Effect of Bed Diffusion and Operating Parameters on Char Combustion in the Context of Underground Coal Gasification

by

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Presentation Outline

- Introduction
- Kinetic Determination
- Boat Reactor Experiments
- Modeling of Boat Reactor Experiments
- Conclusions

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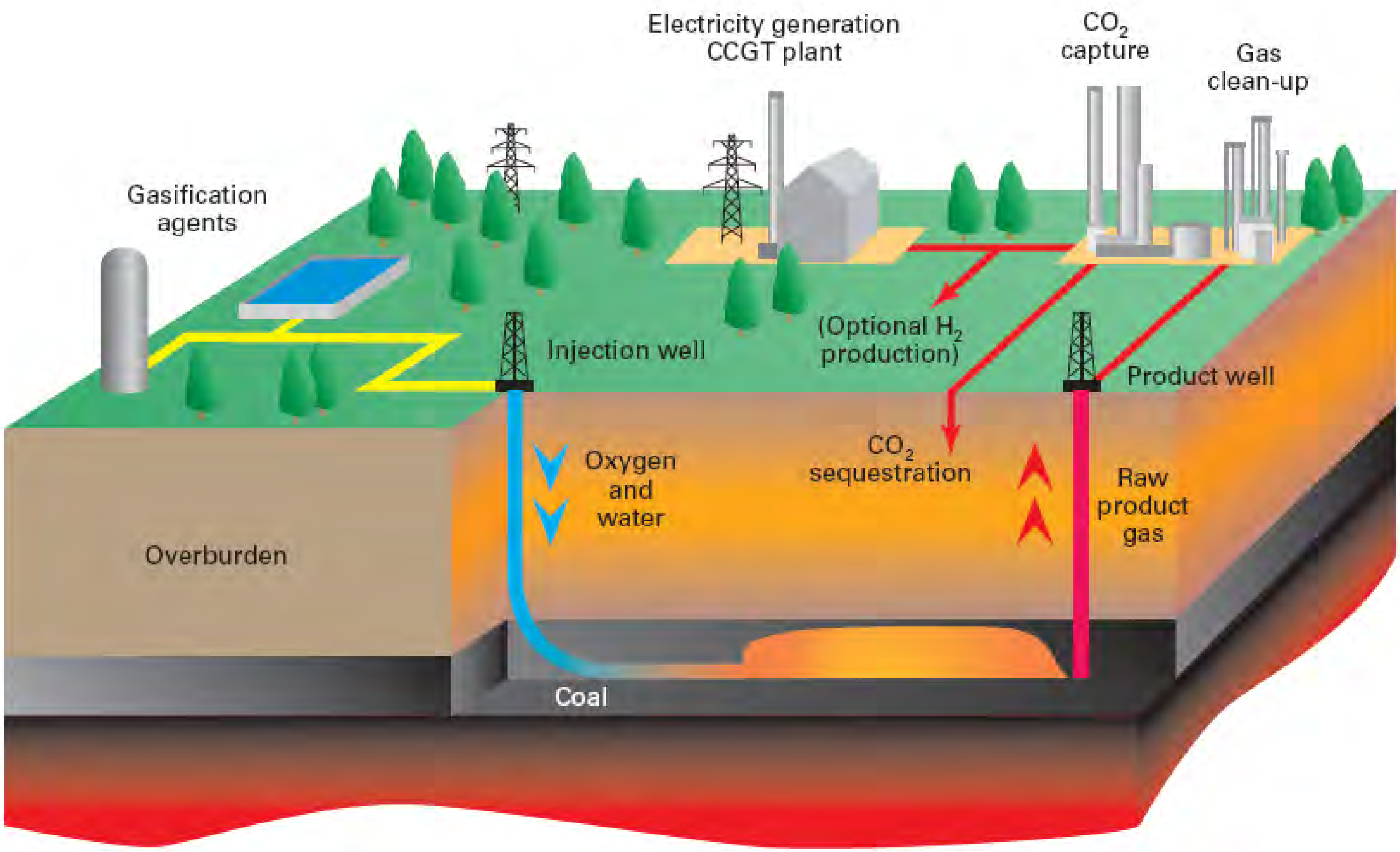
The Process of UCG



http://www.dti.gov.uk/energy/sources/renewables/publications/page19148.html

Importance of Combustion

- It is the essential heat source for endothermic gasification reactions.
- It is the only reaction during early cavity growth.
- So, to study effect of different parameters on combustion reaction becomes a very important part of understanding UCG.

