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Supplementary Material

Impact of Chemistry–Turbulence Interaction Modeling Approach on the CFD Simulations of Entrained Flow Coal Gasification

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Section 2.1 Devolatilization

Model	Short description
	Global models
Single-step first-order (SFOR) [1–3]	Volatiles V that evolve during the devolatilization process are related to the difference between the current V and the ultimate yield of V_∞. $\frac{dV}{dt} = A \cdot exp\left(-\frac{E}{RT}\right) \cdot (V_\infty - V)$
Competing two-step (C2SM) [4]	Mechanism is based on two competing reactions producing char and volatiles from coal. One of the reactions predominates at lower heating rates, whereas the other at higher rates. $coal \xrightarrow{k_1} (1-\alpha_1)char + \alpha_1 volatiles$ $coal \xrightarrow{k_2} (1-\alpha_2)char + \alpha_2 volatiles$ $\frac{dV}{dt} = \left(\alpha_1 A_1\, exp\left(-\frac{E_1}{RT_1}\right) + \alpha_2 A_2\, exp\left(-\frac{E_2}{RT_2}\right)\right) \cdot C$
	Phenomenological network models
FG-DVC [5]	Coal is represented by functional groups. The decomposition occurs through first order reactions to the products of tar, char and gas.
CPD [6–8]	The chemical percolation devolatilization model is based on the characteristics of a coal obtained through a 13-C NMR spectroscopy

Parameters for CPD Model: - BYU Reactor

- Side molecular chain weight – 45
- Cluster molecular weight – 557
- Initial fraction of bridges in coal lattice – 0.33
- Lattice coordination number – 4.9
- Initial fraction of char bridges - 0
- Volatiles – $0.272C_xH_yO_z + 0.2645C_mH_n + 0.2287H_2O + 0.2076CO + 0.0762CO_2$

Parameters for SFOR Model – MHI Reactor

$A = 113700$, $E = 6.094 \times 10^7$

Volatiles – $0.1766C_xH_yO_z + 0.4729C_mH_n + 0.1999H_2O + 0.125CO + 0.0256CO_2$

Parameters for C2SM Model – E-gas Reactor

$\alpha_1 = 0.35$, $\alpha_2 = 1$, $A_1 = 79690$, $E_1 = 5 \times 10^7$, $A_2 = 9305000$, $E_2 = 1.168 \times 10^8$

Volatiles – $0.1022C_xH_yO_z + 0.3321C_mH_n + 0.2818H_2O + 0.1869CO + 0.048CO_2$

Section 4 Ideal Plug Flow Reactor Study

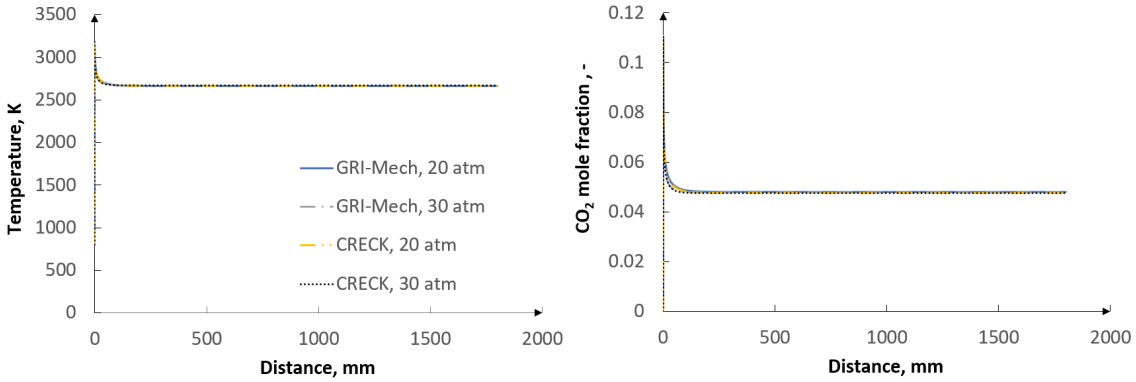

Figure S1. Distributions in PFR for GRI-Mech and CRECK: a) temperature distribution, b) CO_2 mole fraction

Section 6 Mesh Independence Study

Performed for the global approach and the eddy dissipation concept. The results of CO and H_2 mole fraction distribution with respect to the mesh size are presented.

