2012 COMSOL Conference in Bangalore

Diffusion Modeling in TGA in Context of CO_2 Gasification of Char

By

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Presentation Outline

- Introduction
- TGA Experiments
- Model Development and Results
- Conclusion

Introduction

Why CO_2 Gasification ?

- Important reaction in coal gasification (both surface and underground)
- Important reaction in oxy-fuel combustion

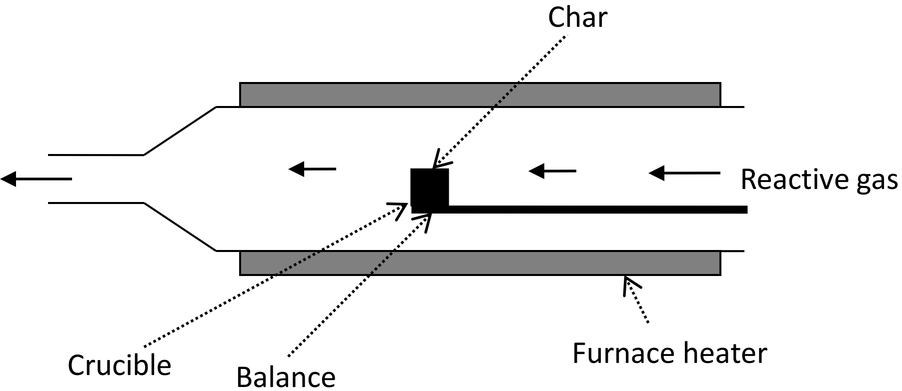
Why Diffusion Effects?

- Reaction may be limited by diffusion through ash layer and to reach to external surface of char particle
- Effect of diffusion becomes dominant in processes where control on particle size is minimal (e.g. UCG)

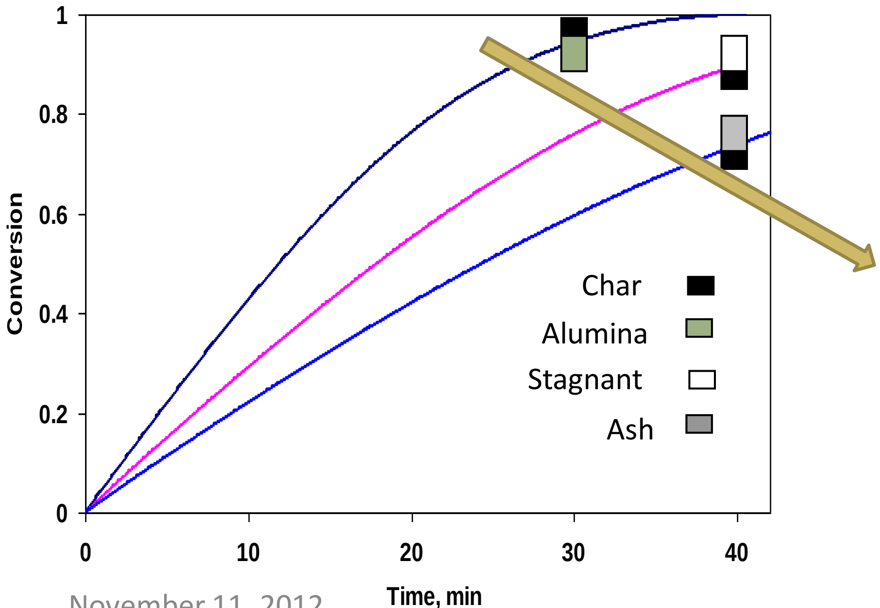
Why TGA ?

- Easy to use and so often used for determination of kinetics

TGA Experiments and Diffusion Effects



Schematic diagram of horizontal arm TGA



Gasification experiments are carried out by using standard methodology.

