Refractory Wear Modeling in Gasification Environments

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Gasification-based Coal Conversion Technology

Steam/
Water

Gasification with Oxygen
$C + {}^{1}/_{2}\, O_2 \longleftrightarrow CO$

Combustion with Oxygen
$C + O_2 \longleftrightarrow CO_2$

Gasification with Carbon Dioxide
$C + CO_2 \longleftrightarrow 2CO$

Gasification with Steam
$C + H_2O \longleftrightarrow CO + H_2$

Gasification with Hydrogen
$C + 2H_2 \longleftrightarrow CH_4$

Water-Gas Shift
$CO + H_2O \longleftrightarrow H_2 + CO_2$

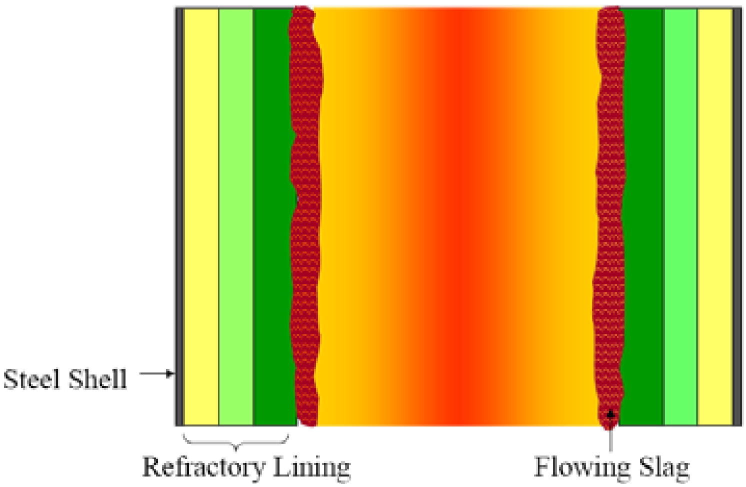
Methanation
$CO + 3H_2 \longleftrightarrow CH_4 + H_2O$

Gasifier Gas Composition (Vol %)

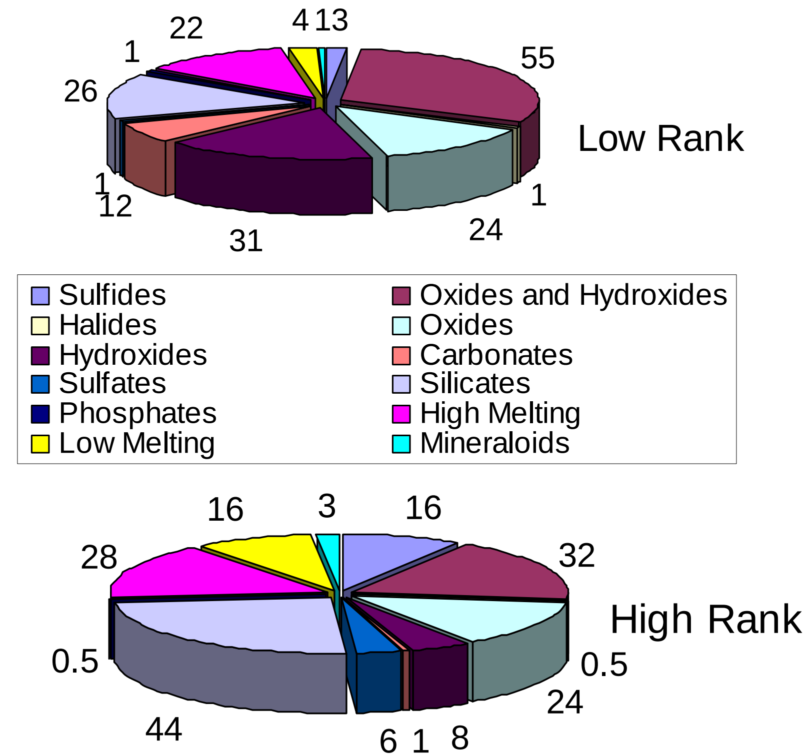
H_2	25 - 30
CO	30 - 60
CO_2	5 - 15
H_2O	2 - 30
CH_4	0 - 5
H_2S	0.2 - 1
COS	0 - 0.1
N_2	0.5 - 4
Ar	0.2 - 1
NH_3 + HCN	0 -0.3

Ash/Slag/PM

Slag and Refractory Wear in Entrained-flow Gasifiers



Slagging in gasifiers



- Inorganic matters in fuel result in slagging problems
- Corrosive nature of slag causes serious chemical corrosion in gasifiers
- Models are needed to simulate and monitor refractory wear in gasification processes

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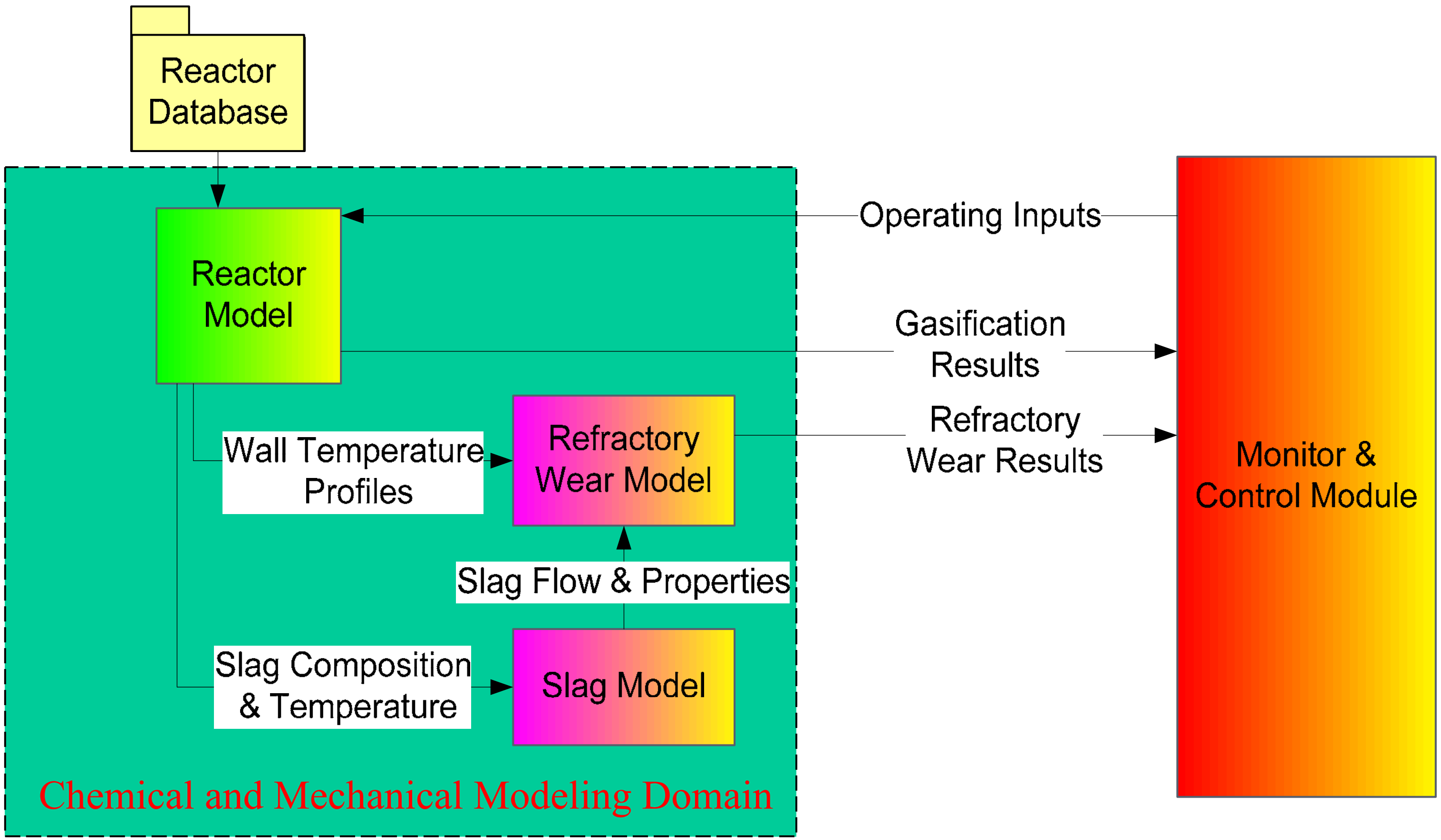
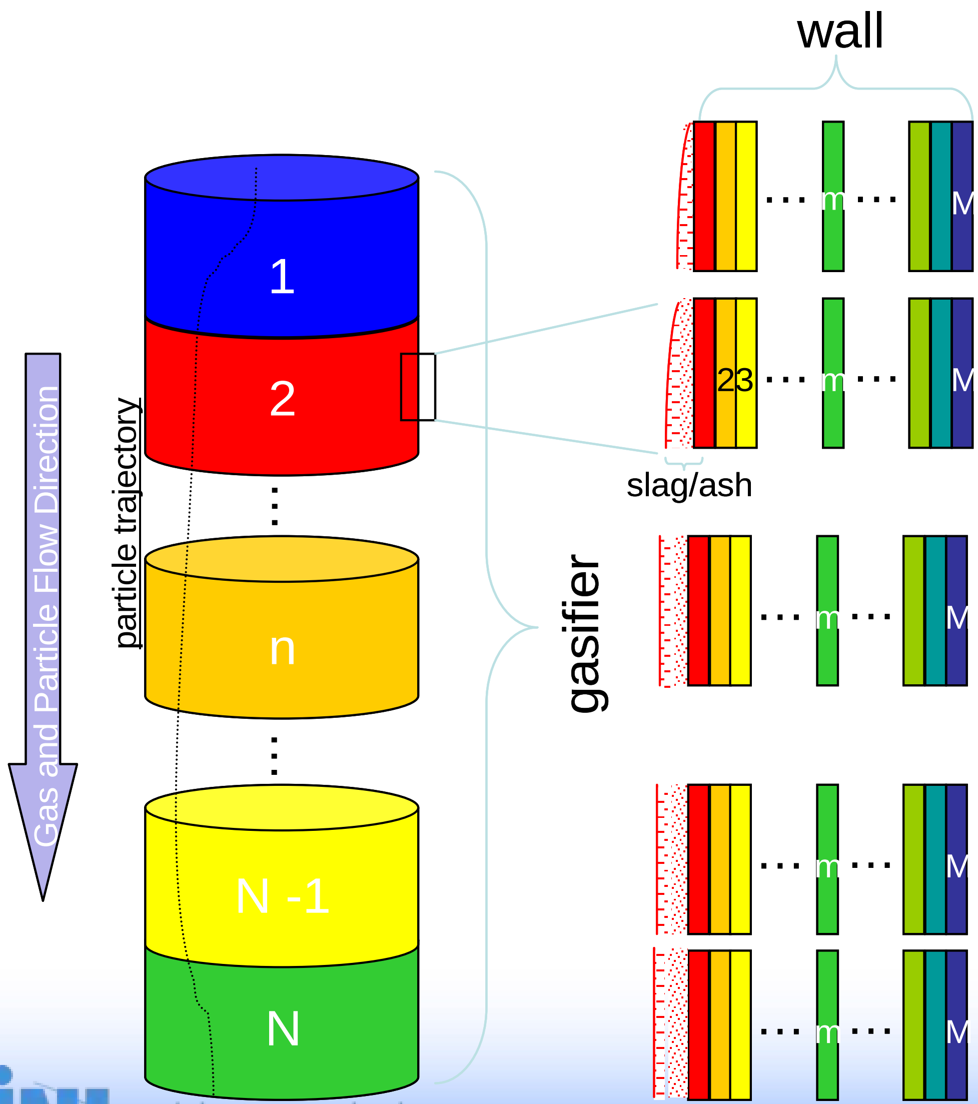
Project Objective

- **Develop a comprehensive model to predict coal gasification process and refractory wear in entrained-flow gasifiers**
  - Gasification reactions
  - Heat and mass transfer
  - Chemical corrosion model
  - Crack/Fracture development
  - Spalling
  - Monitor & control module

Highest Level Data Flow Diagram

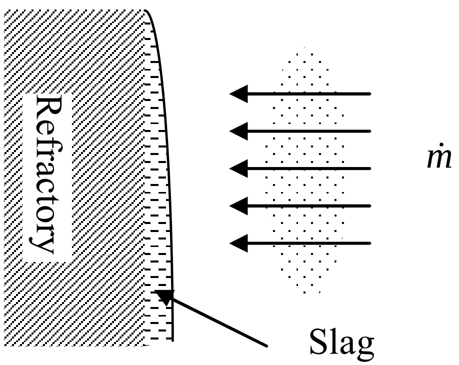


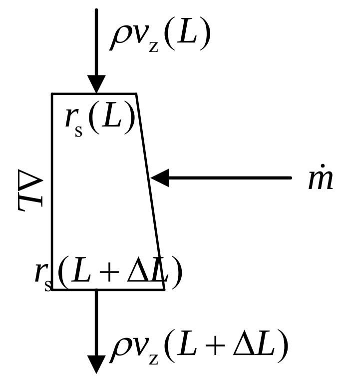
Overall Modeling Concept



- Reactor Model:
  - Gas and particle-related reactions:
    - 1-D steady state model
  - Temperature profiles of refractory and steel walls:
    - 1-D steady state model
    - 2-D steady state model
  - Slag accumulation rate/ash deposition rate
- Refractory Wear Model:
  - Chemical corrosion
  - Fracture & penetration
  - Spalling

Slag Flow Model





Assumptions

- Slag is Newtonian fluid and uniformly distributed around gasifier
- Slag flow is 1-D, laminar, steady-state, and fully developed.
- Shear force between slag and gas is neglected

Momentum equation

$$0 = \frac{1}{r}\frac{d}{dr}\left(r\mu\frac{dv_z}{dr}\right) + \rho g \sin\theta$$

Mass balance equation

$$\dot{m}\Delta L + \int_{R-r_s(L)}^{R} \rho v_z dr = \int_{R-r_s(L+\Delta L)}^{R} \rho v_z dr$$

R: internal radius of refractory layer

μ: slag viscosity

θ: angle between the slag flow direction and gravity direction

L: slag position from the top of the gasifier

ρ: slag density

v_z: slag velocity

r_s: slag thickness

ΔL: control volume length

$\dot{m}$: accumulation mass flux of slag

Corrosion Model

Assumptions

- Solute diffusion dominates refractory dissolution rate
- Solute dissolution occurs only when slag is unsaturated with respect to refractory solute
- Bulk slag concentration is independent of refractory dissolution.

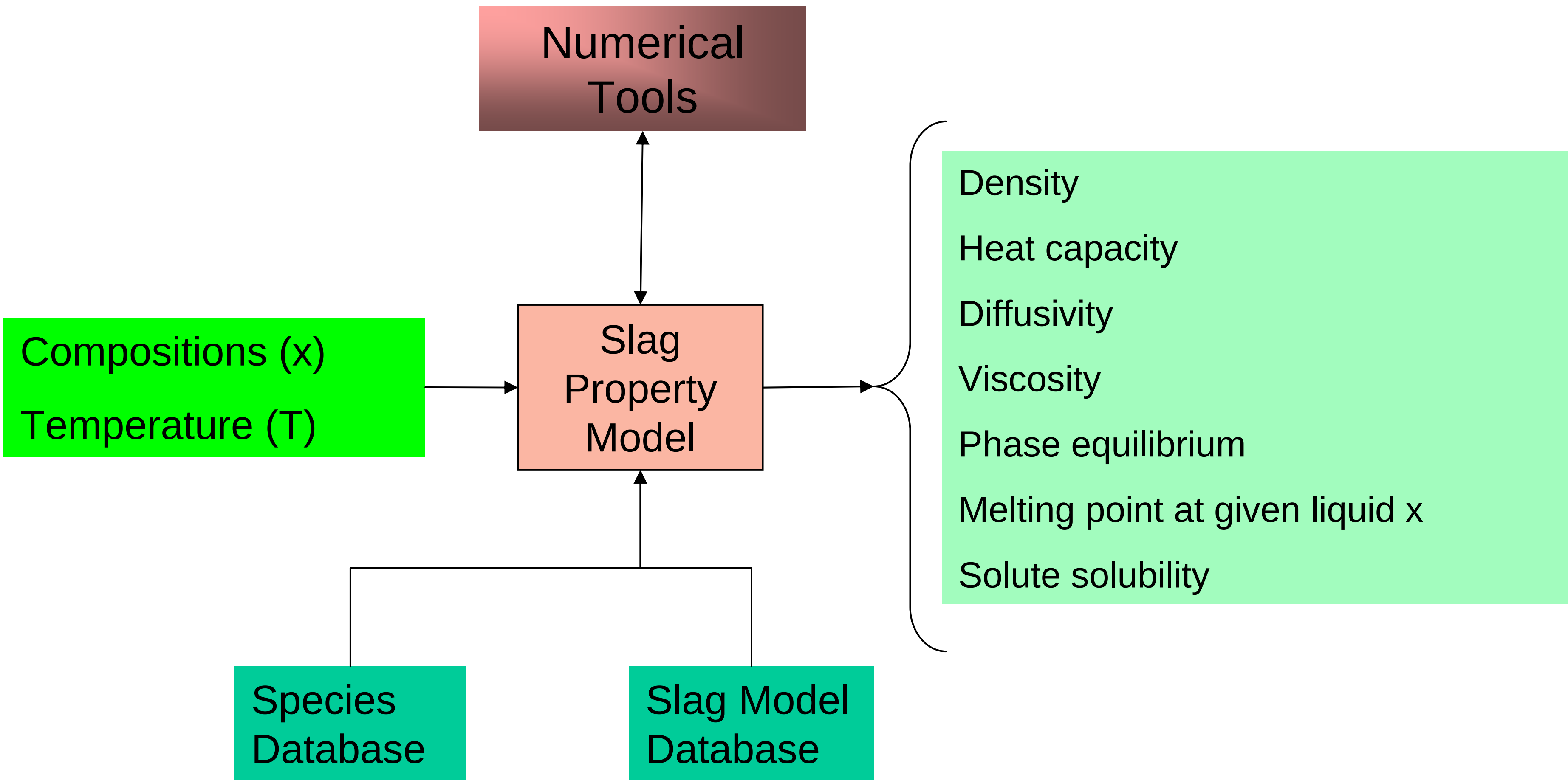
Governing mass transfer equation:

$$N_{\mathrm{A}} = k_{\mathrm{A}} \Delta C_{\mathrm{A}} = k_{\mathrm{A}} (C_{\mathrm{A}}^{*} - C_{\mathrm{Ab}})$$

ΔC_{A}: solute concentration difference between slag-refractory interface and bulk slag.

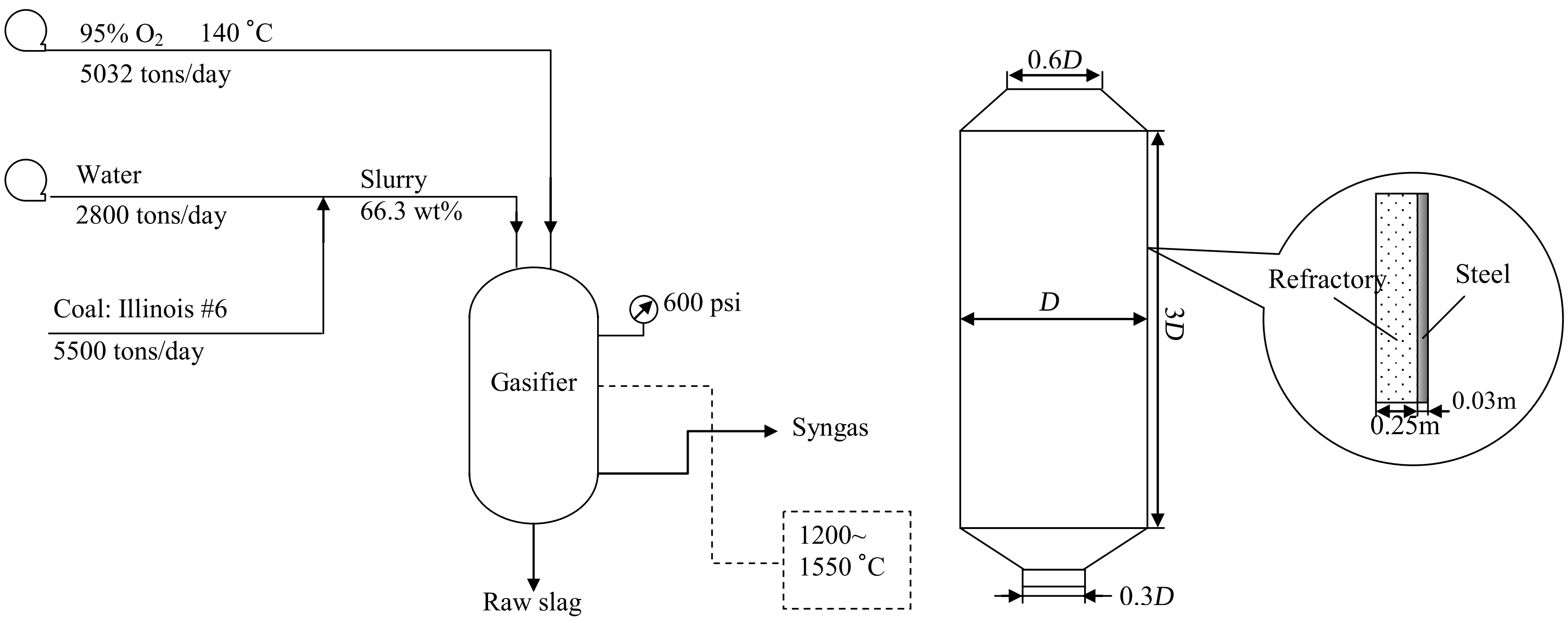
k_{A}: mass transfer coefficient

Slag Property Model



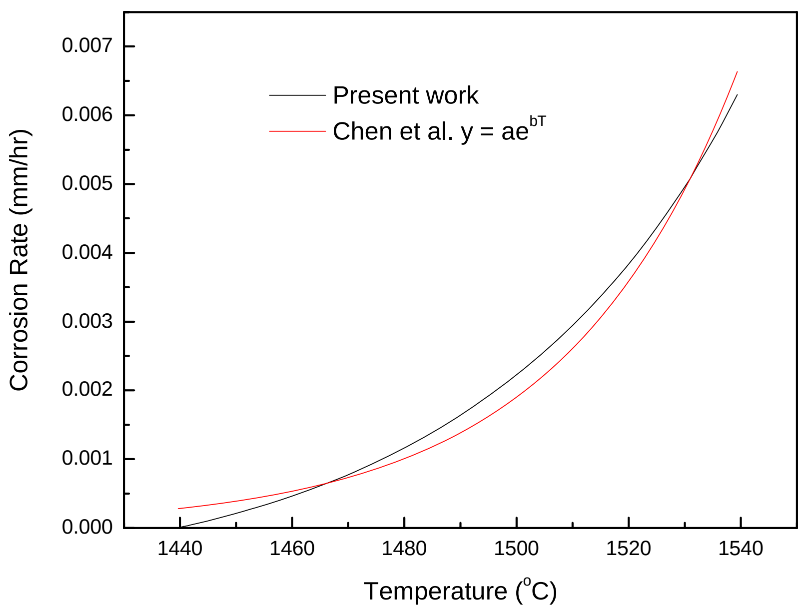
Each output/property of slag is calculated using one or more sub-models.

Gasifier Example Description

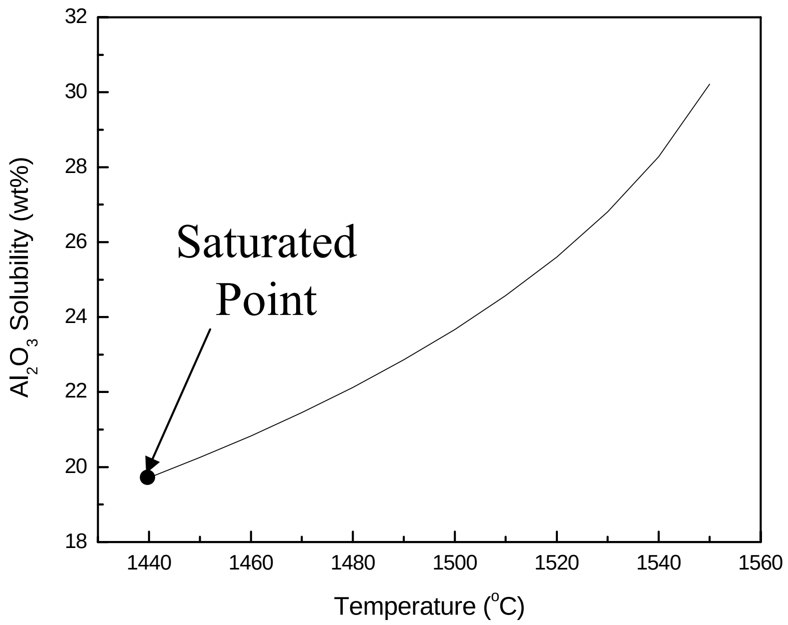


- Single-stage entrained down-flow gasifier
- One refractory layer without cooling jacket/heat exchanger installed in the gasifier
- D = 2.8m
- CaO-Al_2O_3-SiO_2 slag is used in the present work
- Greencast 94 is used as the refractory material (Al_2O_3 > 94wt%)

Corrosion Rate as a Function of Temperature



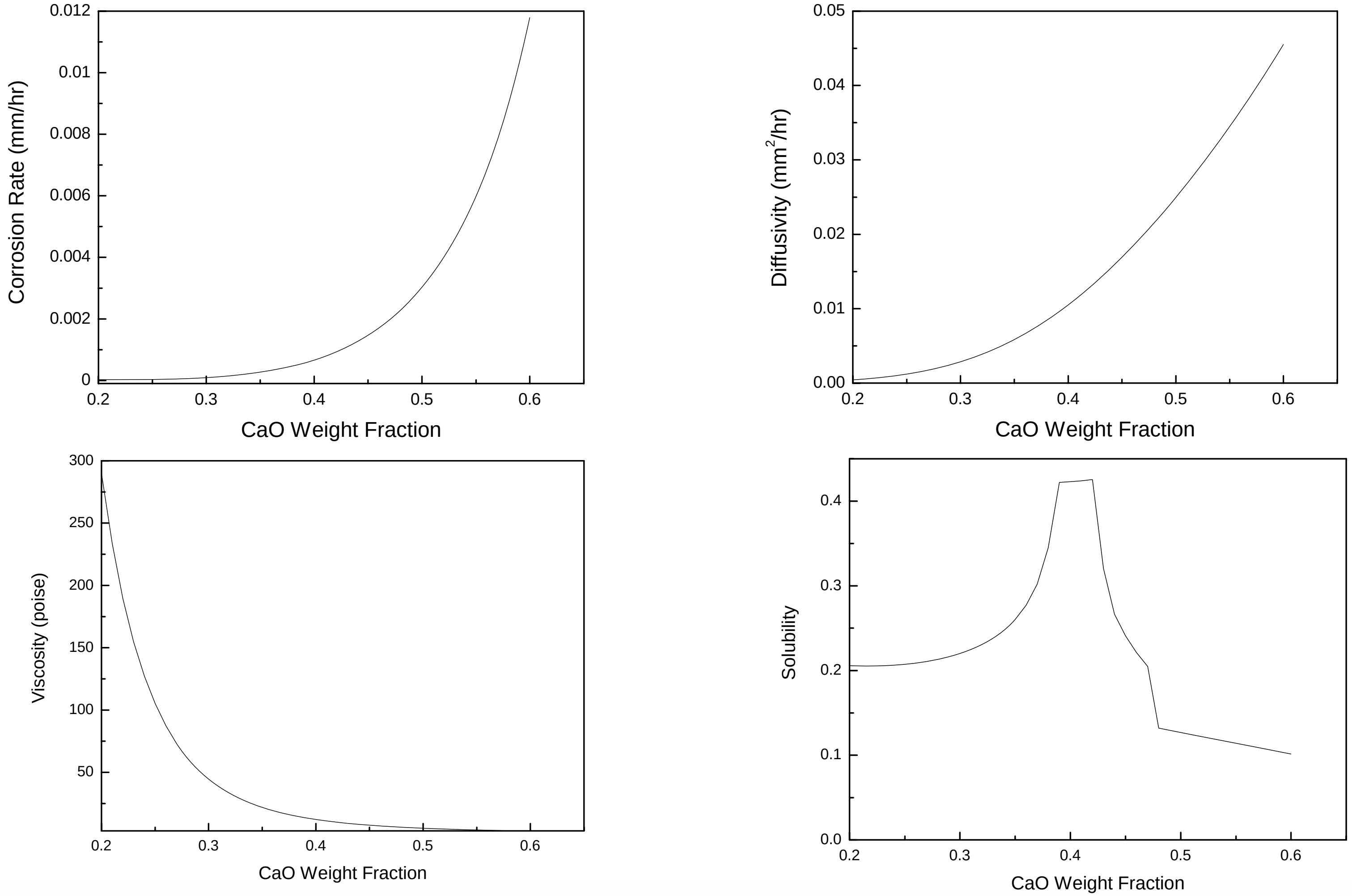
Comparison of corrosion rate calculated using the present model and the Chen et al. equation



Solubility of Al_2O_3 as a function of temperature

- Corrosion rates are computed based on the results of reactor model (refractory temperature profile, slag temperature & composition, etc.) at L = 0.28 m from the top of the gasifier
- Bulk slag composition (weight fraction) used in the figures: 19.7%Al_2O_3-27.6%CaO-52.7%SiO_2
- Solute is assumed to be Al_2O_3 due to its large fraction in Greencast 94 refractory

Effect of CaO Concentration



All four figures are plotted at average gas temperature 1500 ^oC and $Al_2O_3/SiO_2 = 0.34$

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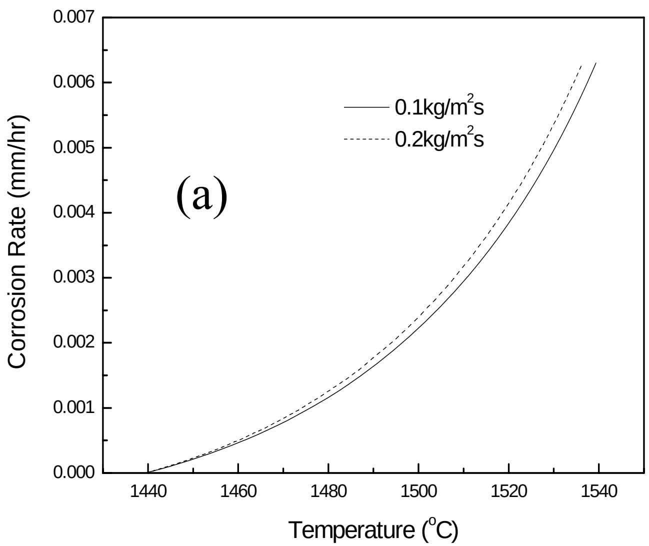
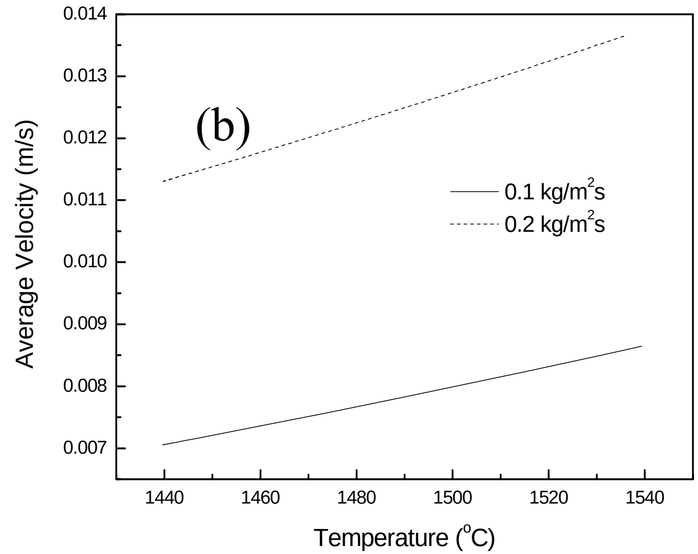
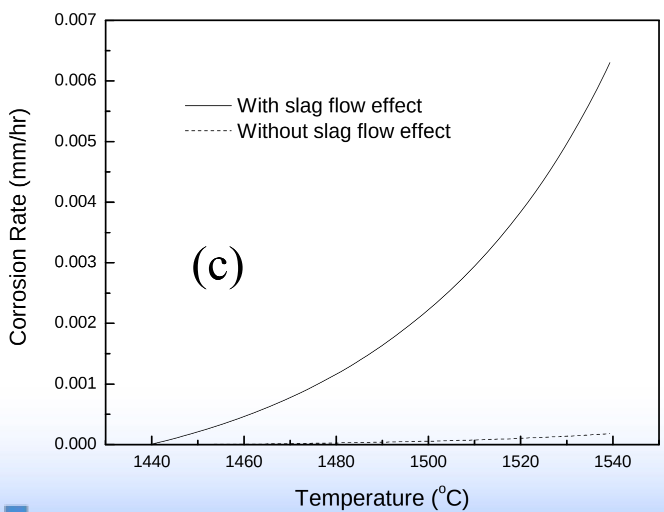
Effect of Slag Flow on Corrosion Rate







(a) **Corrosion rate at slag accumulation mass flux of 0.1 and 0.2 kg/m²s**

(b) **Average slag velocity at slag accumulation flux of 0.1 and 0.2 kg/m²s**

(c) **Comparison of corrosion rates w/o slag flow effect**

(d) **All results are computed at L = 0. 28 m from the top of the gasifier with a slag mass fraction of 19.7%Al_2O_3-27.6%CaO-52.7%SiO_2**

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Conclusions

- **A chemical corrosion model has been developed to account for refractory dissolution rate**
- **Effects of temperature, slag composition, and slag flow have been discussed**
- **Temperature and slag composition have significant effect on corrosion rate**
- **Neglecting slag flow effect underestimates corrosion rate, especially at high temperatures**

Future Work

- Test and validate models using experimental data (may need collaborations from industrial companies, laboratories, universities etc.)
- Explore the effects of oxides containing Fe, Na, K on corrosion rates
- Explore chemical corrosion for Cr_2O_3-based refractory
- Develop mechanical models to account for the effects of fracture, slag penetration, and spalling on refractory wear
- Develop databases needed for refractory wear and reactor models
  - Refractory material database
  - Slag species database
  - Solid and liquid slag solution database
  - