Numerical simulation of coal gasification in a counterflow fluidized bed reactor

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Objective

- Study the counterflow hydrodynamics in the reactor and compare the coal gasification results with experimental data.
- Numerical simulation of the fluidized bed gasifier using Two-Flow Model (TFM).
- Utilizing CFD code, Multiphase Flow with interphase eXchanges (MFiX), along with a new module, Multiphase Chemistry and Reaction Solver (MChaRS) to account for chemical kinetics using time splitting method.

Two-fluid model

- Volume fraction

$$\varepsilon_g + \sum_{m=1}^{M} \varepsilon_{sm} = 1$$

- Continuity equation

$$\frac{\partial\, \varepsilon_g \rho_g}{\partial t} + \nabla.(\varepsilon_g \rho_g \mathbf{v_g}) = \sum_{n=1}^{N_g} R_{gn}$$

$$\frac{\partial\, \varepsilon_{sm} \rho_{sm}}{\partial t} + \nabla.(\varepsilon_{sm} \rho_{sm} \mathbf{v_{sm}}) = \sum_{n=1}^{N_{sm}} R_{smn} \qquad (m = 1, \ldots, M)$$

- Momentum equation

$$\frac{\partial\, \varepsilon_g \rho_g \mathbf{v_g}}{\partial t} + \nabla.(\varepsilon_g \rho_g \mathbf{v_g} \mathbf{v_g}) = \nabla.\sigma_{\mathbf{g}} + \varepsilon_g \rho_g \mathbf{g} - \sum_{m=1}^{M} \mathbf{I_{gm}}$$

$$\frac{\partial\, \varepsilon_{sm} \rho_{sm} \mathbf{v_{sm}}}{\partial t} + \nabla.(\varepsilon_{sm} \rho_{sm} \mathbf{v_{sm}} \mathbf{v_{sm}}) = \nabla.\sigma_{\mathbf{sm}} + \varepsilon_{sm} \rho_{sm} \mathbf{g} + \mathbf{I_{gm}} - \sum_{l=1}^{M} \mathbf{I_{ml}}$$

$$\sigma_{\mathbf{g}} = -\mathbf{P}_{\mathbf{g}}\mathbf{i} + \tau_{\mathbf{g}}, \qquad \sigma_{\mathbf{sm}} = \begin{cases} -\mathbf{P}_{sm}{}^{v}\mathbf{i} + \tau_{sm}{}^{v} & \text{if } \varepsilon_g > \varepsilon_g{}^{*} \\ -\mathbf{P}_{sm}{}^{p}\mathbf{i} + \tau_{sm}{}^{p} & \text{if } \varepsilon_g \leq \varepsilon_g{}^{*} \end{cases}$$

$$\mathbf{I}_{\mathbf{gm}} = -F_{gm}(\mathbf{v}_{\mathbf{sm}} - \mathbf{v}_{\mathbf{g}}) + R_{gm}[\zeta_{gm}\mathbf{v}_{\mathbf{sm}} + \overline{\zeta}_{gm}\mathbf{v}_{\mathbf{g}}]$$

$$\mathbf{I}_{\mathbf{ml}} = -F_{sml}(\mathbf{v}_{\mathbf{sl}} - \mathbf{v}_{\mathbf{sm}}) + R_{ml}[\zeta_{ml}\mathbf{v}_{sl} + \overline{\zeta}_{ml}\mathbf{v}_{sm}]$$

- Species transport equation

$$\frac{\partial(\varepsilon_g \rho_g X_{gn})}{\partial t} + \nabla.(\varepsilon_g \rho_g X_{gn}\mathbf{v}_g) = R_{gn}$$

$$\frac{\partial(\varepsilon_{sm} \rho_{sm} X_{smn})}{\partial t} + \nabla.(\varepsilon_{sm} \rho_{sm} X_{smn}\mathbf{v}_{sm}) = R_{smn}$$

Time-splitting method

- A new reaction module, called Multiphase Chemistry and Reaction Solvers (MChaRS), is developed and coupled with MFiX to handle thermochemistry calculations.
- Chemical reaction source term is integrated using stiff ordinary differential equation solvers.

$$\frac{d\Psi}{dt} = S(\Psi) + T(\Psi) \qquad \Psi = [\rho_k, \varepsilon_k, X_{kn}]$$

$$\frac{d\Psi}{dt} = T(\Psi) \qquad \frac{d\Psi}{dt} = S(\Psi)$$

$$\Psi(t) \ \underset{\rightarrow}{T} \ \Psi^*(t+\delta t) \ \underset{\rightarrow}{S} \ \Psi(t+\delta t)$$

