2-D Modeling of Underground Coal Gasification(UCG)

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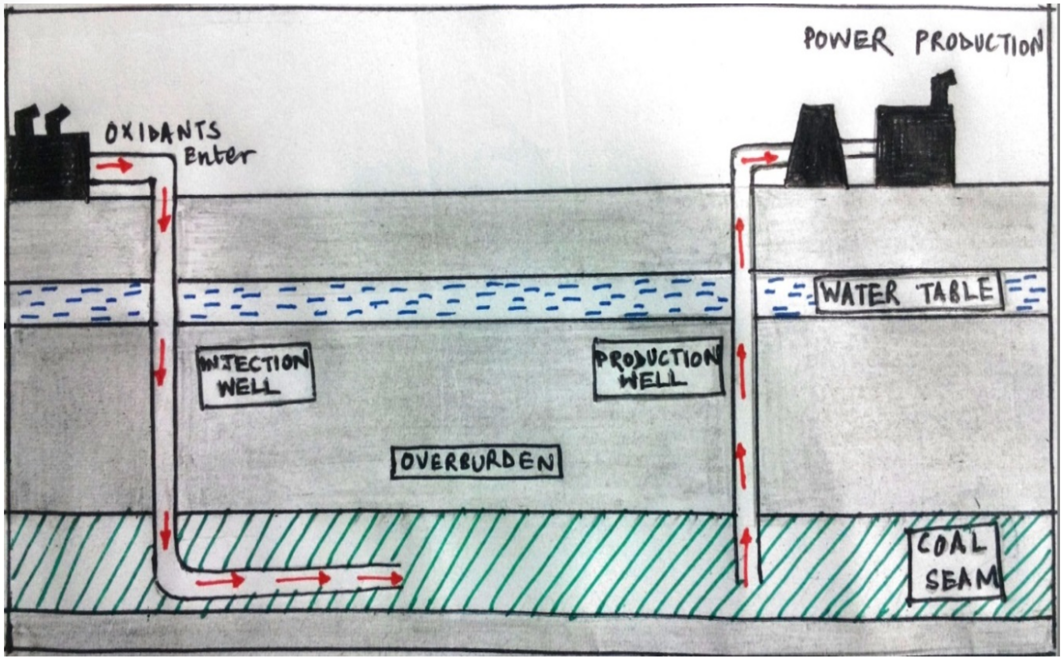
Agenda

- What is UCG?
- Model Geometry
- Reactions and Governing Equations
- COMSOL Modeling
- Results and Discussions

What is UCG and Why UCG?



Schematic of the UCG process - *CRIP* geometry

Advantages	Disadvantages
Environmental	Complexity
Transportation	Subsidence
Deep Coals	Contamination
CCS	Exploration

The successful application of such a process would provide a low to medium heating gas(80-250 kJ/mol), depending on whether air or a mixture of oxygen - steam is used.

What is UCG and Why UCG?

UCG can help meet the rising energy demand by utilizing coal resources that otherwise would be too deep, or of poor quality, or simply not economical to mine.

Why modeling of UCG?

- A cavity is formed; **grows three dimensionally**
- Complex process; **simplified process model** needed
- Develop a **two-dimensional model** of the cavity
- Analyse **cavity growth** and **product gas composition**

This model can foresee the growth of the cavity even after it has hit the overburden, which is the reality for the UCG of thin coal seam.

