Radiative Heat Transfer in Gasifiers for Clean Hydrogen Production

Gautham Krishnamoorthy

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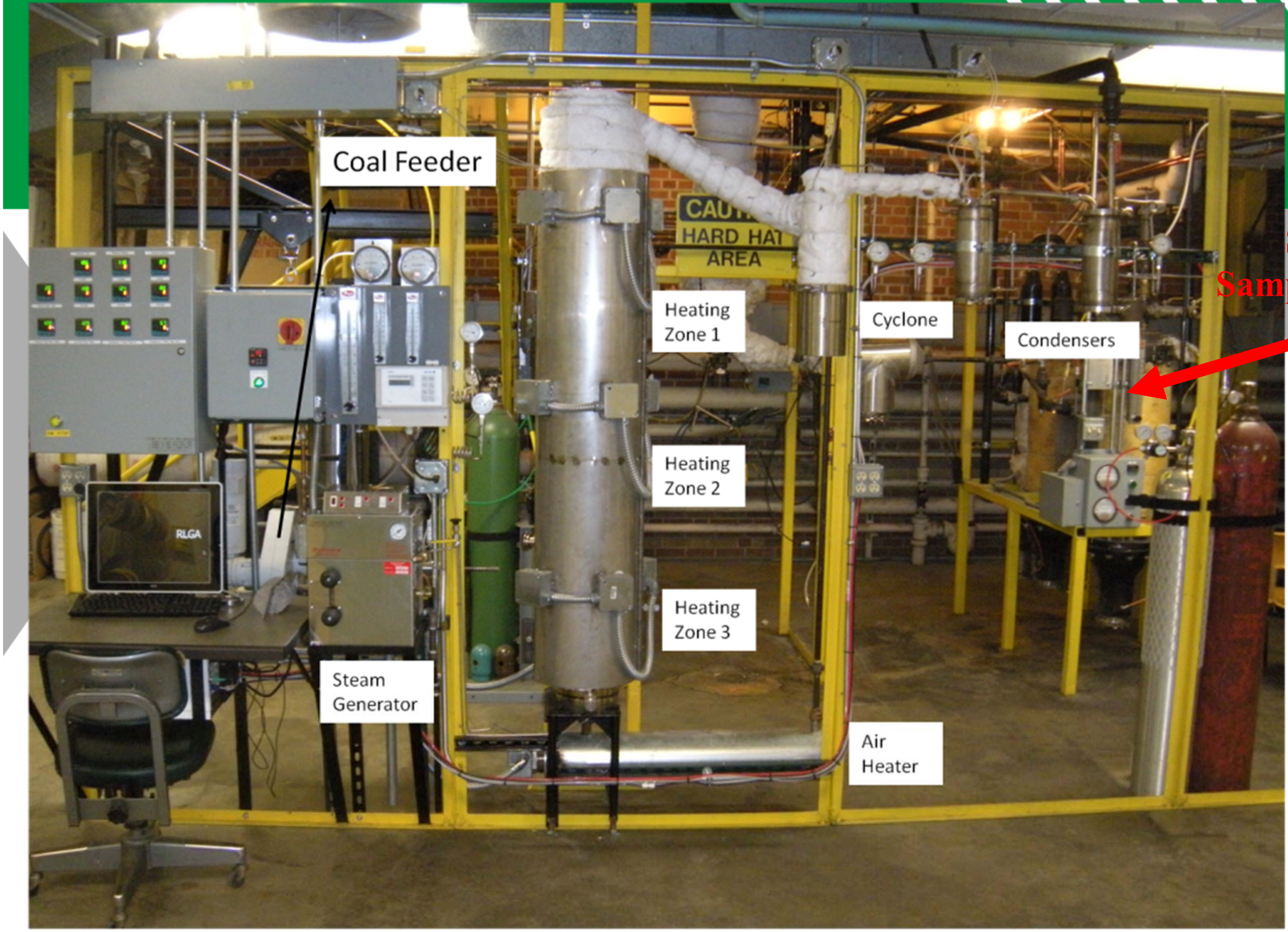
UND UNIVERSITY OF NORTH DAKOTA

LEADERS IN ACTION

Motivation

- Gasifier operations to support our transition to a net-zero greenhouse gas emissions economy requires an ability to manage complex feedstock (coal waste, biomass, plastics and municipal waste)
- The operating temperatures in gasifiers can range from 600 C – 1000 C and need to be carefully monitored and controlled
- Hydrogen production, CO and CH4 concentrations, ash fusion, tar formation all vary quite sharply within this temperature range.
- Radiative transfer is challenging to model. Radiative effects presumed to be insignificant at this lower temperature range (600 C – 1000 C) and small optical path lengths!
- **<u>Question</u>**: Do radiative transfer effects impact the product syngas composition as it is cooled ? Does it impact the location of tar/ash condensation along the sampling train?



Syngas Sample location

Fluidized bed experimental set up
Lignite coal + Sand

Experimental conditions

Run identifier	Coal flow rate (Kg/s)	O_2 flow rate (Kg/s)	Steam flow rate (Kg/s)
O/C = 0.8	2.04e-04	5.31e-05	1.50e-04
O/C = 1.1	2.04e-04	7.43e-05	1.50e-04
O/C = 1.6	2.04e-04	10.61e-05	1.50e-04

Mota, R., Krishnamoorthy, G., Dada, O. and Benson, S.A., Hydrogen rich syngas production from oxy-steam gasification of a lignite coal–A design and optimization study. Applied Thermal Engineering, 90, pp.13-22 (2015).