Reaction steps

Equations solved in MChaRS:

$$\frac{d\varepsilon_{sm}}{dt} = \frac{1}{\rho_{sm}} \sum_{n=1}^{N_{sm}} R_{smn}$$

$$\frac{d\rho_g}{dt} = \frac{1}{1 - \sum_{m=1}^{M} \varepsilon_{sm}} \left(\sum_{n=1}^{N_g} R_{gn} + \rho_g \sum_{m=1}^{M} \frac{1}{\rho_{sm}} \sum_{n=1}^{N_{sm}} R_{smn} \right)$$

$$\frac{d\,X_{gn}}{dt} = \frac{R_{gn}}{\varepsilon_g \rho_g} - \frac{X_{gn}}{\varepsilon_g \rho_g} \sum_{n=1}^{N_g} R_{gn}$$

$$\frac{d\,X_{smn}}{dt} = \frac{R_{smn}}{\varepsilon_{sm}\rho_{sm}} - \frac{X_{smn}}{\varepsilon_{sm}\rho_{sm}} \sum_{n=1}^{N_{sm}} R_{smn}$$

Numerical specification

- Finite volume method
- 3D Cylindrical coordinate system
- Superbee
- Semi-Implicit Method for Pressure-Linked Equations (SIMPLE)
- LSODA (stiff and non stiff ODE solver)
- Iso-thermal
- Constant pressure at outlet
- Partial-slip and no-slip boundary conditions

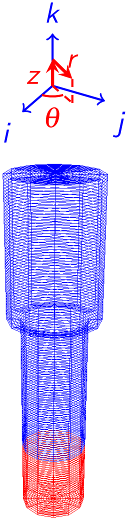


Table: Mesh resolution.

Mesh	$\Delta r\,[cm]$	$\Delta z\,[cm]$	$\Delta\theta\,[rad]$
$20\,d_p$	0.5	1.0	0.52
$15\,d_p$	0.39	0.39	0.44
$12\,d_p$	0.35	0.36	0.34

Experimental study

Neogi (1984)

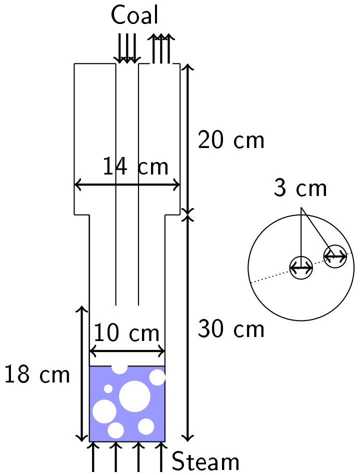


Table: Operating conditions

Feed	
Coal feed rate[g/s]	0.085
Steam supply rate[g/s]	0.22
Operating pressure [atm]	1.0
Entrance temperature [K]	1073
Char surface area [cm^2/g]	13,130
Coal particle diameter [cm]	0.0297
Coal density [g/cm^3]	1.58
Bed	
Operating temperature [K]	1073
Minimum fluidization void fraction	0.43
Minimum fluidization velocity [cm/s]	12
Superficial velocity [cm/s]	16.5
Static bed height [cm]	10
Bed density [g/cm^3]	2.608

Devolatilization analysis

Proximate Analysis %	
Char (DAF*)	55.4
Volatiles (DAF)	44.6
Ash (Dry)	8.4
Moisture	7.8
Ultimate analysis (% DAF)	
C	75
H	5.3
N	1.4
O (by diff.)	10.9
S	7.5

Products	Compositions
Char (wt. % DAF)	65.2
Volatiles (wt. % DAF)	34.8
Volatiles (wt. % DAF)	
Dry gas	15.1
Tar	13.8
Water	5.9
Dry gas (vol. %)	
CO	19.2
CO_2	19.2
H_2	43.1
CH_4	18.5

[*] DAF denotes dry ash free compositions.

Chemical kinetics

- Neogi (1984)

No.	Reaction	$E_i[J/mol]$	A_i	K_{eq}	$R_i[mol/(cm^3.s)]$
1	$C + H_2O \longrightarrow CO + H_2$	121,417	13.9 [cm/s]	-	$A_p k_1^* C_{H_2O}$
2	$C + CO_2 \longrightarrow 2CO$	360,065	$5.56 \times 10^6 [cm/s]$	-	$A_p k_2 C_{CO_2}$
3	$C + 2H_2 \longrightarrow CH_4$	230,274	20.83 [cm/s]	-	$A_p k_3 C_{H_2}$
4	$CO + H_2O \rightleftharpoons CO_2 + H_2$	12,560	$2.78 \times 10^6 [cm^3/mol.s]$	$0.0265 \exp(3955.7/T)$	$\varepsilon_g k_4 (C_{CO} C_{H_2O} - \frac{1}{K_{eq}} C_{CO_2} C_{H_2})$

- Wen et al. (1982)

No.	Reaction	$E_i[J/mol]$	A_i	K_{eq}	$R_i[mol/(cm^3.s)]$
1	$C + H_2O \longrightarrow CO + H_2$	175,560	3,000 [1/(atm.s)]	$\exp(17.29 - 16,330/T)$	$k_1 C_{char}(P_{H_2O} - P_{H_2} P_{CO}/K_{eq})$
2	$C + CO_2 \longrightarrow 2CO$	175,560	3,000 [1/(atm.s)]	$\exp(20.92 - 20,280/T)$	$k_2 C_{char}(P_{CO_2} - P_{CO}/K_{eq})$
3	$C + 2H_2 \longrightarrow CH_4$			$\exp(-13.43 + 10,100/T)$	$C_{char} \exp(-7.087 - 8078/T)$ $(P_{H_2} - (P_{CH_4}/K_{eq})^{0.5})$
4	$CO + H_2O \rightleftharpoons CO_2 + H_2$			$\exp(-3.689 + 4,018.89/T)$	$4459.35 \exp(-116,036.8/(R_u T)) \times$ $\exp(-8.91 + 5553/T) \varepsilon_s \rho_{coal} \times$ $P^{(0.5 - P/250)} \times$ $\exp(-8.91 + 5,553/T) X_{ash} \times$ $(Y_{CO} Y_{H_2O} - Y_{CO_2} Y_{H_2}/K_{eq})$

* $k_i = A_i \exp(\frac{-E_i}{R_u T})$

Table: Enthalpy and entropy at equilibrium condition STANJAN

No.	Reaction	$\Delta h(1073K)[J/mol]$	$\Delta s(1073K)[J/mol.K]$	K_{eq}
1	Gasification	-189,833.43	-3.017	-
2	Water-gas shift	-1.61	0	1

Mesh independence study

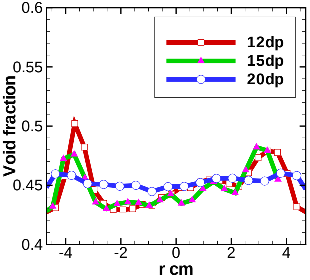


Figure: Mean void fraction at z=5 cm

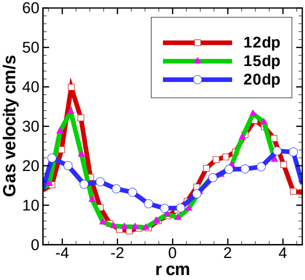


Figure: Mean axial gas velocity at z=5 cm

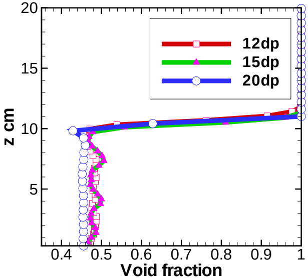


Figure: Mean void fraction at r=2.5 cm

Mean void fraction through azimuthal direction at z=5 cm

Figure: $12d_p$

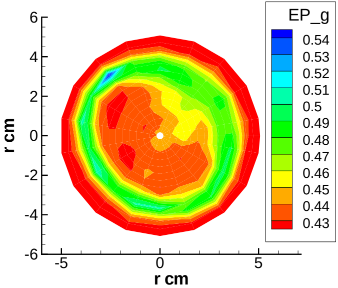


Figure: $15d_p$

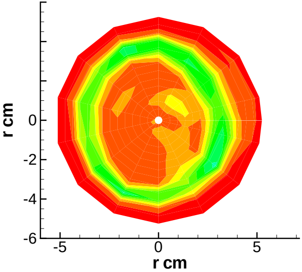
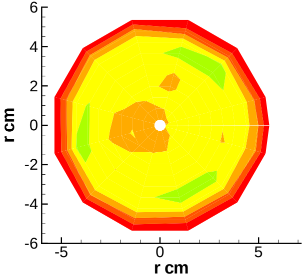
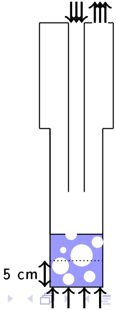
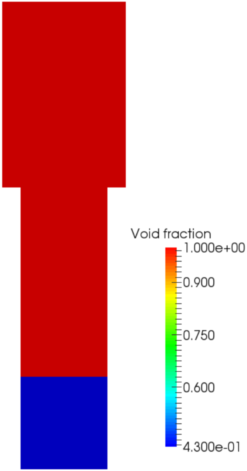