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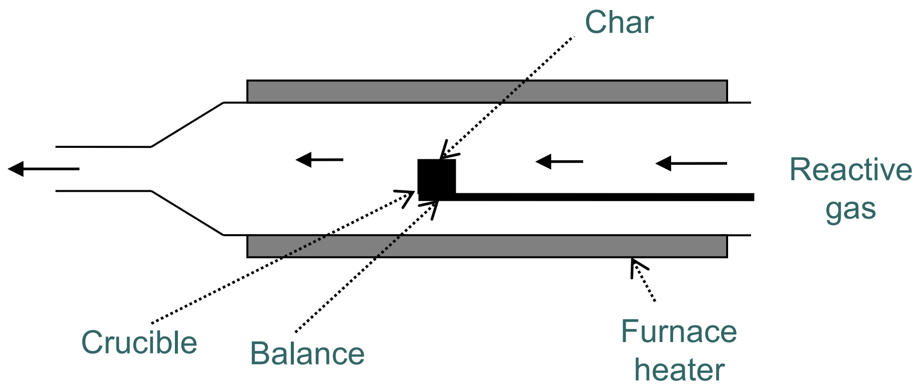
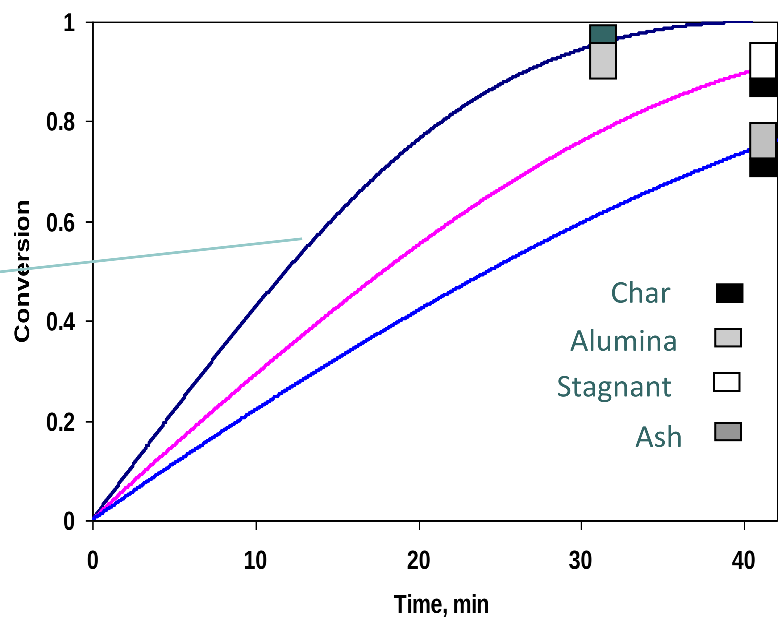
TGA Experiments for Kinetics



Schematic diagram of horizontal arm TGA

- Preliminary experiments conducted with different crucible fillings

Conversion profiles for different fillings

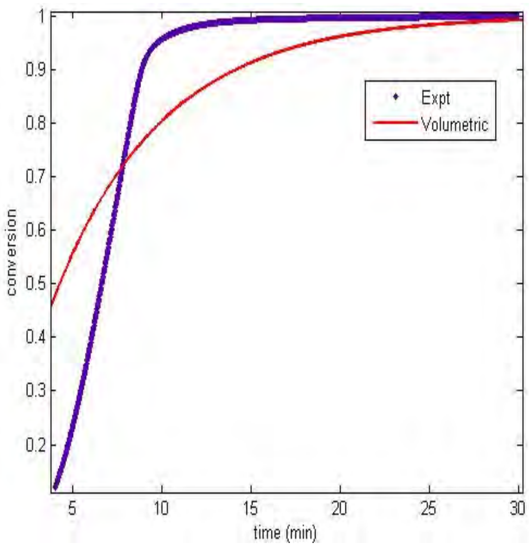


The crucible filling of char on the top of alumina gives the true intrinsic kinetics