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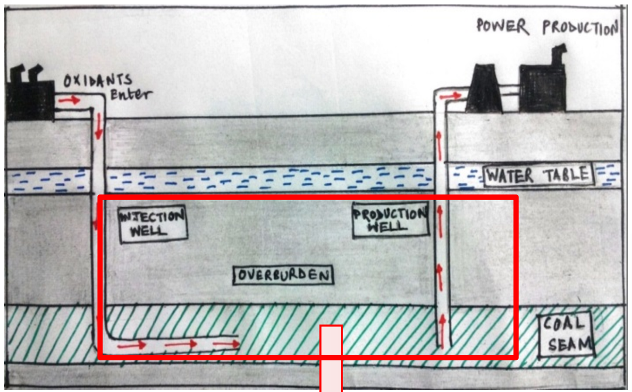
UCG Process Model Geometry



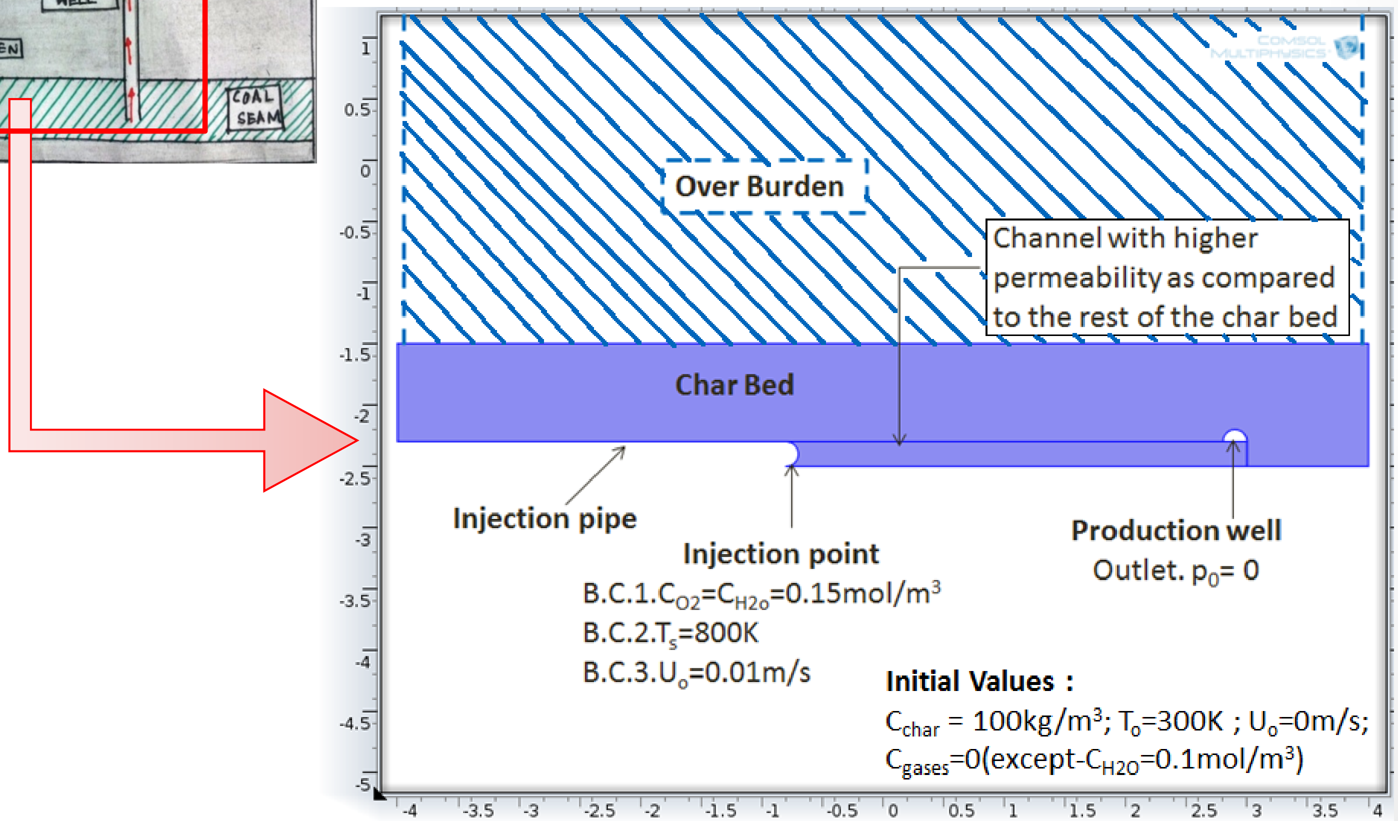


Figure 2 2-D Geometry of UCG process (COMSOL model)

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Reactions in UCG

Oxidation of Char -

$$C + O_2 \rightarrow CO_2 \qquad (i)$$

Steam gasification of Char -

$$C + H_2O \rightarrow CO + H_2 \qquad (ii)$$

Boudouard reaction -

$$C + CO_2 \rightarrow 2\,CO \qquad (iii)$$

Water-gas shift reaction -

$$CO + H_2O \leftrightarrow CO_2 + 2H_2O \qquad (iv)$$

Oxidation of Hydrogen gas-

$$H_2 + {}^{1}/_{2}\,O_2 \rightarrow H_2O \qquad (v)$$

Oxidation of Carbon monoxide-

$$CO + {}^{1}/_{2}\,O_2 \rightarrow CO_2 \qquad (vi)$$

Governing Equations

1) Brinkman's Equation (Modified Darcy's Law)

$$\frac{\partial(\rho\epsilon_p)}{\partial t} + \beta\nabla^2(u) + \nabla.(\rho u) = Q_{br}$$

Where, $u = \frac{-k}{\mu}\nabla p$

2) Mass balance of Solid Char

$$\frac{\partial C_{Char}}{\partial t} = R_{Char}$$

Where, $R_{Char} = -r_1 - r_2 - r_3$

Governing Equations

3) Mass balance of Gas phase species

$$\frac{\partial C_i}{\partial t} + \nabla.(-D_i \nabla C_i) + u.\nabla C_i = R_i$$

i - O_2 , CO_2, CO, H_2, H_2O

4) Heat transfer in the porous media

$$(\rho C_p)_{eff}\frac{\partial T_s}{\partial t} + \nabla.(\rho_g u C_{p,g} T_s) = \nabla.\left(-k_{eff}\nabla T_s\right) + \sum_{i=1}^{3}(\Delta H_i * R_i)$$

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COMSOL Modeling

- Add Physics
  - **Chemical Species Transport** – 'Transport of Dilute Species'
  - **Fluid flow** – 'Porous Media and Sub surface Flow' – *'Brinkman'*
  - **Heat Transfer** – 'Heat Transfer in Porous Media'

- Mesh
  - ***'User Controlled'*** sequence type
  - **Maximum** and **Minimum** element size of **0.03cm** and **1.6e-4cm** each

- 2 Study Steps
  - **Stationary** – Fully coupled PARDISO solver; Brinkman Equations
  - **Time Dependent** – Segregated PARDISO solver; All models

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Results and Discussion

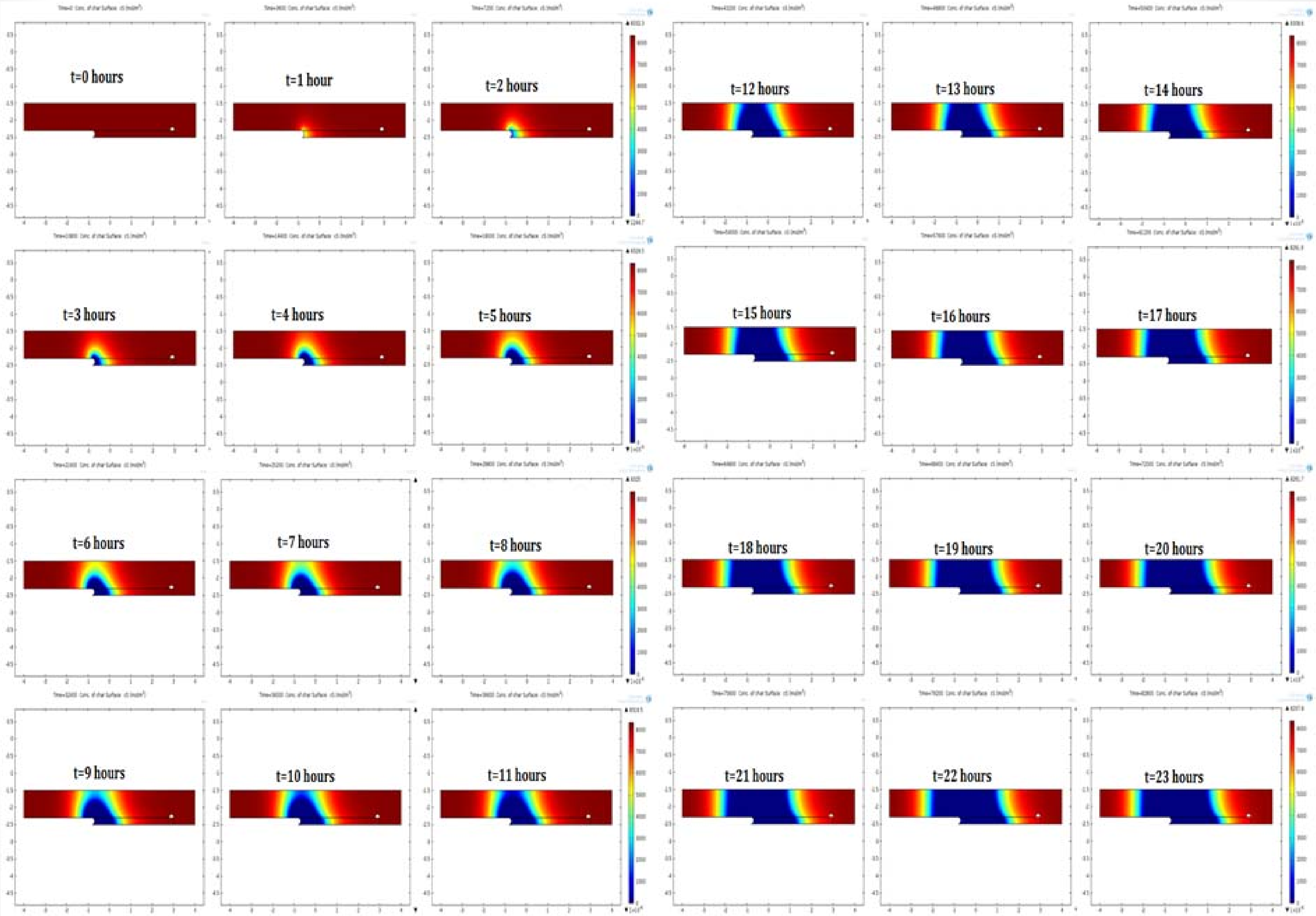

Figure 3 : Concentration of Char (Cavity growth) from time = 0 to 24 hours during UCG

Results and Discussion

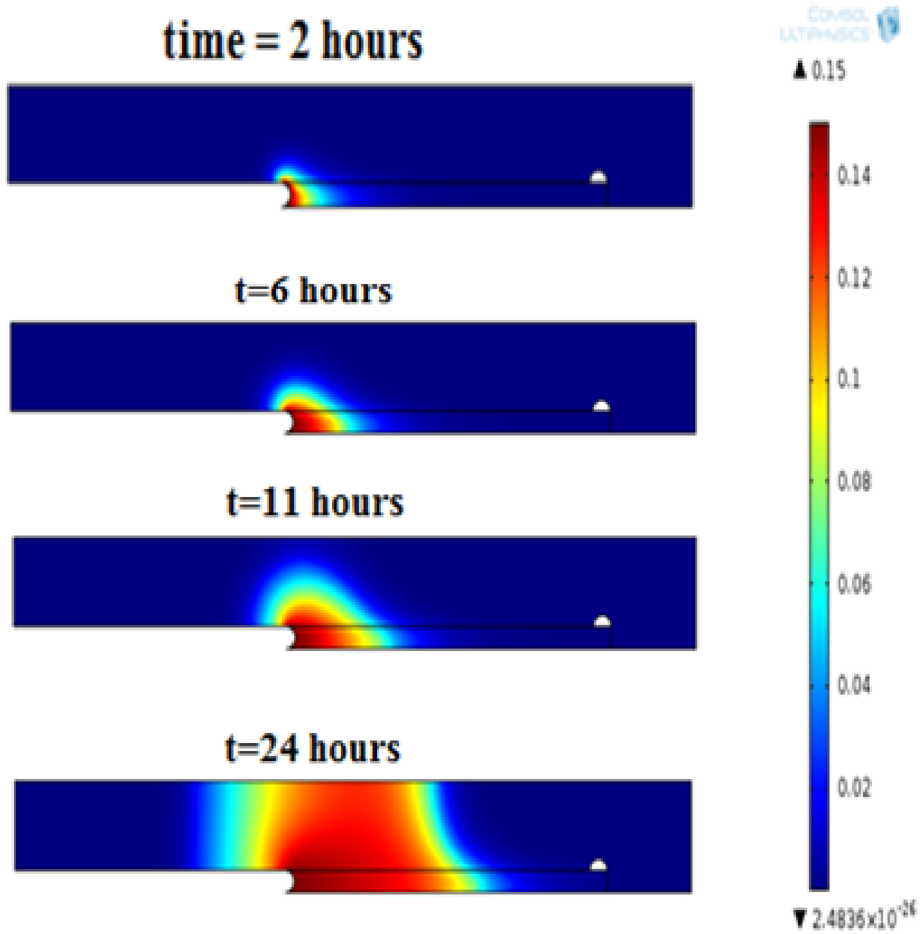

Figure 4 Concentration of Oxygen(O_2) at time = 2, 6, 11 and 24 hours during UCG

Results and Discussion

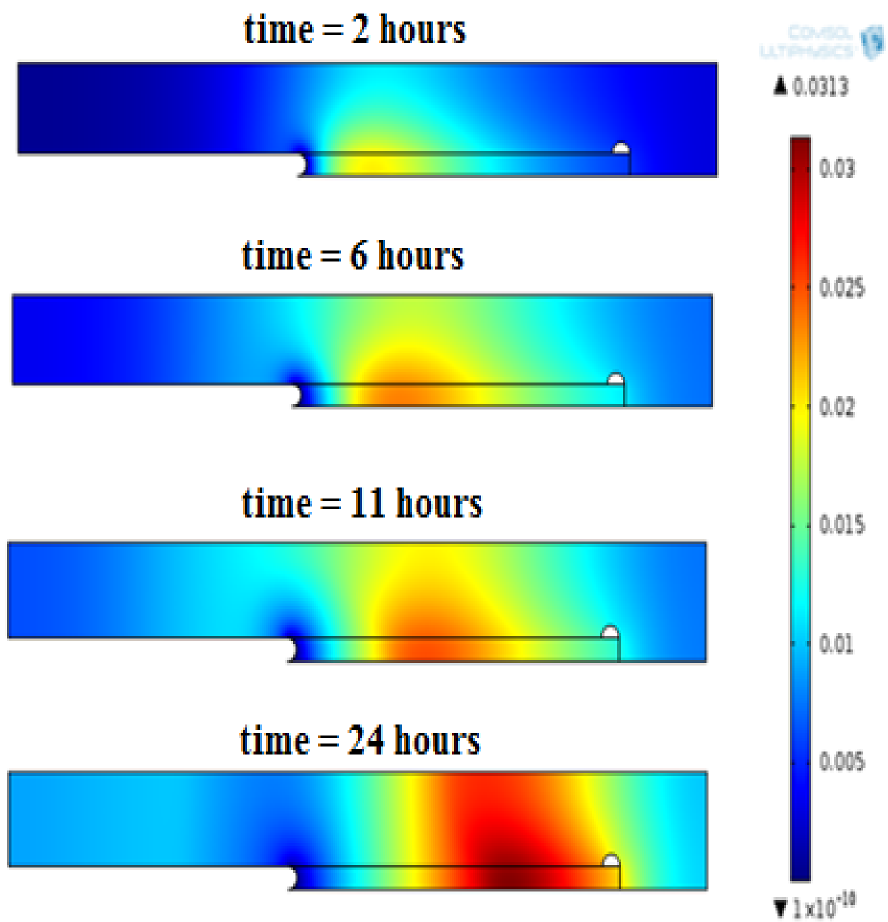

Figure 5 Conc. of Carbon dioxide(CO_2) at time = 2, 6, 11 and 24 hours during UCG

Side and Top view of the Cavity

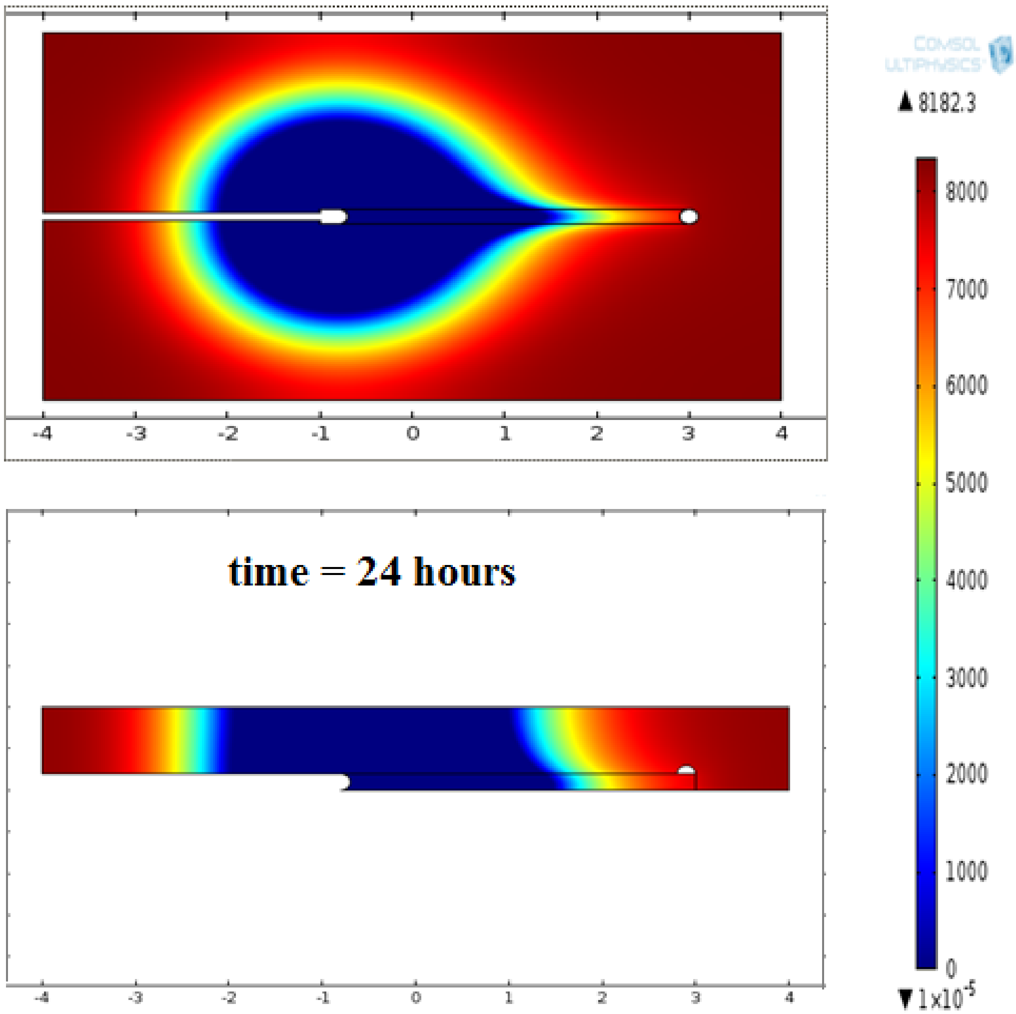

Figure 6 Shape of cavity in top and side view at t=24 hours

Conclusion & Future Work

- Detailed 2-D model for the UCG process has been developed
- Six (post drying and pyrolysis) reactions have been considered
- Predicted Cavity shape matches with experimental results
- The two 2-D model results provide a 3-D perspective

- Parametric analysis
  - Steam to Oxygen ratio
  - Flow rate at inlet
- The effect of geometry scale up is being analysed so as to study the possibility of extrapolation to any size of coal bed and inlet/outlet well positions during UCG

Conclusion & Future Work

This complete UCG COMSOL model is the 2-D top view and side view models with all reactions, parameters, geometry, scales and meshes

The model can verify experimental results and substantiate the MATLAB process model.

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Thank You ☺

Back-up Slides (Q&A)

Reactions Kinetics

$$C + O_2 \rightarrow CO_2 \qquad \textbf{(i)}$$

$$C + H_2O \rightarrow CO + H_2 \qquad \textbf{(ii)}$$

$$C + CO_2 \rightarrow 2\,CO \qquad \textbf{(iii)}$$

These three are **heterogeneous reactions**, i.e. solid – gas reactions representing various oxidation and gasification reactions.

The rates for Eq.(i)-(iii) are influenced by **3 mechanisms:**

- Mass-transport limitation from bulk-gas to solid surface
- Limitation in mass-transport in any internal particle porosity/ash layer
- Kinetic-limitations for reactions at solid surface

Here, the latter two are lumped into one effective chemical rate expression. Otherwise, intra-particle balances would need to be written.

Reaction Kinetics

Eq.(i) –(iii)

- Total rate can thus be obtained by taking the **external transport in series** with the lumped(kinetic+internal transport) rate

$$R_T = \frac{1}{\left({}^{1}/_{(1-\epsilon_p)R_c} + {}^{1}/_{R_m}\right)}$$

- R_c - effective chemical rate evaluated using gas compositions of bulk gas
- R_m - mass-transfer rate of limiting reactant

Standard form of the effective chemical rate -

$$R_c = k * \exp\left(-{}^{E}/_{RT}\right) * yg * Ptotal * Cchar * \sqrt{1 - 3.74\left({}^{Cchar}/_{Cchar_{in}}\right)}$$

Standard form of mass transfer rate -

$R_m = k_y * yg$

Reaction Kinetics

$\boldsymbol{CO + H_2O \leftrightarrow CO_2 + 2H_2O}$ **(iv)**

This is the water-gas shift reaction which is reversible and occurs only in the gas phase.

$$R_4 = R_4{}^+ - R_4{}^- = k_4{}^+ \left[C_{CO} C_{H_2O} - \frac{C_{CO_2} C_{H_2}}{K_{E4}} \right]$$

$\boldsymbol{H_2 + {}^1/_2 O_2 \rightarrow H_2O}$ **(v)**

$\boldsymbol{CO + {}^1/_2 O_2 \rightarrow CO_2}$ **(vi)**

If $C_{O_2} < C_{CO}, C_{H_2};\quad R_5 = R_6 = R_{oxn}$

If $C_{O_2} > C_{CO}, C_{H_2};\quad R_5 = \frac{R_{oxn} * C_{H_2}}{2C_{O_2}}; R_6 = \frac{R_{oxn} * C_{CO}}{2C_{O_2}}$

Where, $R_{oxn} = k_{oxn} * C_{O_2}$, for $T_s > 650K$

Rates of all reactions

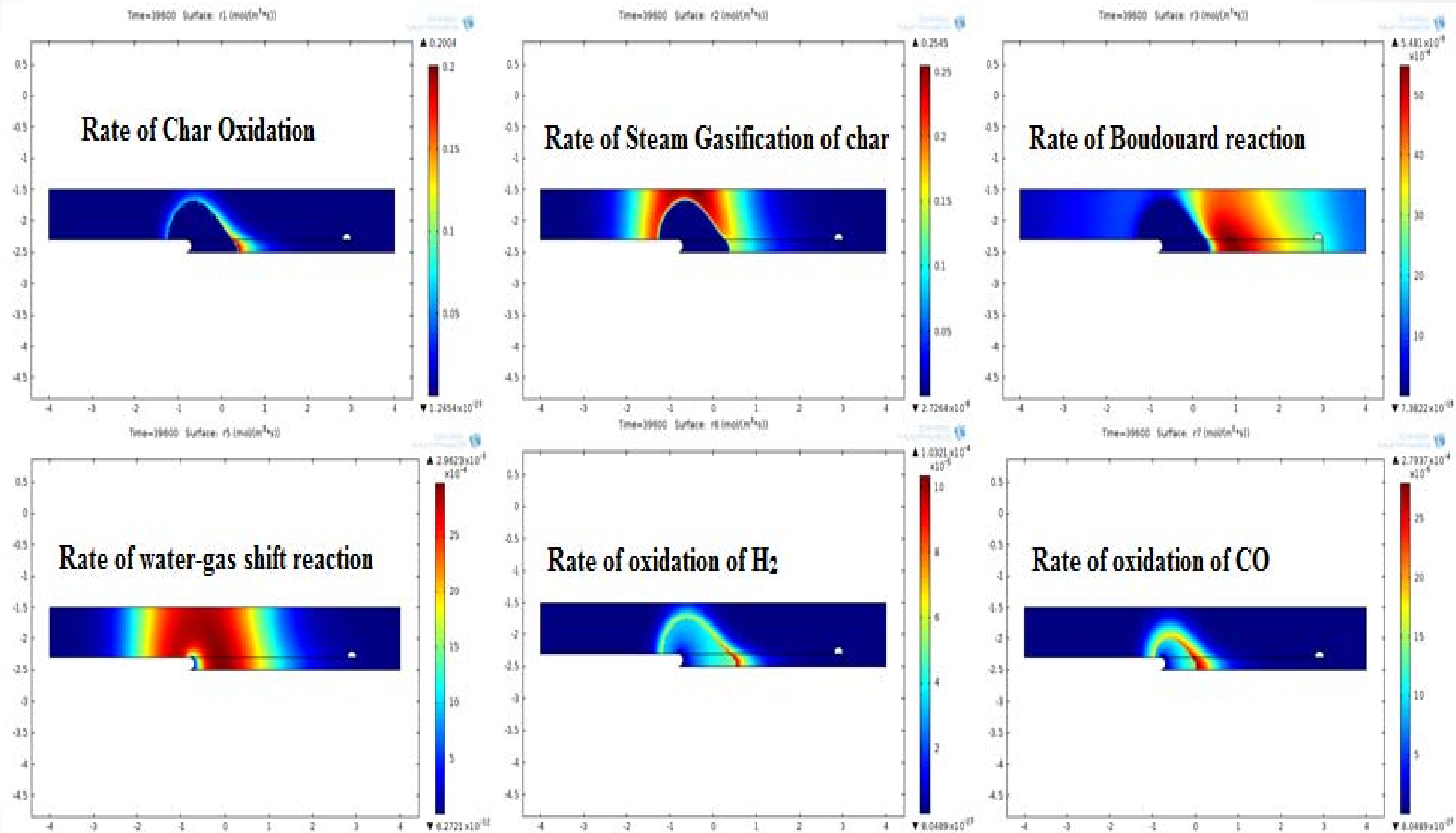

Figure 6 Rates of all 6 reactions at time = 11 hours