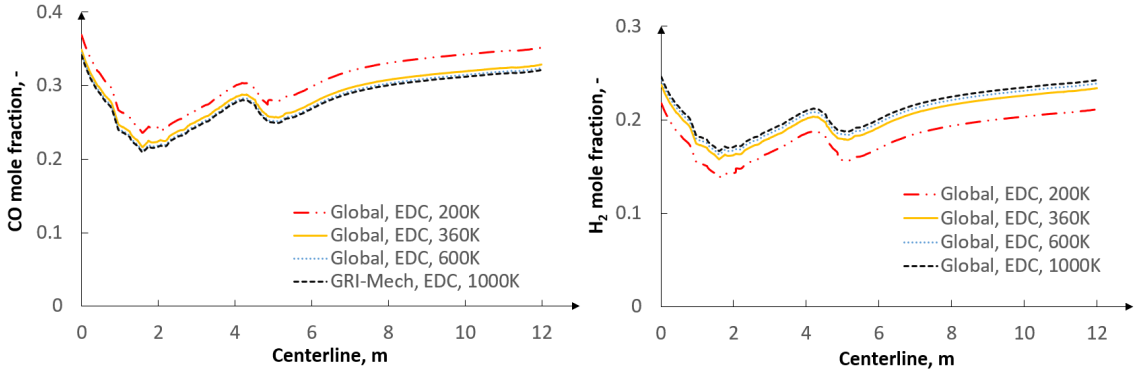

Figure S2. Mesh independence study for E-gas reactor – a) CO mole fraction and b) H_2 mole fraction distributions.

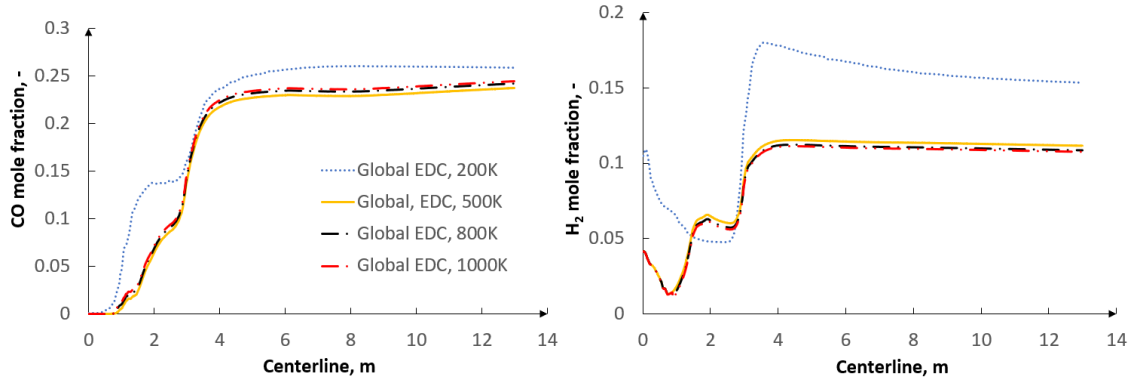

Figure S3. Mesh independence study for MHI reactor – a) CO mole fraction and H_2 mole fraction distribution.

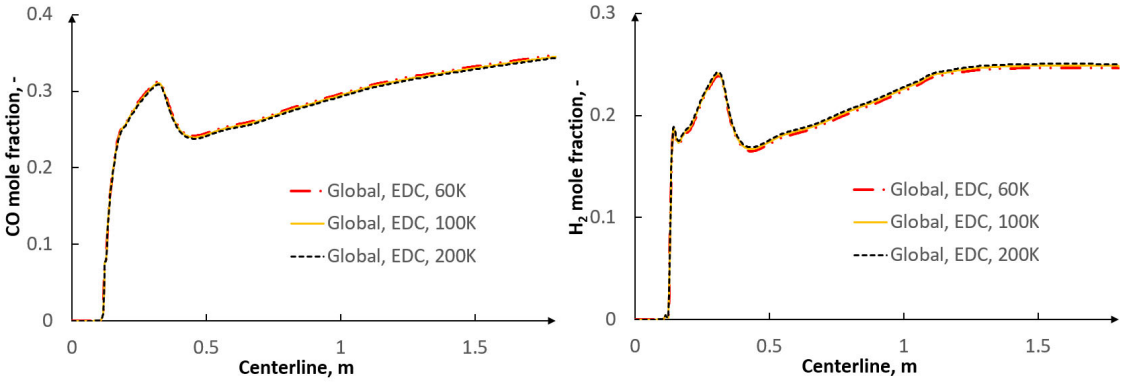

Figure S4. Mesh independence study for BYU reactor – a) CO mole fraction and H_2 mole fraction distribution.

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