Schematic of crucible filling

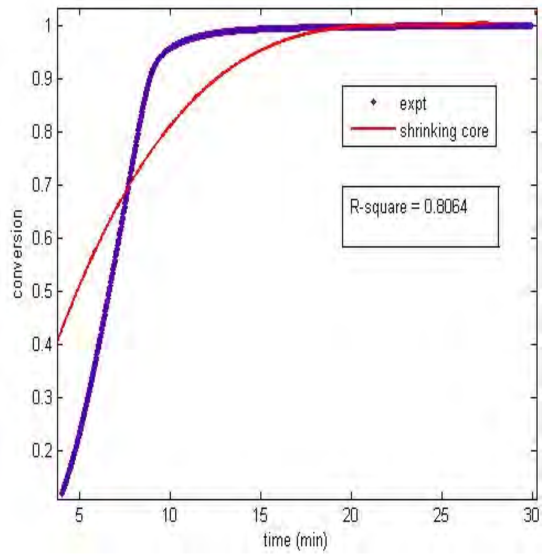
Model Fitting

Conversion vs. time at 600 ˚C



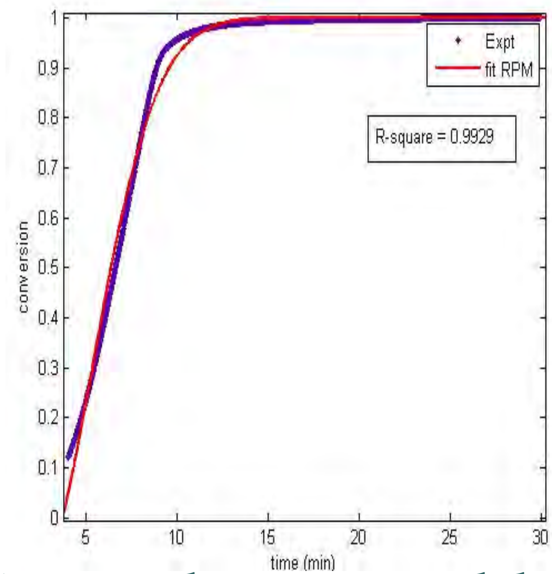
Volumetric model

$$\frac{dx}{dt} = K\, P_g^n\, (1 - x)$$



Shrinking core model

$$\frac{dx}{dt} = K\, (1 - x)^{2/3}$$



Random pore model

$$\frac{dX}{dt} = \frac{k s S_0}{(1 - \varepsilon_0)} (1 - X) \sqrt{1 - \psi \ln(1 - X)}$$

Random pore model gives the best fitting !!

Kinetic Parameters

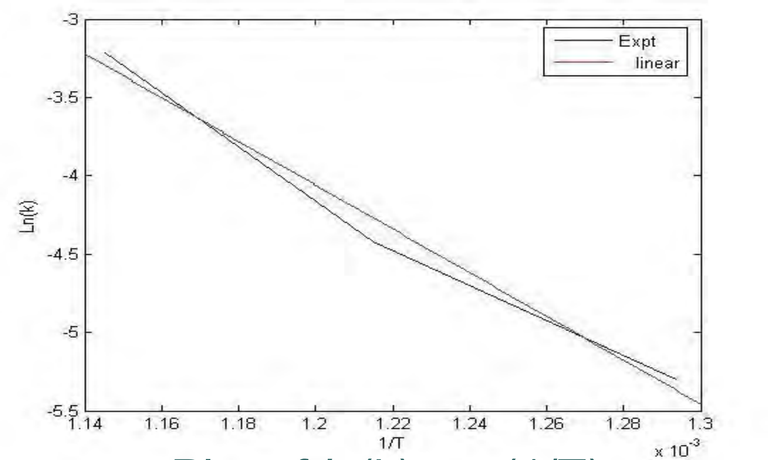
BET Results :

BET surface area (S_0) = 179.16 m^2/g $\psi = \frac{4\pi L_0(1-\varepsilon_0)}{S_0^2} = 3.8485$

From pore size distribution:

ε_0 = 0.2531 ; L_0= 2.754 x 10^{12} cr

Temperature (˚C)	K $\frac{k_s S_0}{(1-\varepsilon_0)}$ (1/sec)
500	5×10^{-3}
550	1.2×10^{-2}
600	4×10^{-2}



Plot of *ln*(k) vs. (1/T)

k_o	E_a
0.2 x 10^6 (sec^{-1})	116.7 kJ/mol

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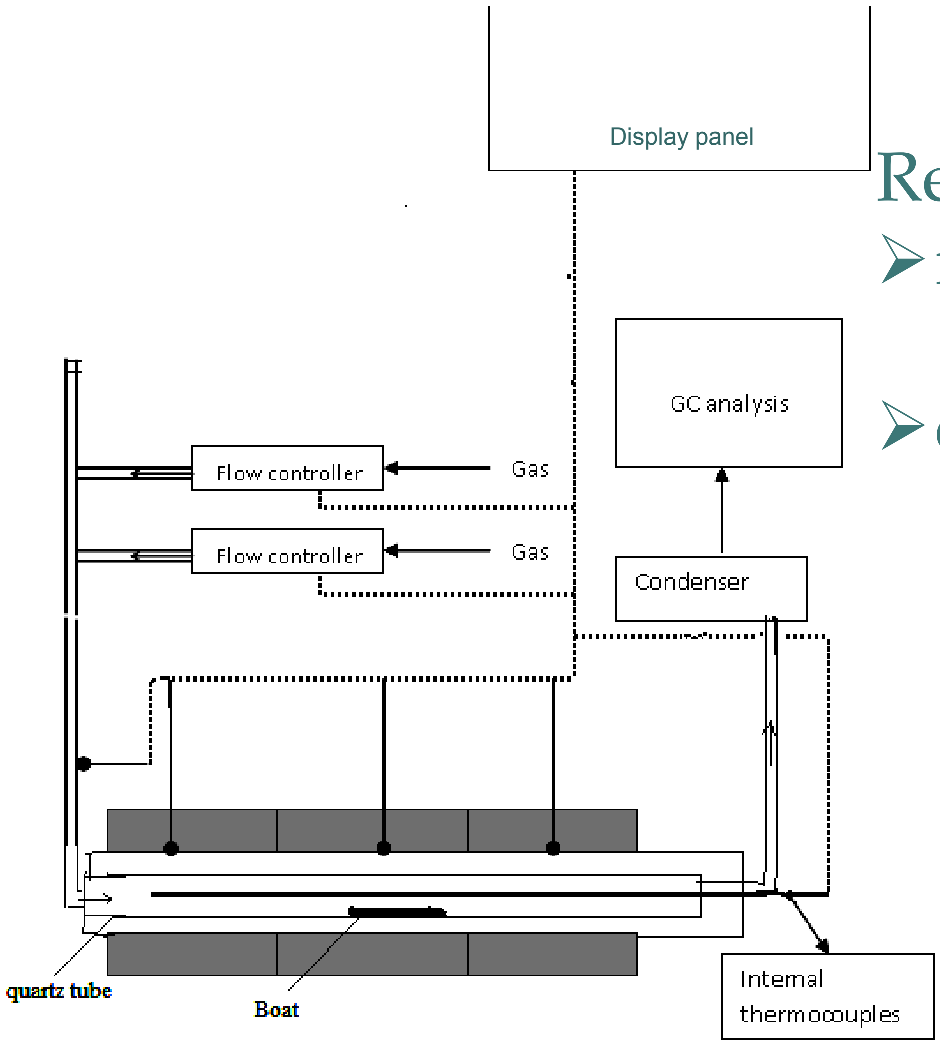
Experimental Setup