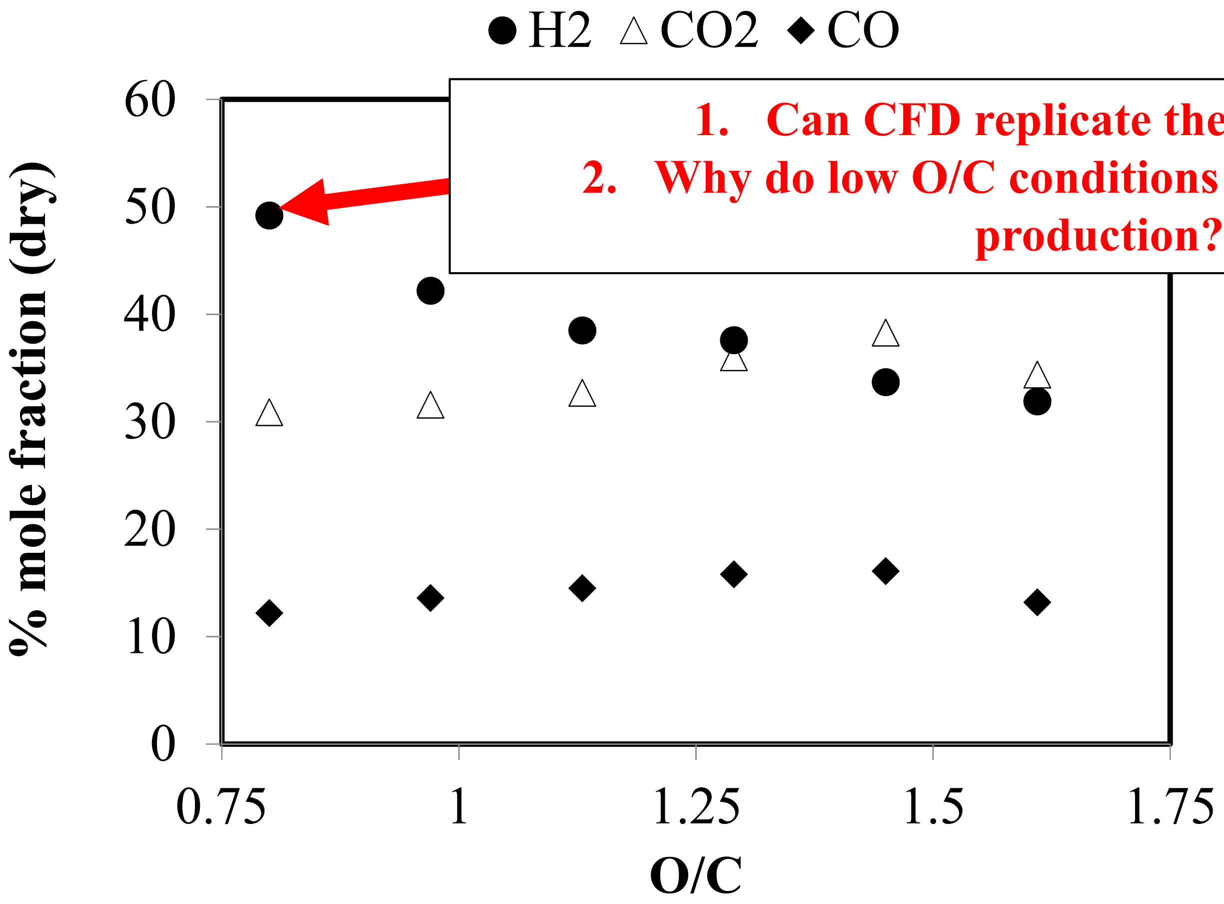
A summary of models employed in the CFD simulations

Physics being modeled	**Modeling option**
Multiphase hydrodynamics	Euler-Euler
Turbulence	Standard k-ε (per phase)
Gas-phase chemistry	Finite rate/Eddy dissipation
Heterogeneous chemistry	Finite rate
Drag law (Gas – Sand)	Wen-Yu
Drag law (Gas – Coal)	Wen-Yu
Drag law (Coal – Sand)	Schiller-Naumann
Radiative heat transfer	P-1 with Planck mean absorption coefficients for CO, CO2, H2O

Finite rate reactions

	Equation
Heterogeneous reactions	
Devolatilization	Volatiles $\rightarrow$ 0.13 CO + 0.044 CO_2 + 0.238 H_2O + 0.034 CH_4 + 0.403 H_2
Char combustion	$C + O_2 \rightarrow CO_2$
Steam gasification	$C + H_2O \rightarrow CO + H_2$
Boudouard reaction	$C + CO_2 \rightarrow 2CO$
Homogeneous reactions	
CO Oxidation	$2CO + O_2 \rightarrow 2CO_2$
H_2 Oxidation	$H_2 + 0.5O_2 \rightarrow H_2O$
CH_4 Oxidation	$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$
WGS Forward	**$CO + H_2O \rightarrow CO_2 + H_2$**
WGS Reverse	**$CO_2 + H_2 \rightarrow CO + H_2O$**
Methane-Shift Forward	$CH_4 + H_2O \rightarrow CO + 3H_2$
Methane-Shift Reverse	$CO + 3H_2 \rightarrow CH_4 + H_2O$

