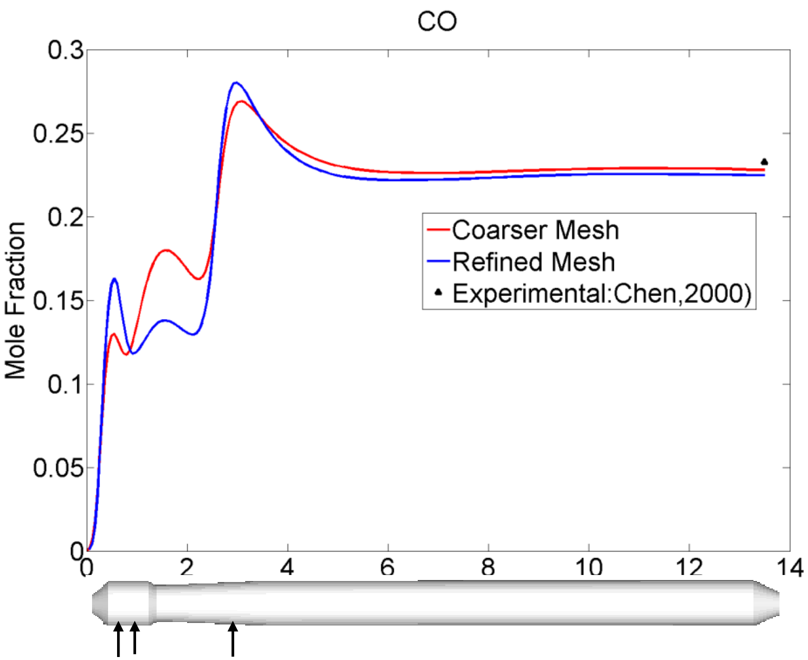
Char concentration (kg/m^3)

k-ε vs k-ω model

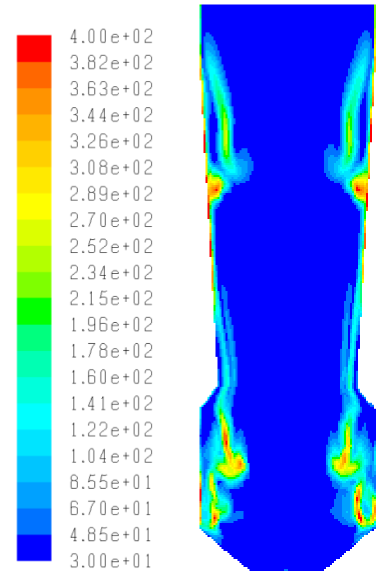


Mesh Refinement





Solution-adaptive Refinement



Temperature Gradients
(above refinement threshold)