Standardized the methodology to eliminate the diffusion resistance for determination of intrinsic kinetics

The alumina filling at the bottom gives true intrinsic kinetics

--Kinetics determined by this approach (Mandapati et al., 2012)

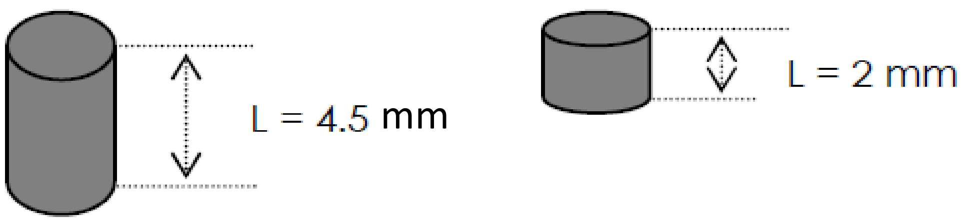
Material and Methods

Proximate and ultimate analysis of the coal samples (Dry basis)

Proximate Analysis		Ultimate Analysis	
Volatile matter	44.92%	Carbon	40.59%
Fixed Carbon	46.61%	Hydrogen	5.67%
Ash	8.47%		

Experiments:

The cylindrical crucibles are completely filled with char as shown in figure:



Experimental results are compared with model results to validate the model (using predetermined intrinsic kinetics)

Model Development

Assumptions:

- Continuum description of the porous solid bed
- The system is two-dimensional and axisymmetric
- The solid is composed of reactive char and inert ash
- There is no disintegration process within the char bed structure
- Perfect gas behavior is assumed for the gasifying agent
- Constant partial pressure of CO_2 at the top of TGA crucible
- Random pore model is applicable at local positions inside the bed
- External mass transfer and diffusion inside particle are not considered

Governing Equations

$$\frac{\partial C_{CO_2}}{\partial t} + \nabla \cdot \left(- \frac{\mathrm{D_{eff}}}{1 + \mathrm{x}_{CO_2}} \nabla C_{CO_2} \right) = R_{CO_2}$$ → **Gas phase balance**

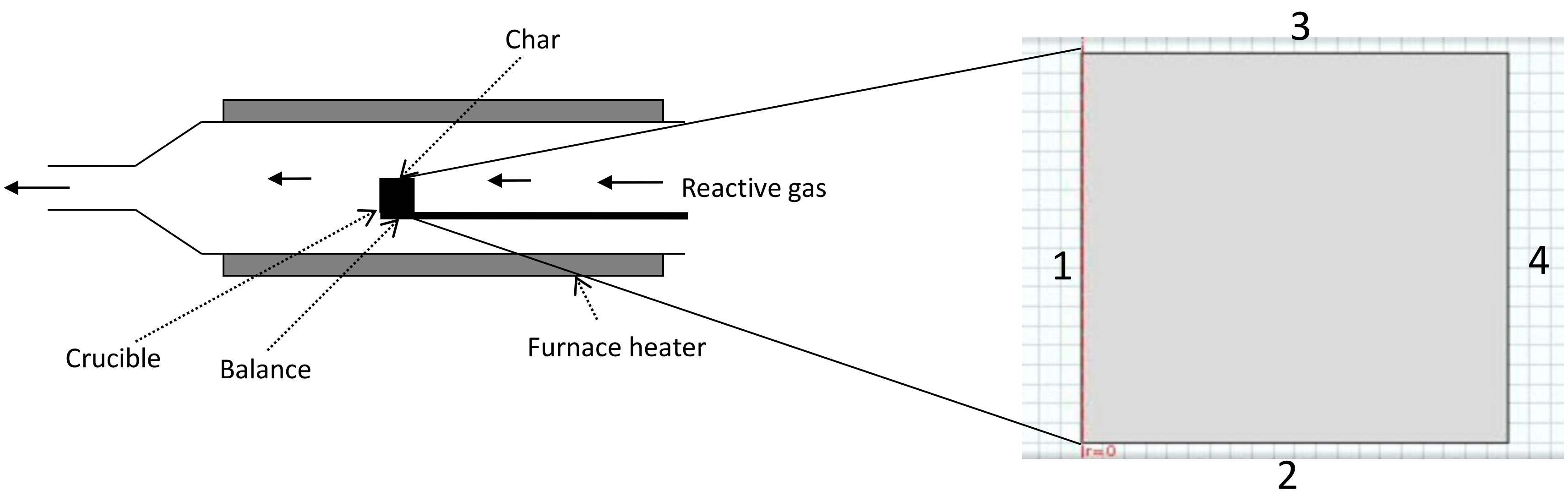
$$\frac{\partial C_{char}}{\partial t} = R_{char}$$ → **Char balance**

$$\rho_{eff}\, C_{p-eff} \frac{\partial T}{\partial t} + \nabla \cdot (-\,\mathrm{k_{eff}}\, \nabla\, \mathrm{T}) = \Delta H * R_{char}$$ → **Heat balance**

Where,

$$Rate = k_0 e^{-\frac{E}{RT}} P_{CO2}^{n} (1 - x)\sqrt{1 - \psi \ln(1 - x)}$$

Boundary Conditions and Initial Conditions



B.C. =

1	symmetry
2, 4	No flux for CO_2, CO and constant T
3	P_{CO_2} = 1 atm, P_{CO} = 0, T = 1239.16 K

I.C. =

char = 10.791 mg, $P_{CO_2} = P_{CO} = 0$,

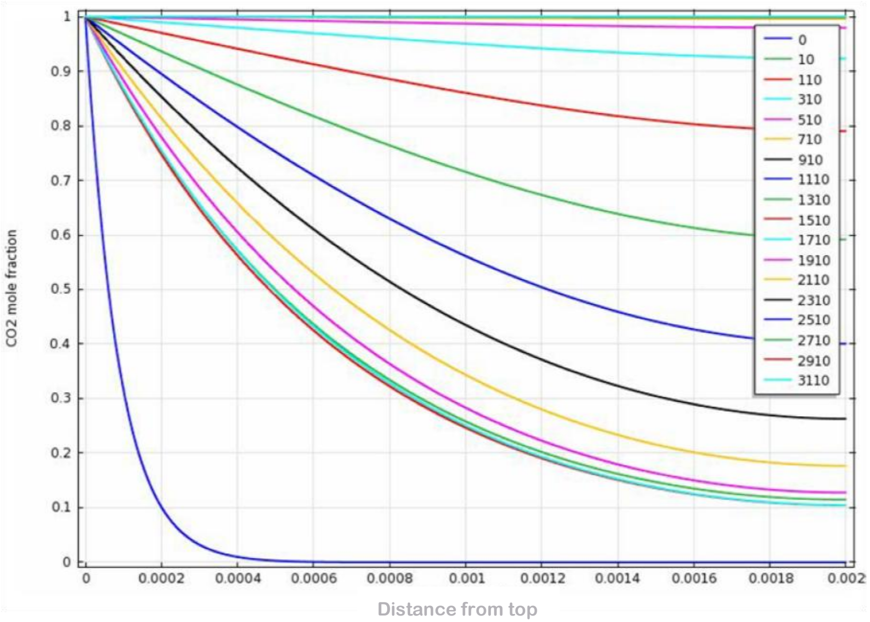
T = 1239.16 K

List of Important Variables

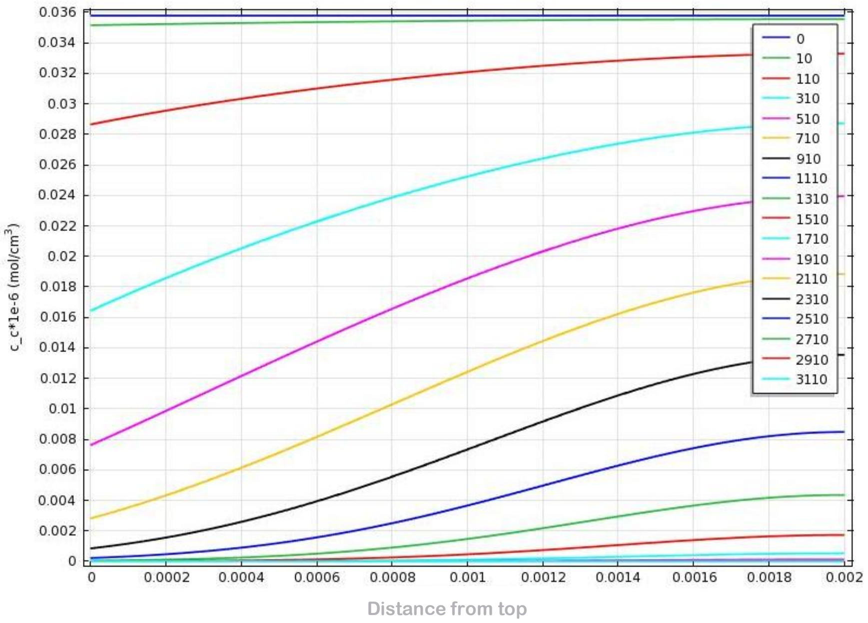
Name	Expression	Description
rate	k*pco2^(.4679)*sqrt(1-psi*log(1-X))*c_c	rate
k	k0*exp(-E/R_g/T)	rate constant
X	max((c_cinit-c_c)/c_cinit,0)	conversion
c_cinit	weight/volume/mol_wt	initial char conc
c_co2init	p_co2/R_g/T	initial CO_2 conc
rho_eff	c_c*mol_wt+ash_wt/volume	effective density
Cp_eff	1000[J/kg/K]	effective sp. Heat
x_ash	ash_wt/(ash_wt+weight)	mass fraction
eps	1-((1-por_init)*(1-(1-x_ash)*X))	porosity
k_eff	(1-eps)/((1/k_s)+(1/(k_gas/psi_+dp*hrs)))	conductivity
hrs	.1952*(p/(2-p))*(1239/100)^3	solid to solid

Simulation Results

CO_2 mole fraction profile

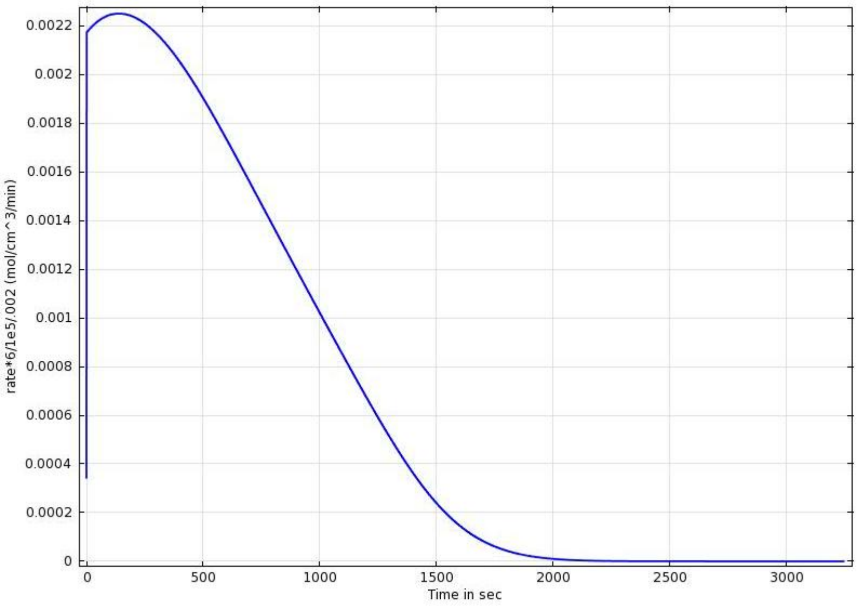


Char concentration profile

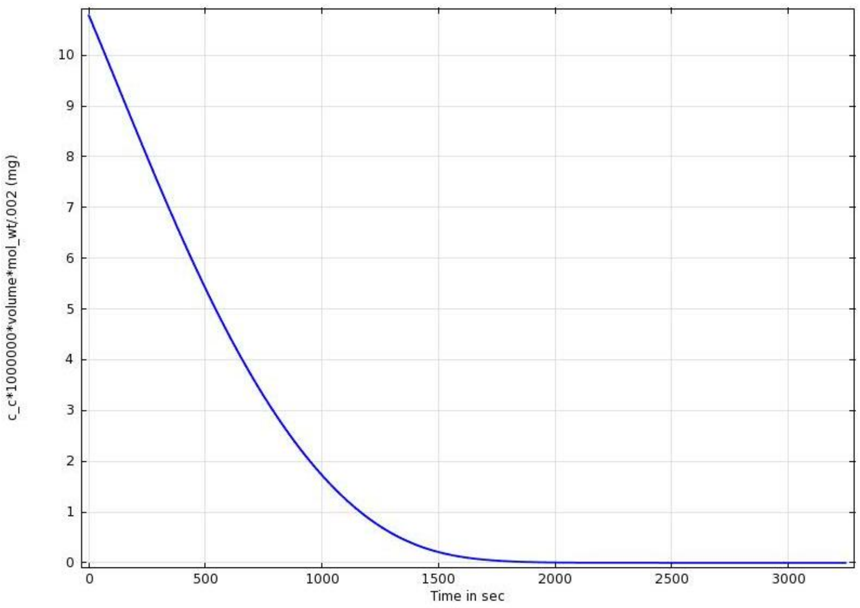


Simulation Results

Total rate profile

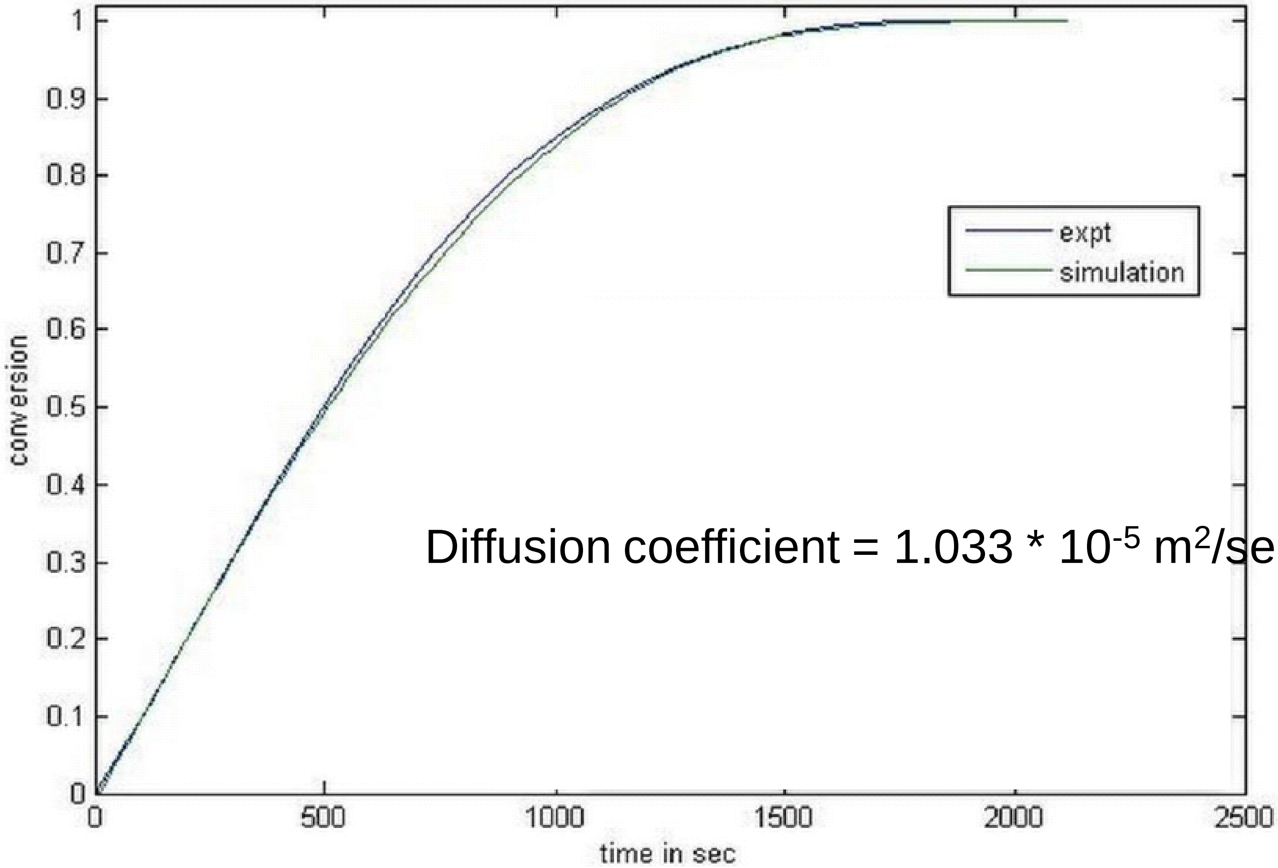


Char weight profile



Simulation Results

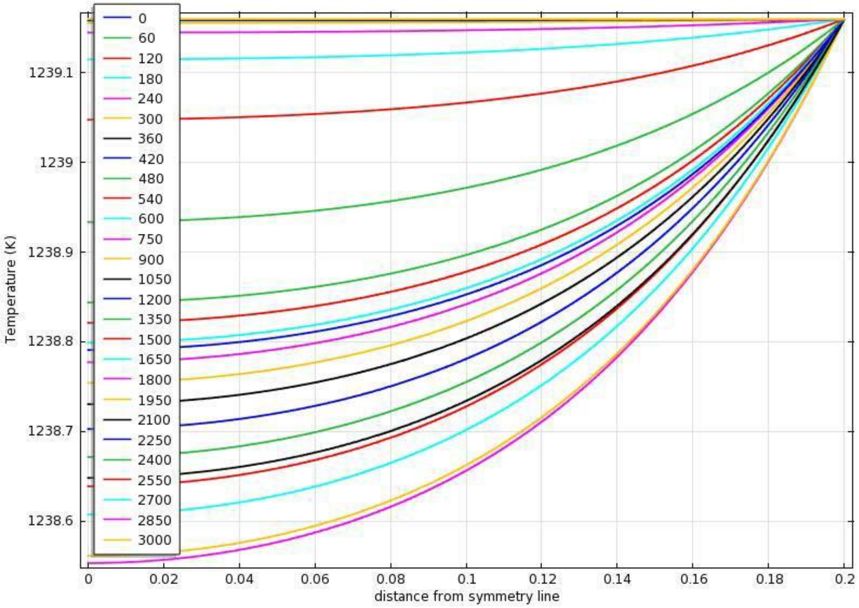
Comparing char conversion by experiment and simulation



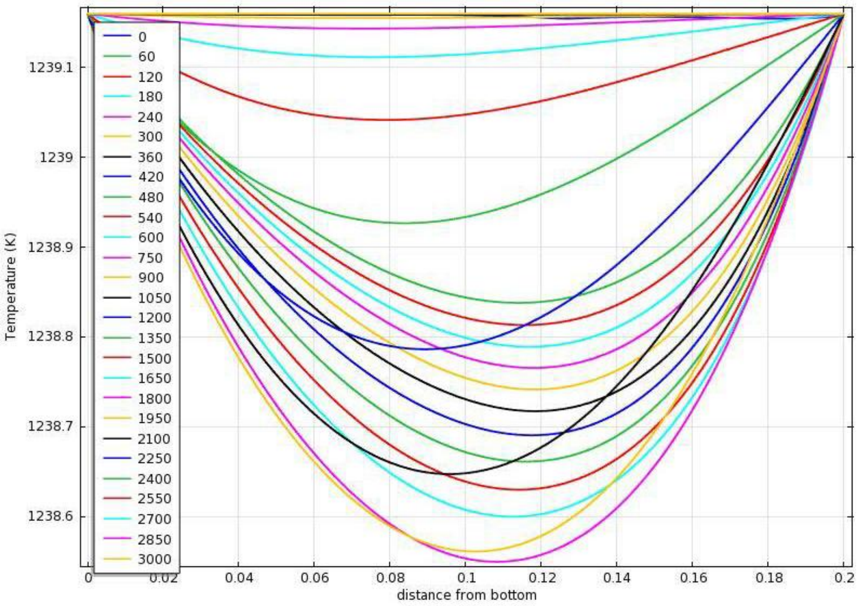
Diffusion coefficient = 1.033 * 10^{-5} m^2/sec

Results

Temperature profile



Temperature profile



Profile of temperature along a horizontal and a vertical line passing through centre of crucible

Conclusion

- Bed diffusion resistance is significant and can not be neglected while determining the reaction kinetics.
- This resistance is successfully modeled for the Vastan coal samples using a diffusion-reaction model.
- Rate constants and diffusivities are successfully estimated for the coals of interest as regards to UCG
- The kinetic model developed in the present work can be suitably incorporated in other process models

Thank you !