Measurements



1. **Can CFD replicate these trends?**
2. **Why do low O/C conditions favor hydrogen production?**

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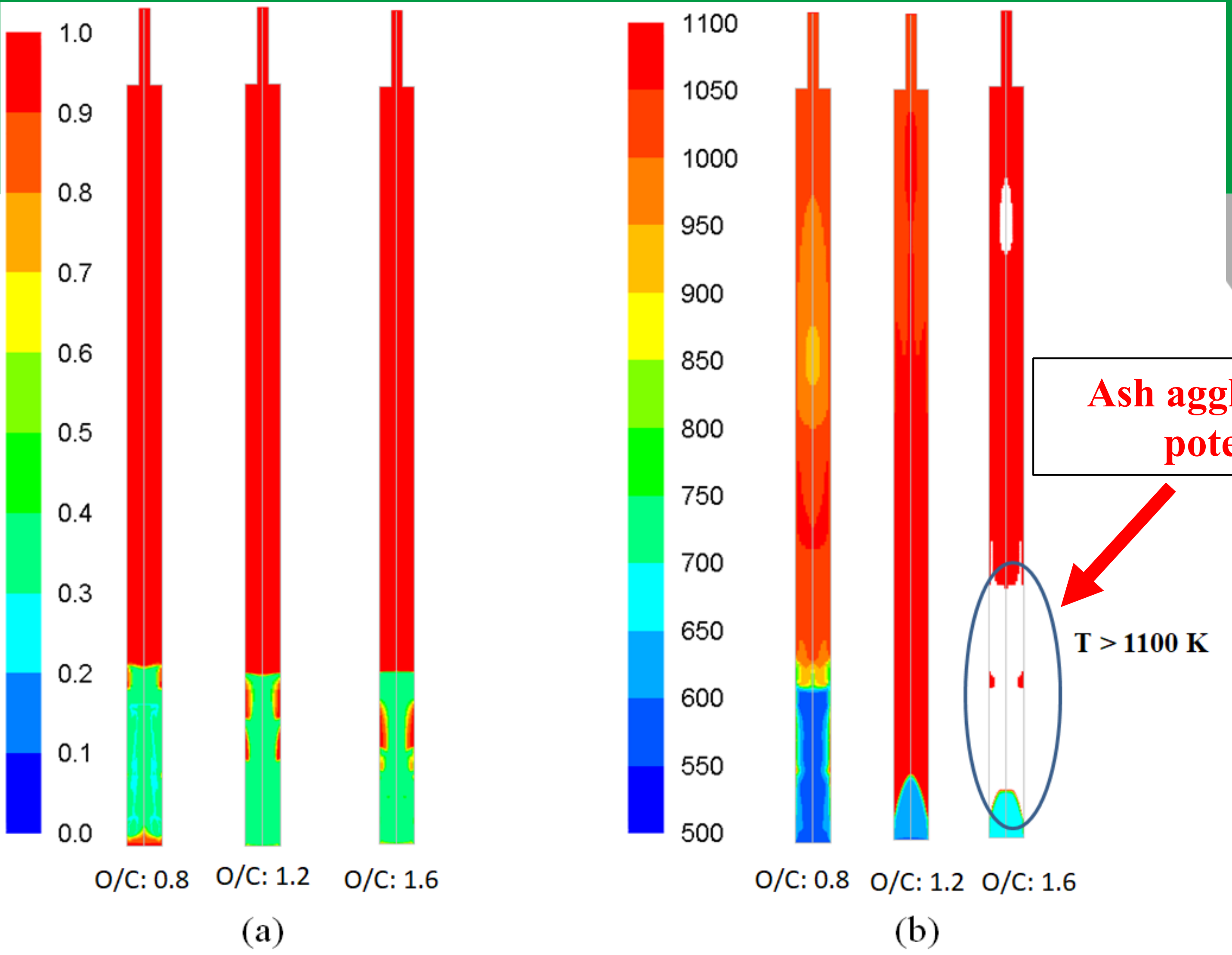
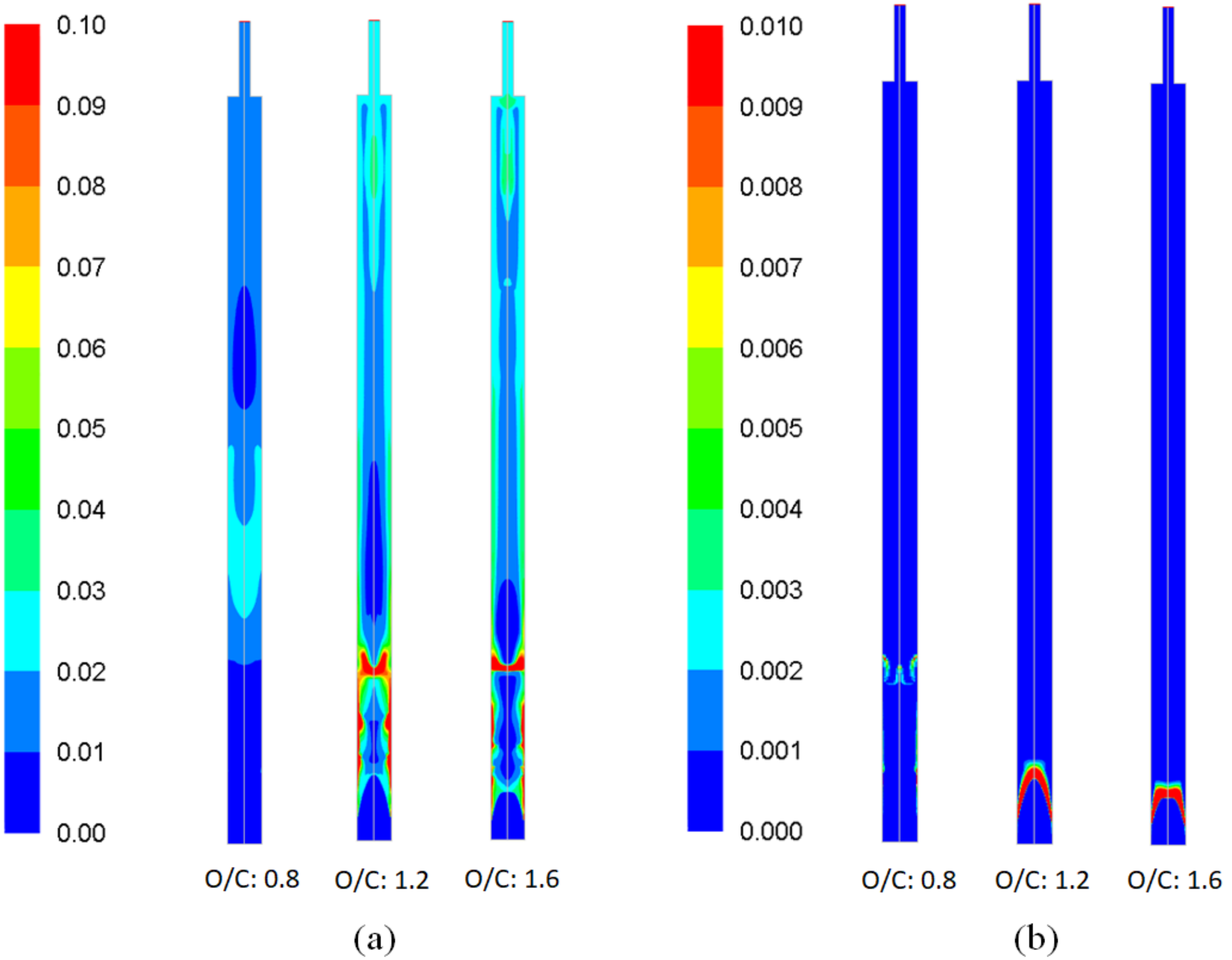