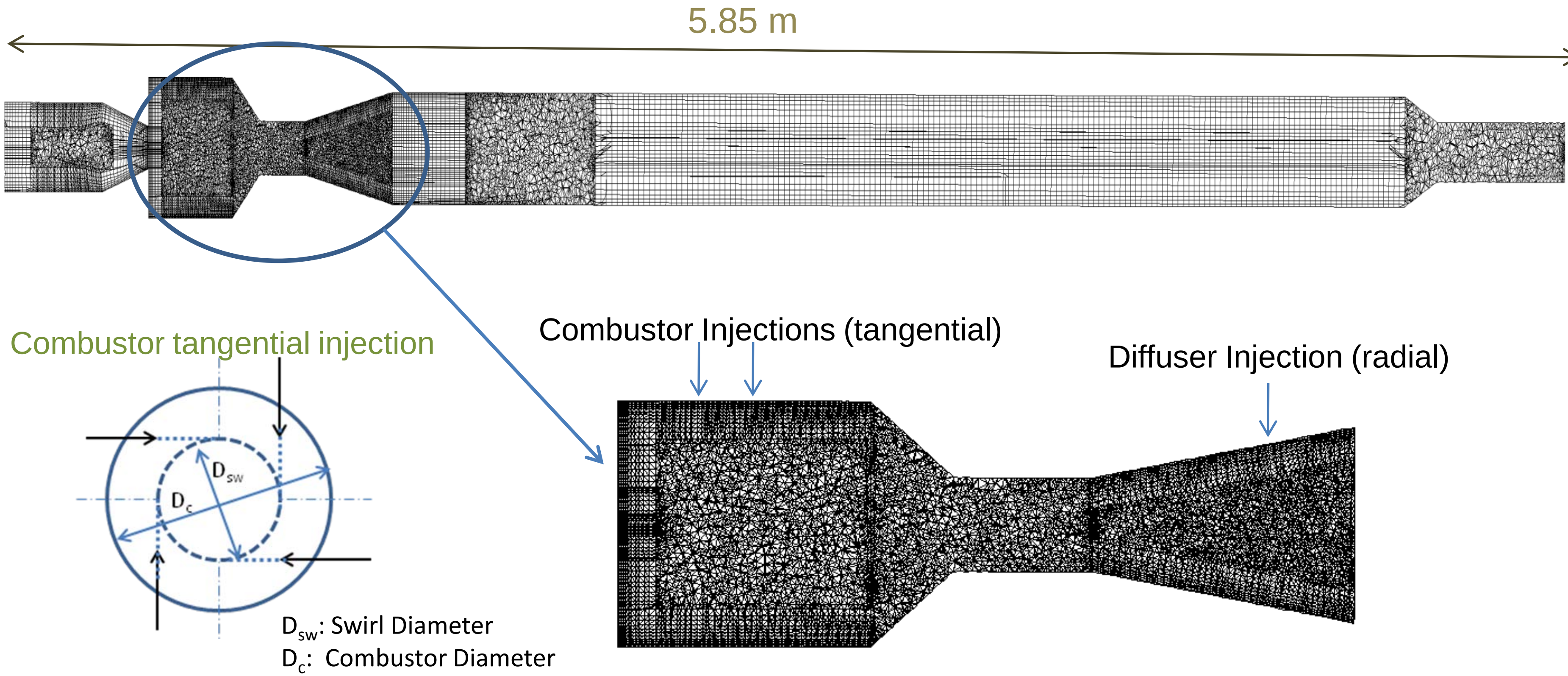
- Refined Mesh is created by solution-adaptive refinement – refining in areas of sharpest temperature gradients.
- Refined Mesh2 is created by refining uniformly by a factor of 2.

- Coarser Mesh: 208,000 nodes
  Refined Mesh: 430,000 nodes
  Refined Mesh2: 1,530,000 nodes

Refined Mesh case is unstable/ cumbersome to converge!

Refined Mesh2 case is impossible to converge!!

Research Scale Gasifier



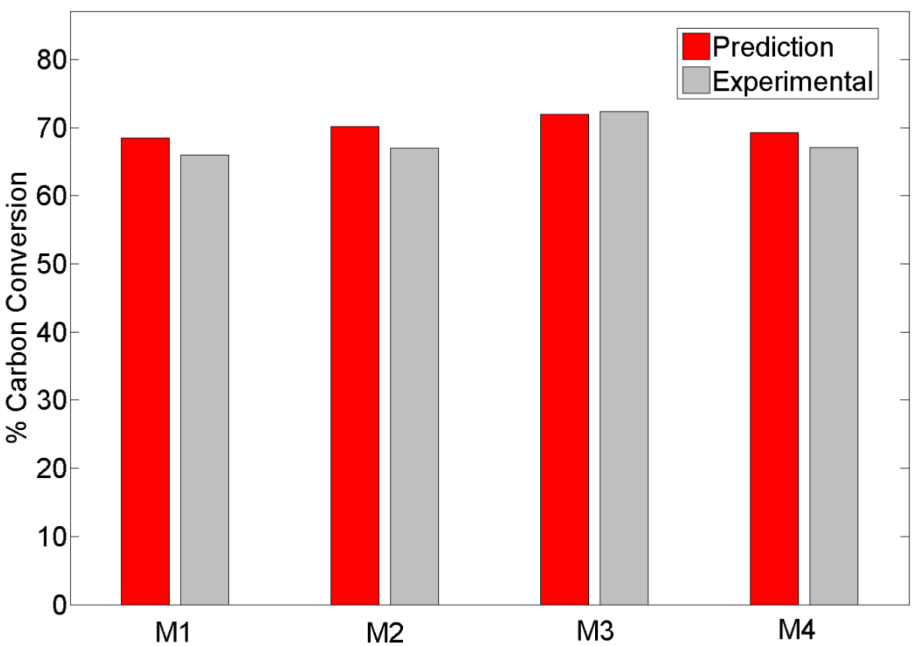
- The research scale (2T/D) design is 5.85m long as opposed to the 13 m long pilot scale (200T/D) design
- High mesh density in the combustor, throat and diffuser regions (7.5 mm). Mesh is coarser in the reductor region (2 cm).
- In addition, mesh is at least 4 times finer close to all the walls.
- Each injector has about 10-12 mesh volumes.

670000 grid points – again, case is unstable, especially when using k-ω model.

MHI Research Scale Gasifier: Results

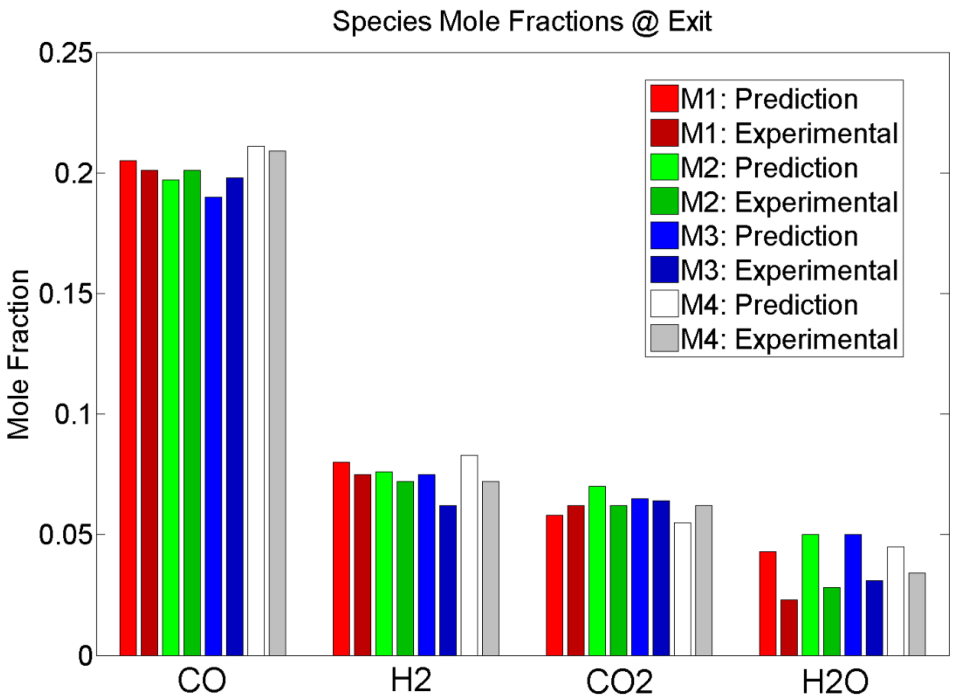
Test cases with Australian bituminous coal: M1, M2, M3, M4

		M1	M2	M3	M4
Inputs (air/coal/char)					
Combustor coal	kg/hr	40.7	41.4	40.6	41.2
Reductor coal	kg/hr	60.3	59.3	58.3	61.3
Recycled char	kg/hr	38.1	36.3	34.8	37.8
Combustor air	kg/hr	391.7	418.4	436.6	409.7
Reductor air	kg/hr	66.96	66.58	66.49	66.68
Gasifier air ratio		0.358	0.381	0.409	0.367

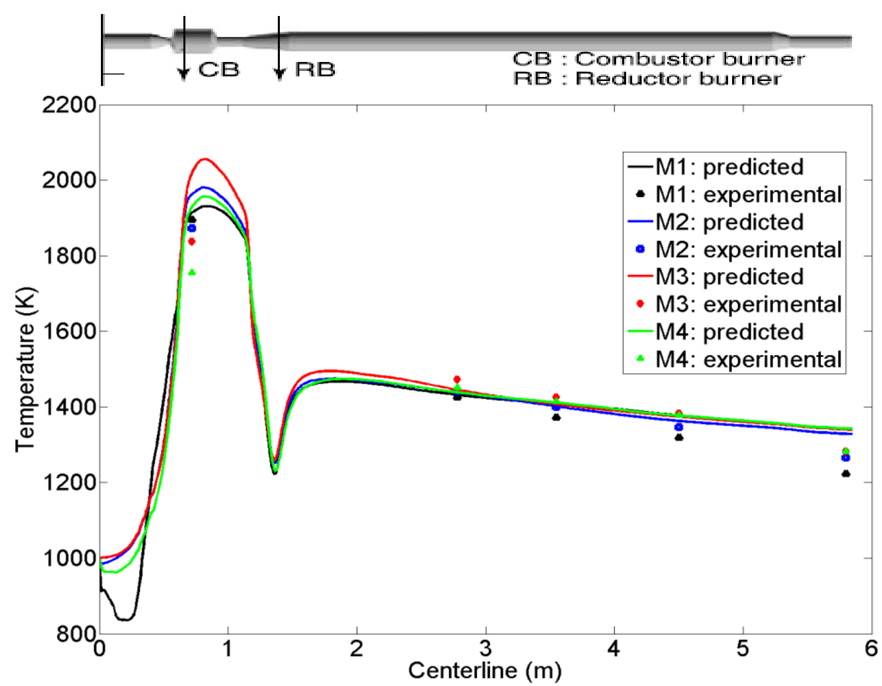


- Gasifier air ratio is the ratio of the input air flow rate to the stoichiometric air flow rate for the total coal/char fed into the gasifier.
- Prediction of carbon conversion is reasonably accurate.
- k-ω model is used for turbulence.

MHI Research Scale Gasifier: Results



Species are well predicted, H_2O is overpredicted.



Temperature is predicted with reasonable accuracy.

Exit temperature is overpredicted by 50-100K.

Conclusions

- Both Research scale and Pilot scale gasifiers can be modeled with reasonable accuracy with the current model using commercial software Fluent.
- Fluent is observed to suffer from numerical instabilites when dealing with finer meshes > 700k grid points. Further, LES of two-phase reacting flow is not feasible in Fluent. It is also not amenable to implementation of sophisticated improvements in the char consumption model.
- Flow solver validation in the swirling sudden axisymmetric expansion case indicates that the standard RANS k-ε model may be inadequate when dealing with co-axial swirling injections with high swirl numbers. The RANS k-ω is observed to perform better.
- Flow solver validation with the non-swirling sudden expansion case and the two-phase bluff body case indicates that the RANS models can reproduce the essential flow structures is many complex flows including those involving formation of external and internal recirculating ones. Such flow structure formations typically occur in many gasifiers.

Other Pieces of the Puzzle

- Char consumption model : requires modeling of both kinetics and transport to/within a single char particle – **Poster session**
- Combustion model : subgrid, premixed/non-premixed, interaction of char flame with gas phase
- Slag model : rate of slag formation, melting/solidification, flow behavior
- Wall heat transfer model : wall thermal resistance, water cooling
- Radiation Model : particle radiative properties
- Development, validation, analysis of expense/utility of next generation LES solver

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