Using CFD and an Overlapping Grid to Model the Low Temperature Oxidation Process in a Coal Discard Heap

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Advanced Mathematical Modelling

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Outline

Coal Discard Heaps
  The Problem
  The Chemistry

Methodology
  The Tools
  Overlapping Grids
  Chemistry

Results
  Method Comparison
  Simulated Results
  The Solution

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  Problems
Coal Discard Heaps - The Problem

- What is Low Grade Coal?
  - "Brown Coal"
  - Low Carbon, High Moisture
  - High Ash Content
  - Already burned/used

- Spontaneous Low-temperature Oxidation

- Heap configurations
Coal Discard Heaps - The Problem

- Emits CO$_2$
  - Discard heap emits$^1$ 12 – 8200 kgCO$_2$m$^{-2}$y$^{-1}$
  - Carbon Commodity Market: 2013-2020, Carbon credits could average €12 per ton CO$_2$

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Coal Discard Heaps - The Problem

- Emits $CO_2$
  - Discard heap emits$^1$ $12 - 8200 \, kg CO_2 \, m^{-2} \, y^{-1}$
  - Carbon Commodity Market: 2013-2020, Carbon credits could average €12 per ton $CO_2$
- Chemical Processes also produces Heat
  - can lead to combustion

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Chemical Reactions

**Oxidation**

\[1.05C(s) + O_2(g) \rightarrow 0.1CO(g) + 0.95CO_2(g)\]

**Gasification**

\[H_2O(g) + C(s) \rightarrow CO(g) + H_2(g)\]

**Hydrogenation**

\[H_2(g) + C(s) \rightarrow CH_4(g)\]

**Water-Gas Shift**

\[H_2O(g) + CO(g) \rightarrow CO_2(g) + H_2(g)\]

**Methanation**

\[CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(g)\]

**Boudouard**

\[CO_2(g) + C(s) \rightarrow CO(g)\]
Coal Discard Heaps - The Chemistry

▶ Chemical Reactions

**Oxidation**  
\[ 1.05C(s) + O_2(g) \rightarrow 0.1CO(g) + 0.95CO_2(g) \]

Reaction Rate:  
\[ R_1 = 2 \times 10^6 nO_2 e^{-\frac{57400}{8.314T}} \text{ [mol.s}^{-1}] \]

Heat Source:  
\[ E_1 = (-300 \times 10^3) R_1 \text{ [J.s}^{-1}] \]

**Gasification**  
\[ H_2O(g) + C(s) \rightarrow CO(g) + H_2(g) \]

\[ R_2 = 810n_{H_2O} e^{-\frac{147000}{8.314T}} \text{, } E_2 = (131 \times 10^3) R_2 \]

**Hydrogenation**  
\[ H_2(g) + C(s) \rightarrow CH_4(g) \]

\[ R_3 = 0.0061n_{H_2} e^{-\frac{80400}{8.314T}} \text{, } E_3 = (-74.85 \times 10^3) R_3 \]

**Water-Gas Shift**  
\[ H_2O(g) + CO(g) \rightarrow CO_2(g) + H_2(g) \]

**Methanation**  
\[ CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(g) \]

**Boudouard**  
\[ CO_2(g) + C(s) \rightarrow CO(g) \]
Methodology - The Tools

- Requirements
  - Chemical Reactions
  - Conjugate Heat Transfer
- Computational Fluid Dynamics
- OpenFOAM
  - Open Source
Methodology - Overlapping Grids

- Model discard heap as a porous medium
- Assume spherical particles
- Overlapping grid represent porous section
- ‘Split’ porous into solid (red) and fluid (green) sections
  - Solid: Conduction, heat generated by chemical processes
  - Fluid: Convection
  - Conjugate heat transfer between phases
- Conventional methods assume thermal equilibrium between the gas and solid phases.
Methodology - Chemistry

- Heat generated calculated based on the content of oxygen available
- Heat transfer:
  \[ \nabla \cdot (\rho hu) = \nabla \cdot (k_{eff} \nabla T_f) + \int_V \frac{h_a}{V} (T_{S_s} - T_f) dV + (1 - \epsilon) r_{O_2} \Delta H_{O_2} \]
- Heat of reaction of oxygen: \( \Delta H_{O_2} \)
- Rate of oxidation: \( r_{O_2} = K_1 C_{O_2} \)
  where \( K_1 = (8.828 \times 10^6) e^{-6950/T_{gas}} \) and \( C_{O_2} \) is oxygen’s mass fraction.
- Specie equation for oxygen: \( \nabla \cdot (\rho C_{O_2} u) = \nabla \cdot (D_{O_2} \nabla C_{O_2}) - r_{O_2} \)
Results - Method Comparison

- Analytical: 753.53 K
- Fluent: 754 K
- OpenFoam: 757 K (Solid), 740 K (Gas)
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Results - Simulated Results

- Initial 2D solution
- Assumptions:
  - A homogeneous, porous trapezoid
  - Only 3 chemical processes present
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![Coal Simulation]

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Results - Simulated Results

- Initial 2D solution
- Assumptions:
  - A homogeneous, porous trapezoid
  - Only 3 chemical processes present

Porous
Results - Simulated Results
Results - Simulated Results

- 3D
Results - Simulated Results

- 3D

Contours of Static Temperature (k)
Results - Simulated Results

3D

Contours of Molar Concentration of co2 (kmol/m3)
Results - The Solution

- To prevent chemical reaction
- Heat
- $O_2$

Results - The Solution

▶ To prevent chemical reaction

▶ Heat
  ▶ Water: Increase methane production, 21x more potent than CO2 as greenhouse gas;
    Acid mine drainage
  ▶ Extract Heat: Produce Electricity

▶ O2

Results - The Solution

- To prevent chemical reaction

- Heat
  - Water: Increase methane production, 21x more potent than $CO_2$ as greenhouse gas;
    Acid mine drainage
  - Extract Heat: Produce Electricity

- $O_2$
  - Cover heap with layer of soil

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Results - The Solution

- To prevent chemical reaction

- Heat
  - Water: Increase methane production, 21x more potent than CO₂ as greenhouse gas;
    Acid mine drainage
  - Extract Heat: Produce Electricity

- O₂
  - Cover heap with layer of soil²
  - Compact coal after dumped²
  - Redesign heap to limit O₂ ingress

Future Work - Problems

- Method
  - Complex chemical reactions
  - Heterogeneous porous medium
  - Transient simulation - take weather conditions into account
  - Reduce reactive coal content over time
Future Work - Problems

- Method
  - Complex chemical reactions
  - Heterogeneous porous medium
  - Transient simulation - take weather conditions into account
  - Reduce reactive coal content over time
- Do not fully understand heap:
  - Internal Structure (old/ large heaps)
  - All mechanism responsible for emissions, chemical or environmental
Thank You

- Njabulo Siyatshana, CSIR:MDS
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