Ash agglomeration potential !

T > 1100 K

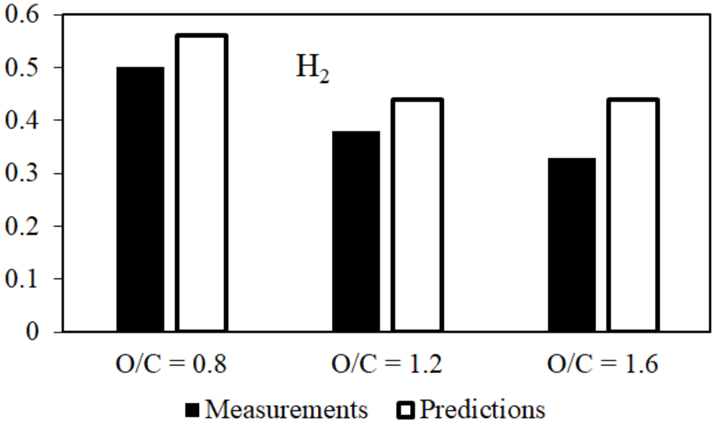
(a) Gas volume fraction; (b) Gas temperature (in K) at different O/C ratios.



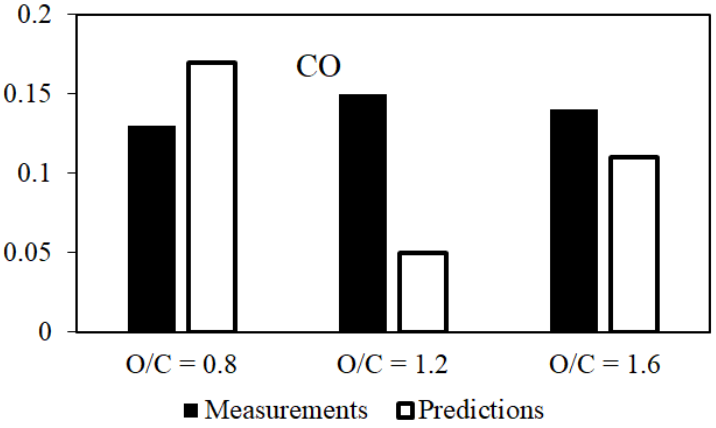
Rates of reactions (kmol/m^3-s) (a) WGS Reverse; (b) Sum of all oxidation reactions (CO, H_2 and CH_4) at different O/C ratios.

WGS Reverse: $CO_2 + H_2 \rightarrow CO + H_2O$ [endothermic]

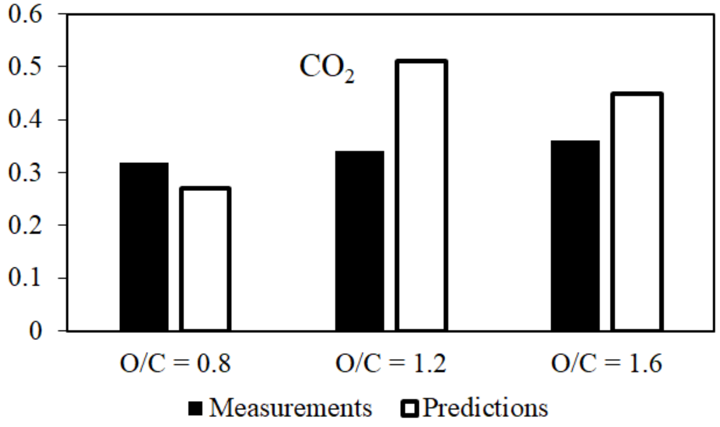
Measurements vs Predictions



(a)

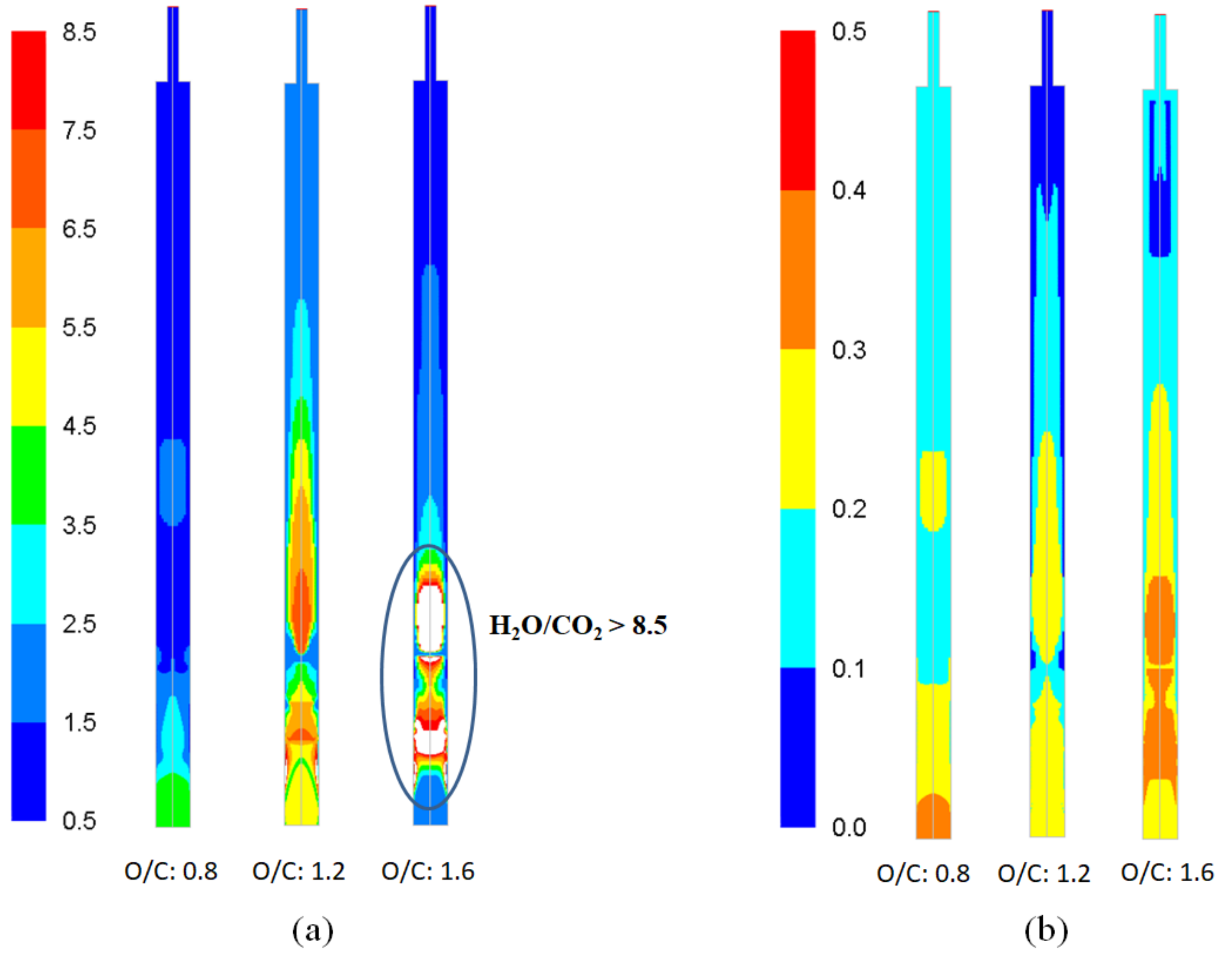


(b)

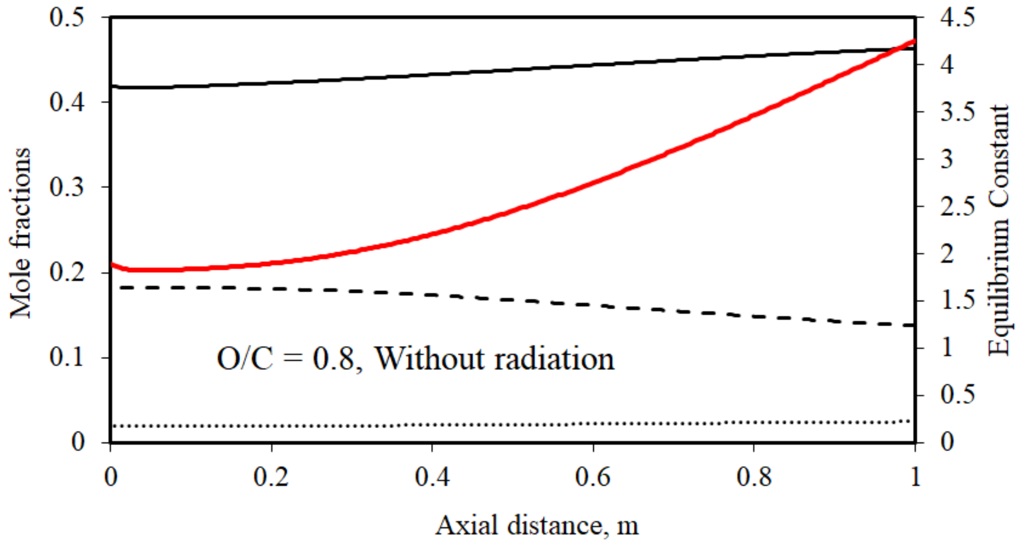


(c)

Need for improved gas radiation models?



(a) H_2O/CO_2 mole fraction ratio; (b) CO mole fraction at different O/C ratios.



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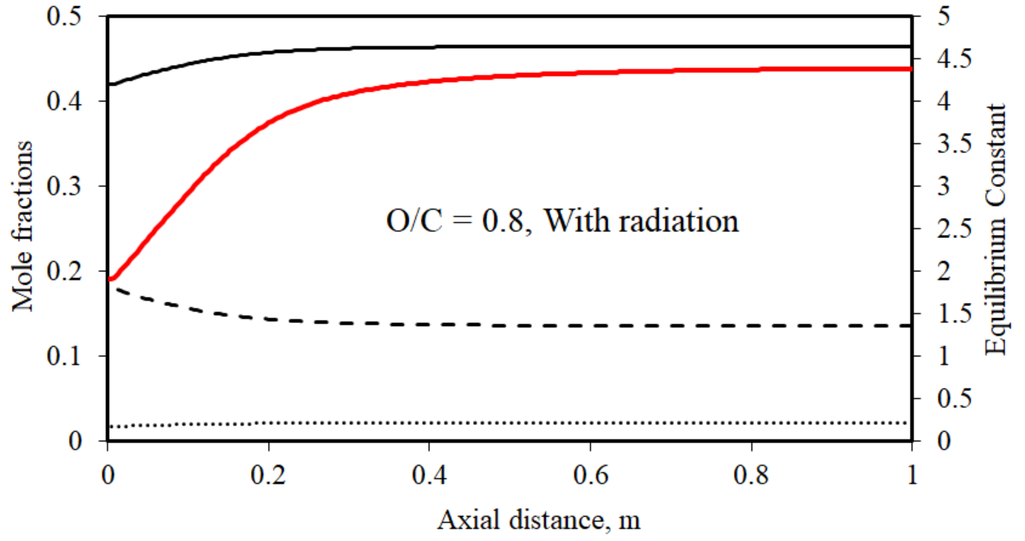


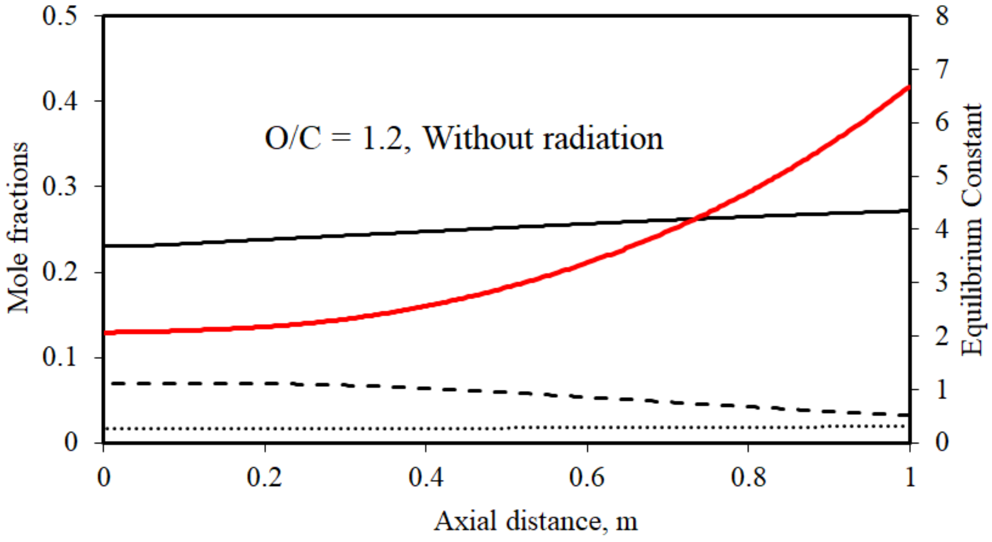
(b)

$$K = \frac{[CO2][H2]}{[CO][H2O]}$$

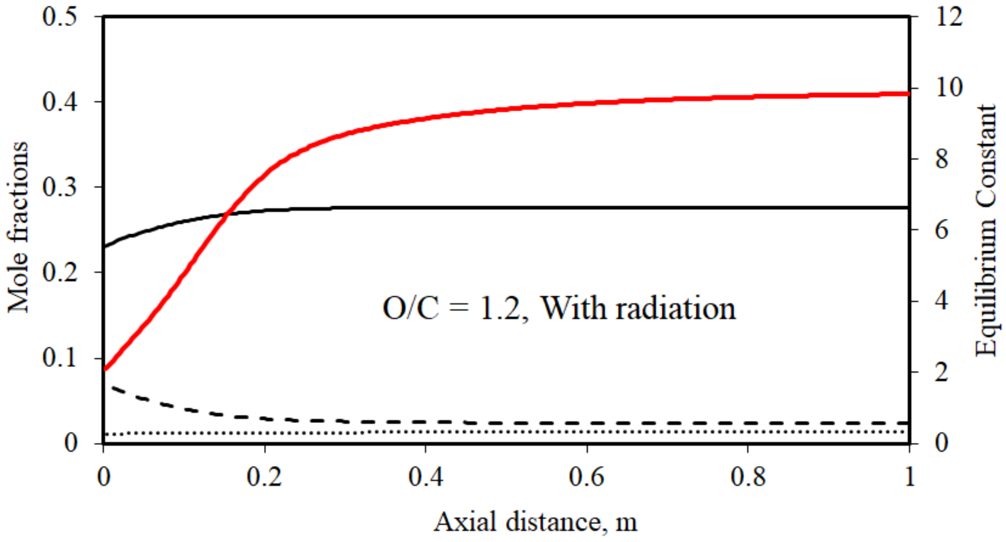
Forward WGS [Exothermic]

$CO + H_2O \rightarrow CO_2 + H_2$

— H2 – – CO ······ CO2 — Equilibrium Constant



(c)



(d)

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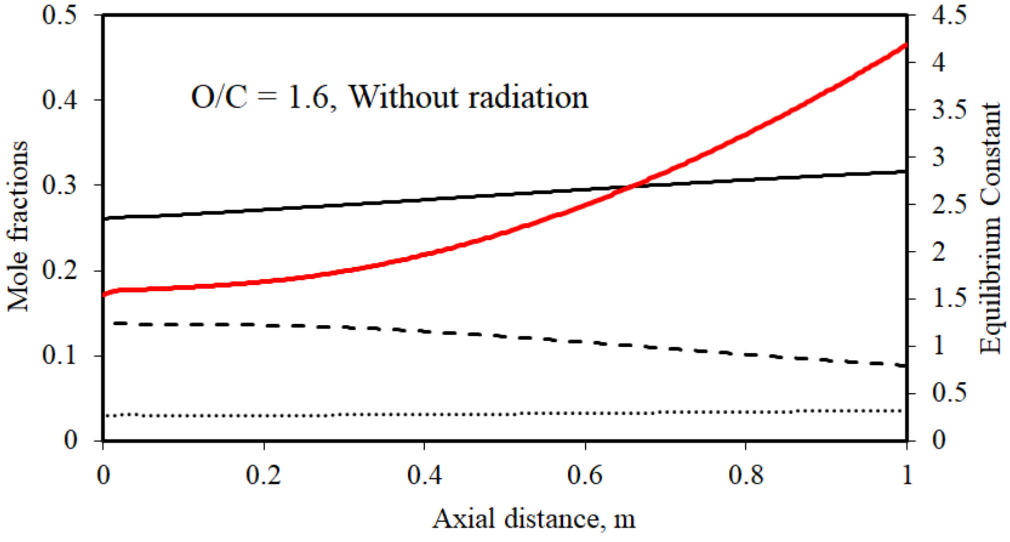
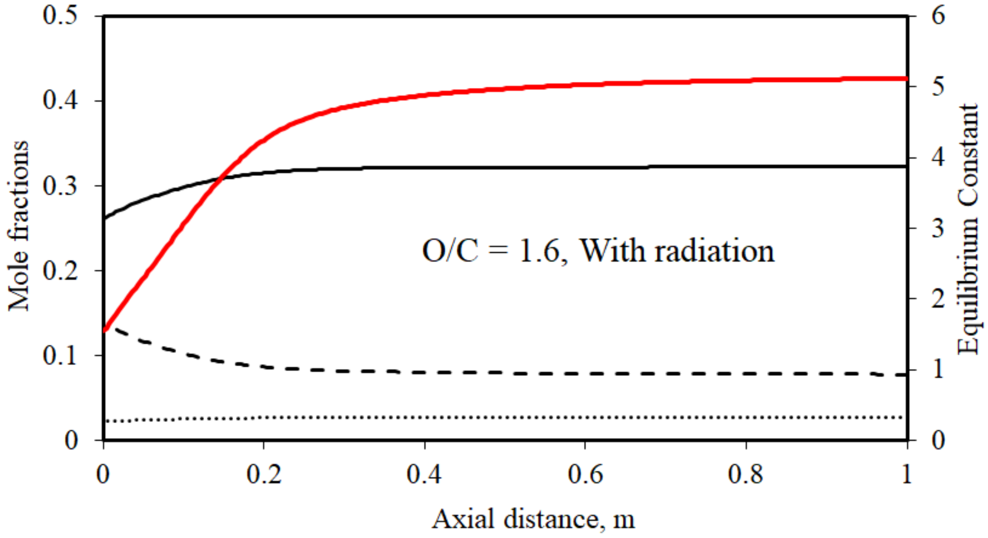


(e)



(f)

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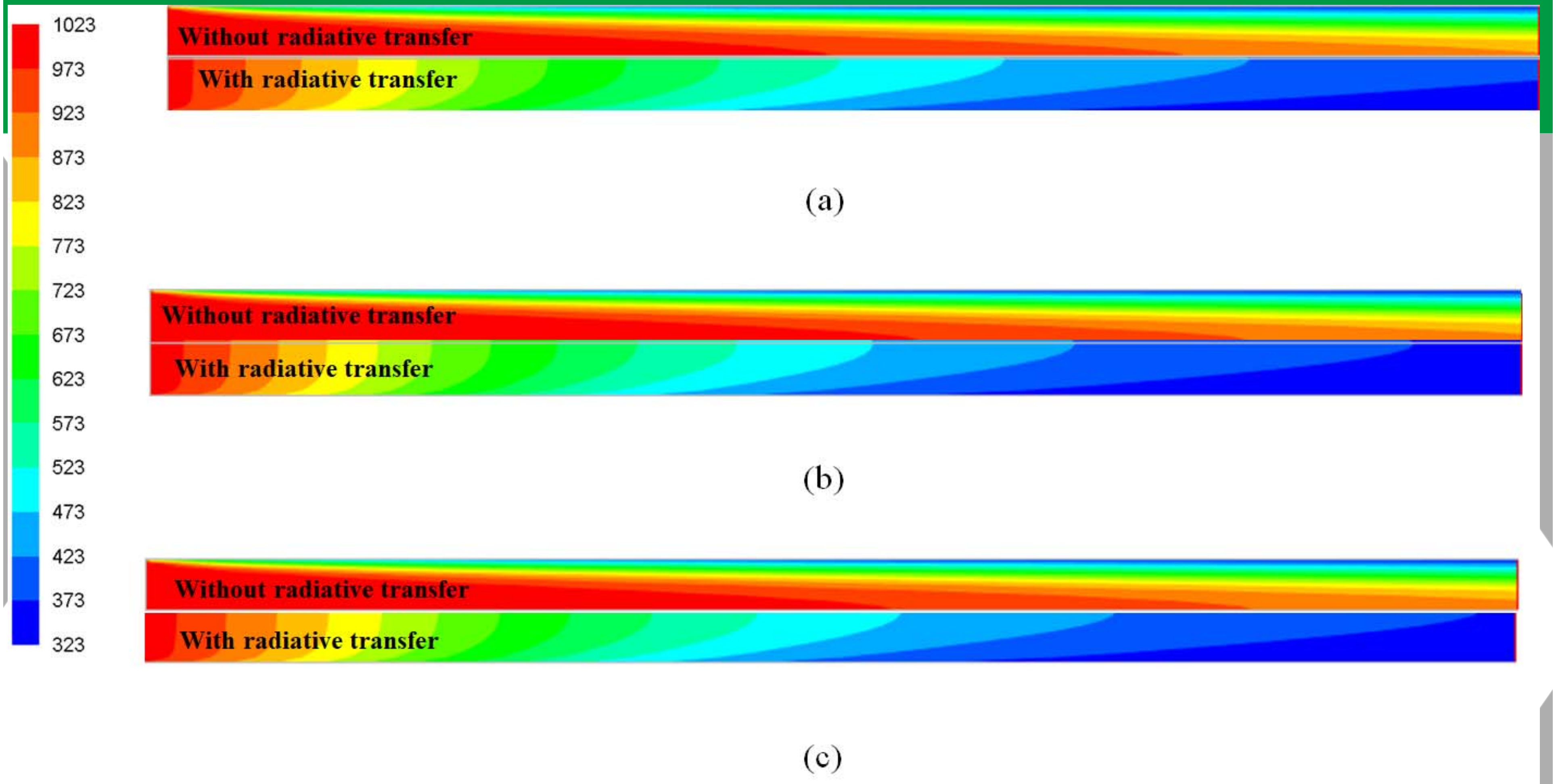

Gas temperatures (K) along the sampling train pipe (a) O/C = 0.8; (b) O/C = 1.2; (c) O/C = 1.6

Conclusions

1. Maximum hydrogen concentration of 50% (dry-basis) was predicted at low oxygen to carbon ratios (O/C = 0.8). Thereby, the validity of the various multiphase reacting flow models employed in the modeling process was established.
2. There were significant variations in the H_2O/CO_2 ratios (0.5 – 8.5) within the gasifier and the CO mole fractions were as high as 0.5 in some regions. Therefore there is a need for developing and validating customized models for the gas radiative properties that can be employed in these scenarios.
3. The water-gas-shift reactions persisted throughout the gasifier and along the syngas sampling train as reflected by its compositional variations during the cooling process.
4. Accounting for radiative losses accelerated the syngas cooling process and attainment of equilibrium concentrations along the sampling train. This may also have implications on the ash and tar condensation processes along the sample lines and help identify potential operational challenges.