Reactor is

- insulated from outside
- equipped with
  - heaters at top and bottom
  - internal thermocouples
  - flow controllers
  - an online GC

Experimental Conditions

- At low temperature & relatively higher flow rates
- Char particle size < 150 micron
- Temperature = 500 ^{o}c, 550 ^{o}c, 600 ^{o}c
- Flow rate = 75 ml/min, 100 ml/min, 125 ml/min
- Bed height = fully filled and monolayer

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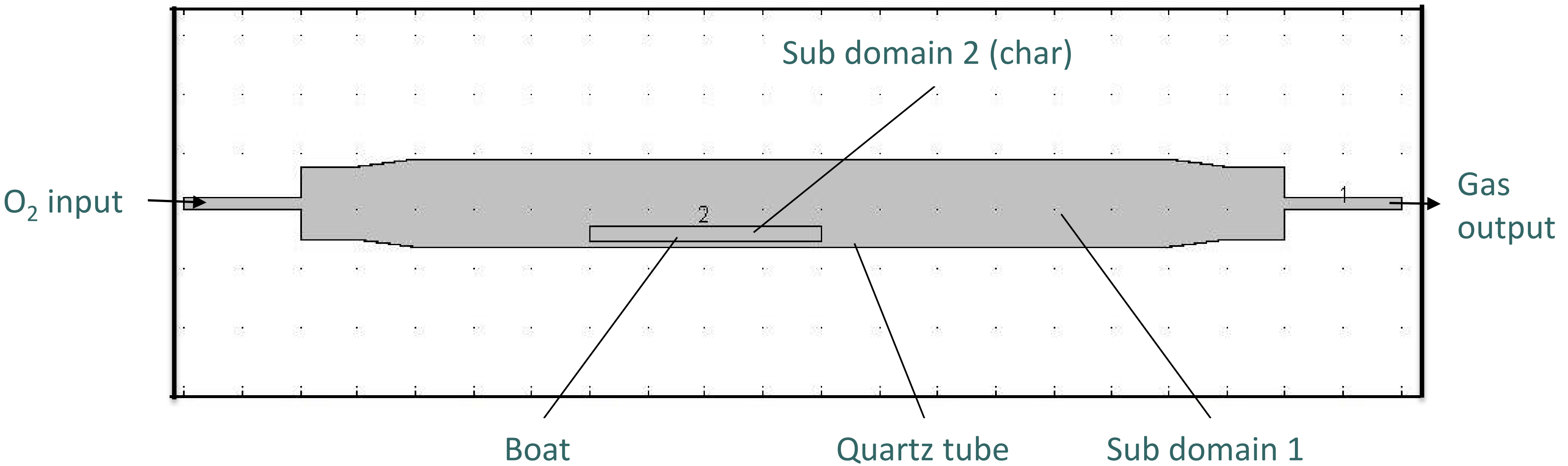
Boat Reactor Geometry for Modeling



Schematic of boat reactor

Governing Equations

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \tau] + \mathbf{F}$$

Navier Stokes equation

$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = \nabla\cdot(D\nabla c)$$

Mass transport equation in quartz tube

$$\frac{\partial c}{\partial t} = \nabla\cdot(D\nabla c) + R$$

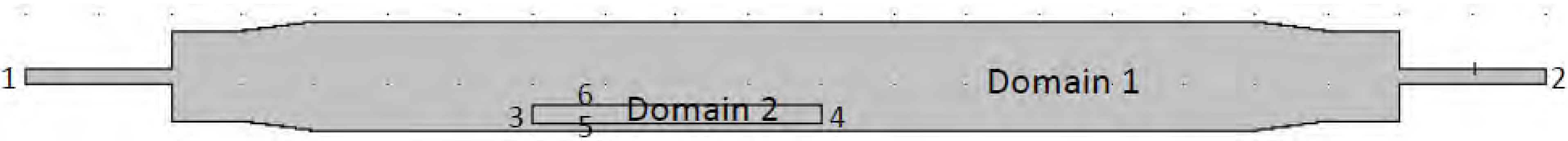
Mass transport equation in boat

Reaction: $C + O_2 \rightarrow CO_2$

Boundary Conditions

boundary no.	velocity	O_2	CO_2	char
1	u_in	c_o2_fluxin		NA
2	outlet	convective flow		NA
3,4,5	wall	zero flux (wall)		
6		continuity		no flux
all other		zero flux (wall)		NA

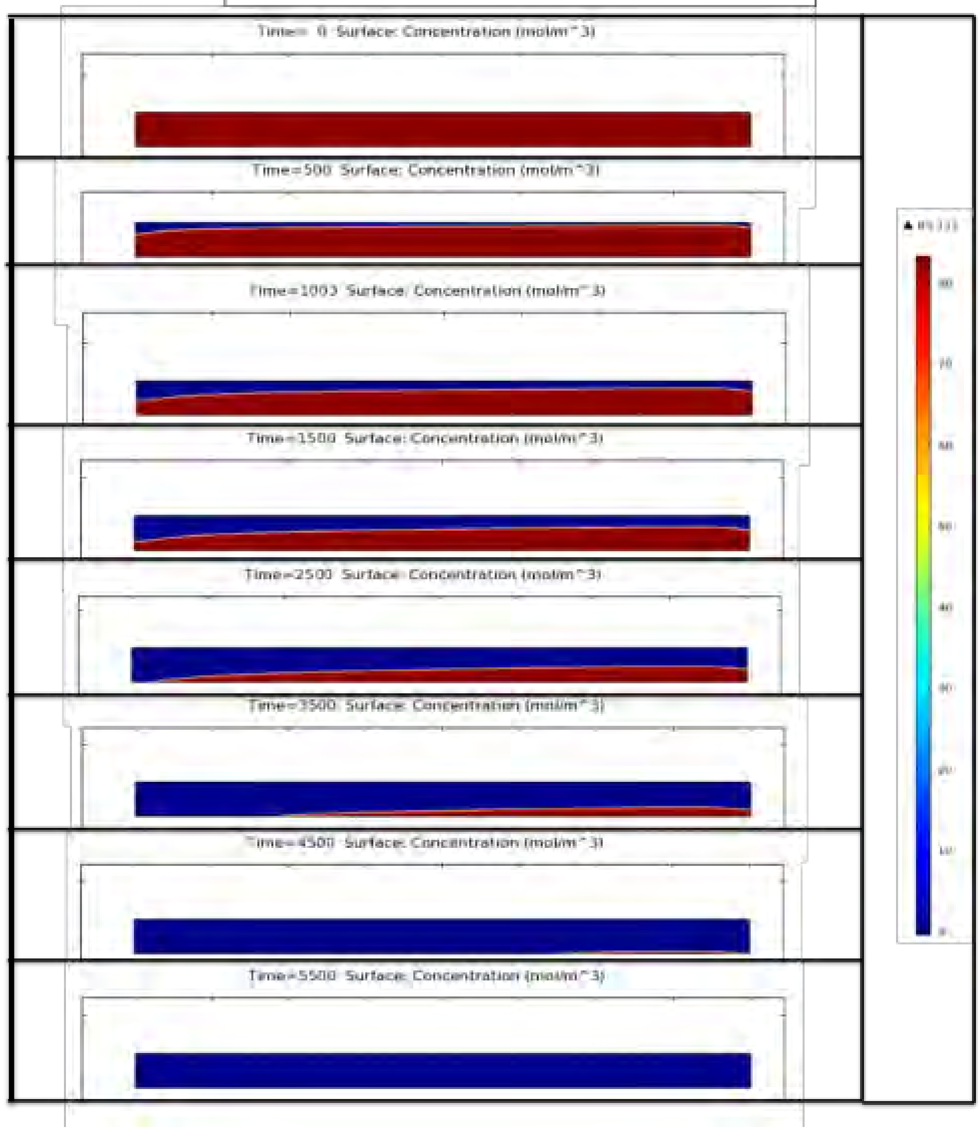
Initial Conditions



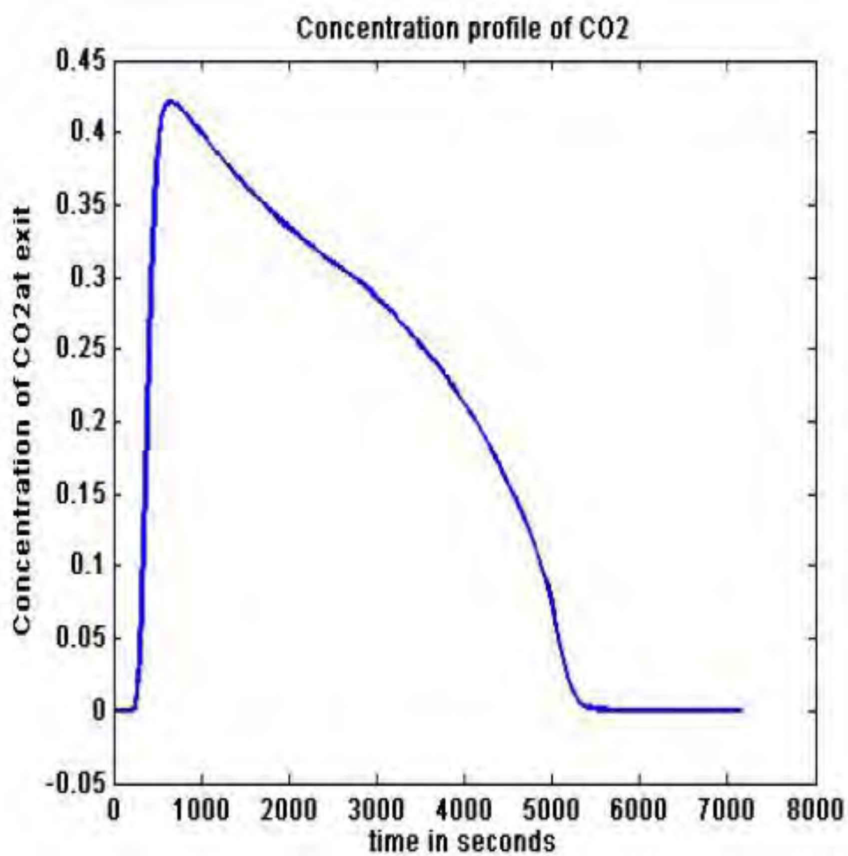
domain no.	velocity	O_2	CO_2	char
1	0	Zero concentration		NA
2	NA	Zero concentration		c_cinit

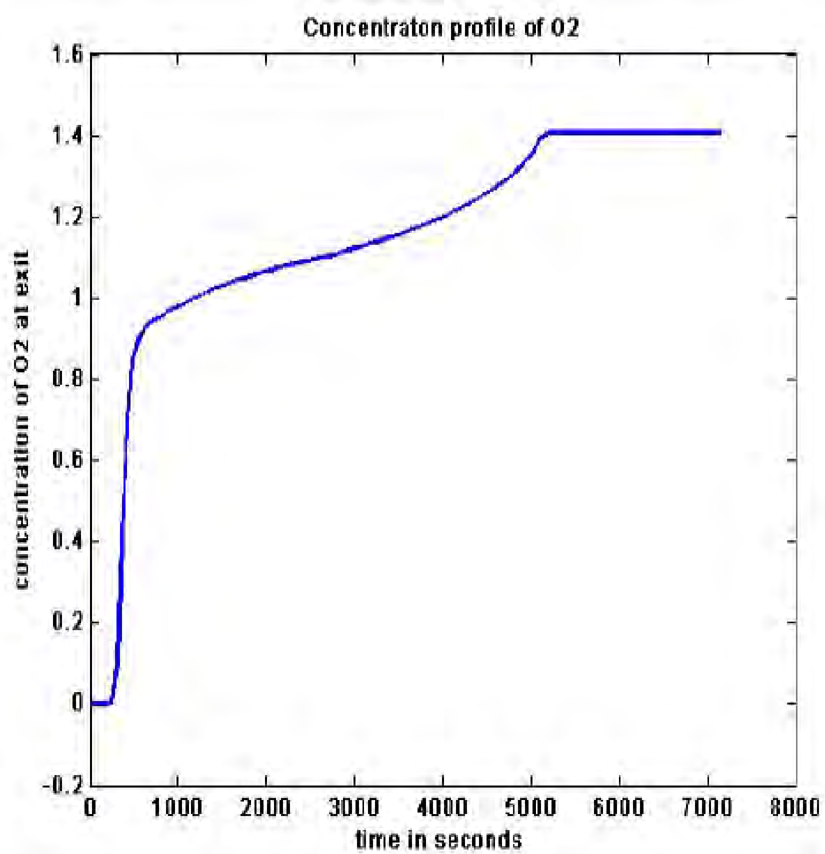
Results:

Evolution of char concentration in boat over time



Results: Outlet Gas Concentration





Qualitatively matches with experimental results !!

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Conclusion

- Effect of different operating parameters and bed diffusivity/bed height on the char combustion in UCG like condition are evaluated.

- Multiphysics modeling using COMSOL provided an insight of the experiments.

- Dependence on partial pressure of oxygen is to be determined and modeled.

- Modeling strategy is to be extended to real UCG conditions for early cavity growth.

Thank you !

References

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[6] Daggupati, S, Mandapati, R., Mahajani, S.M., Ganesh, A., Mathur, D.K., Sharma, R.K. and Aghalayam, P., 2009, “Laboratory Studies On Combustion Cavity Growth In Lignite Coal Blocks In The Context Of Underground Coal Gasification” in *Energy*, **35**, 2374-2386, (2010)
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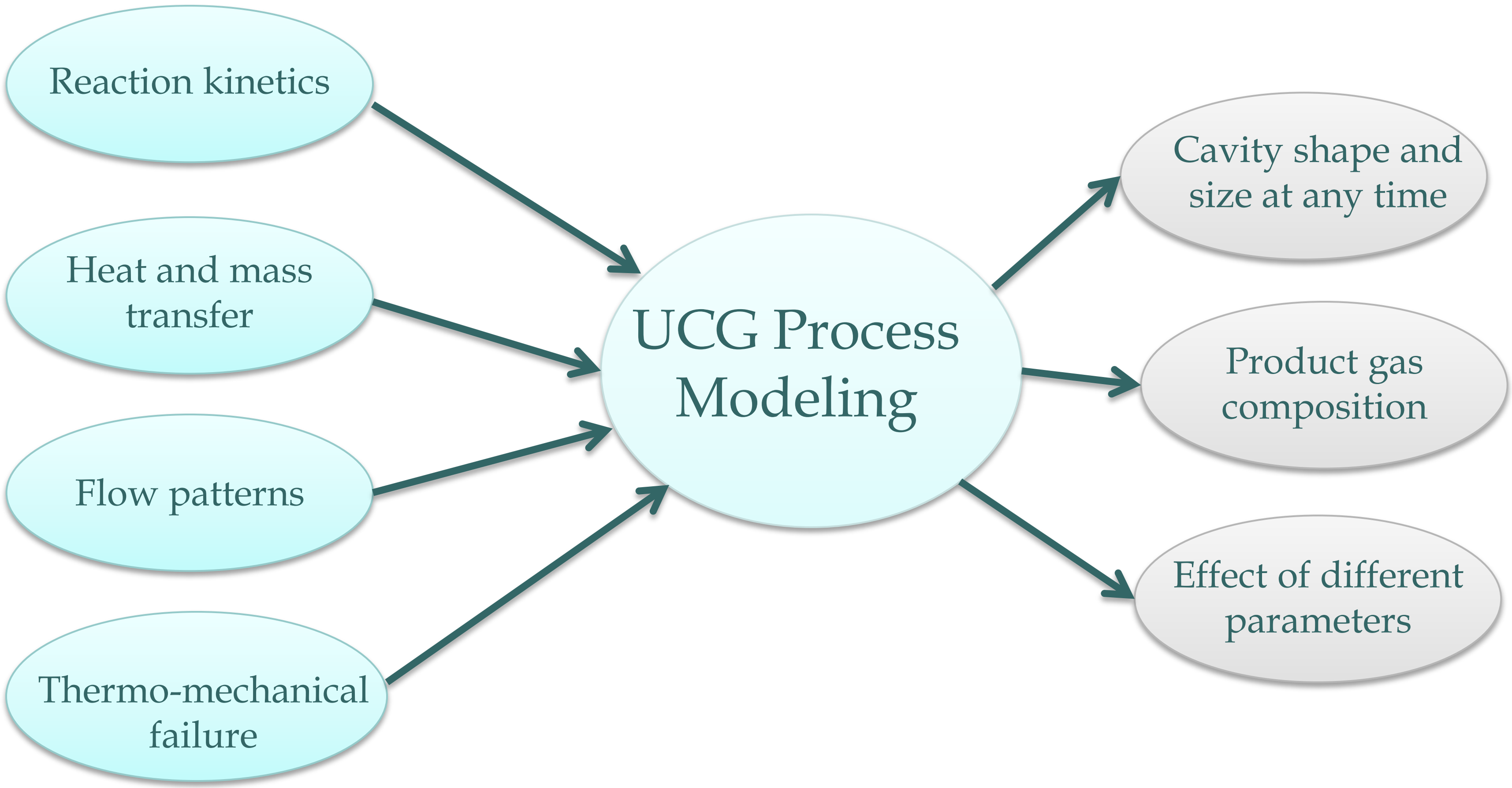
Extra Slides

Boat reactor

Name	Expression
rho	(100000*32/1000/8.314/873) [kg/m^3]
eta	(70e-6/rho) [Pa/s*kg/m^3]
u_in	.05[m/s]
D1_o2	5e-5[m^2/s]
D2_o2	1e-5[m^2/s]
c_cinit	(1/12e-3) [mole/m^3]
D1_co2	5e-5[m^2/s]
D2_co2	1e-5[m^2/s]
c_o2_fluxin	.1[mol/m^2/s]
psi	3.85
k0	2e9
E	95700
R_g	8.314
T	600 [K]

Name	Expression
R_c	-k1*c_o2
R_o2	-k1*c_o2
R_co2	k1*c_o2
k1	ka1*(1-psi*log(1-X))^.5*flc2hs(X, 1e-3)
X	max((c_cinit-c_c)/c_cinit,0)
ka1	k0*exp(-E/R_g/T)

Process Modeling of UCG



The boat reactor set up consists of

a cylindrical quartz tube (length 0.8 m and diameter 0.05 m),
and
a rectangular quartz boat is placed inside the quartz tube. Boat dimensions are: length 0.15m, breadth 0.035m and thickness 0.005m.

Table 1 Coal properties

	Dry basis	
Proximate Analysis	Volatile matter	44.92%
	Fixed Carbon	46.61%
	Ash	8.47%
Ultimate Analysis	Carbon	40.594%
	Hydrogen	5.672%

Experimental Results

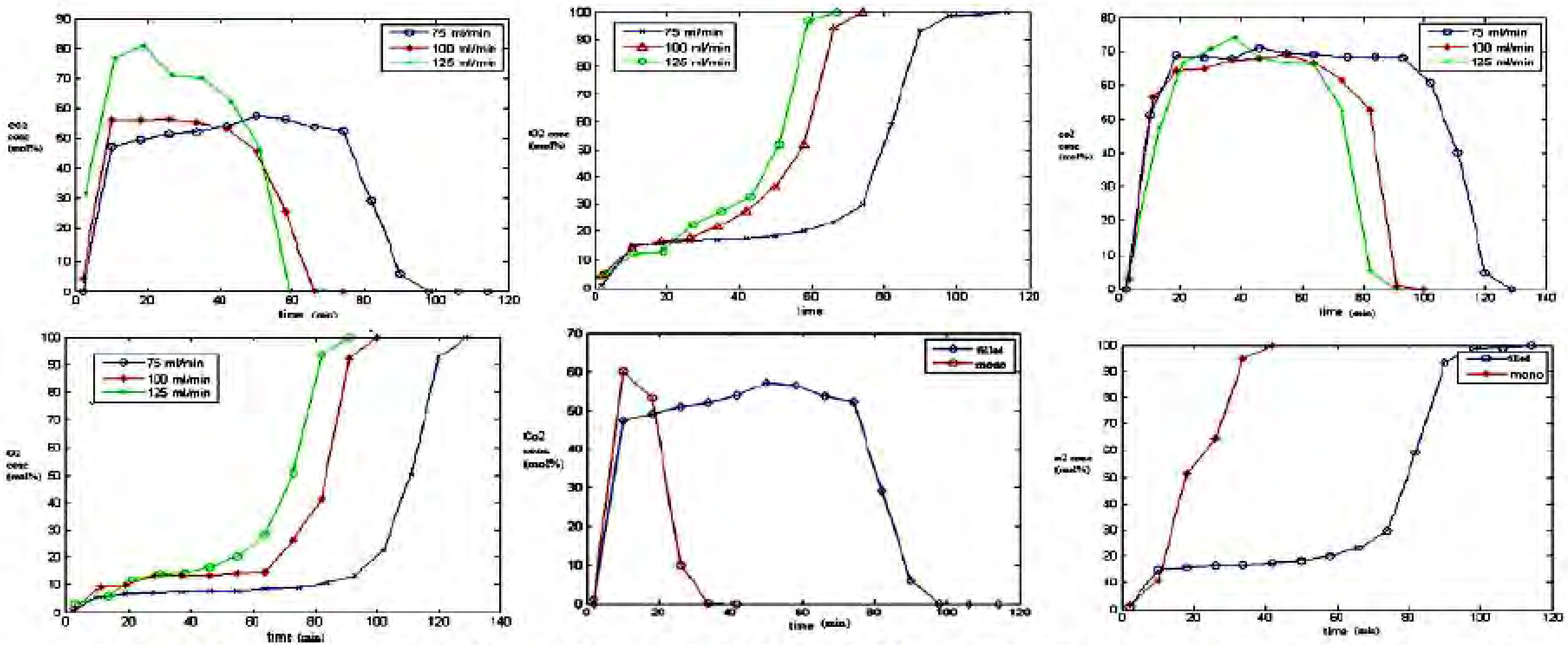


Figure 2 Concentration of CO2 and O2 vs. time at 500 and 550°C respectively (fig. a, b, c, d), comparison of monolayer and complete filling at 500°C, 100 ml/min (fig. e, f)

Assumptions:

- Incompressible laminar flow
- Inlet gas is pure oxygen
- Flow of gas in the channel,
- Diffusion and combustion in the boat.
- 2-D geometry modelled.

The mesh quality and quantity is as following: minimum element quality: 0.6689, average element quality: 0.9909, triangular elements: 151779.