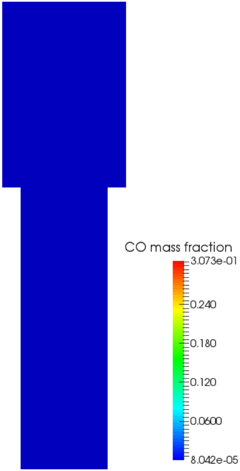
Figure: $20d_p$





Flow pattern





Instantaneous iso-surfaces for $\varepsilon_g = 0.7$

Figure: t=0.2 s

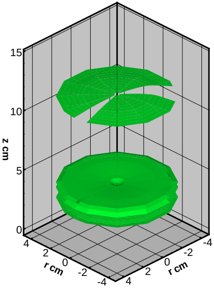


Figure: t=0.4 s

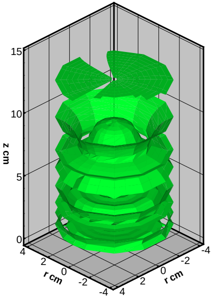
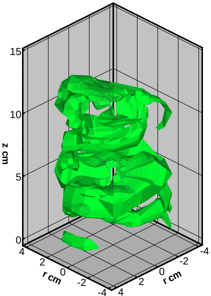


Figure: t=3.3 s



Gas and particle hydrodynamics

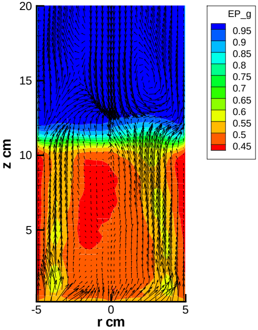


Figure: Mean gas velocity vectors

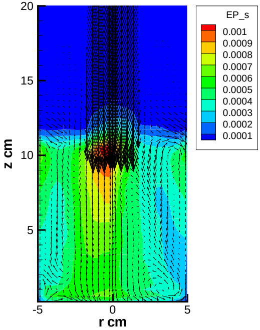


Figure: Mean coal velocity vectors

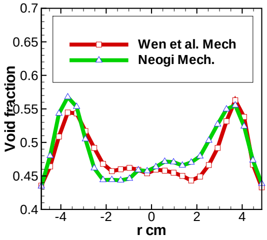


Figure: Mean void fraction profiles at z=5 cm

Gaseous species concentrations

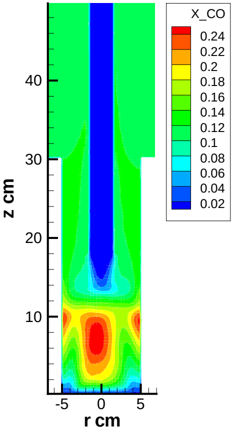


Figure: Mean CO mass fractions contour using Neogi mech.

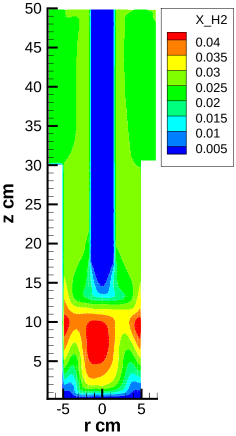


Figure: Mean H_2 mass fractions contour using Neogi mech.

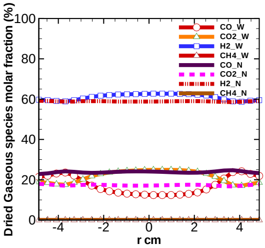
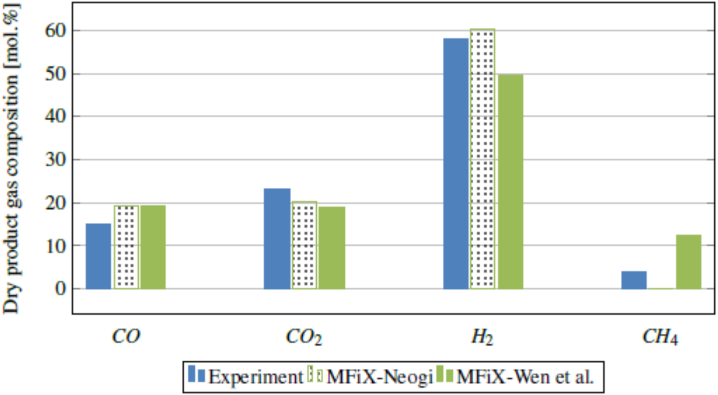


Figure: Mean species molar fraction profiles at z=5 cm

W: Wen et al. Mech.
N: Neogi Mech.

Comparison with experimental data



Conclusions

- Simulation of coal gasification in a counterflow bubbling fluidized bed is conducted using MFiX.
- Gasification chemistry is handled using time-splitting method via a chemistry module (MChaRS) coupled with MFiX.
- Computational results show good agreement with the available experimental data.
- Two chemical mechanisms are implemented by MChaRS method.

Future work

- Optimizing the code parallelization.
- Validating with more detailed experimental data.

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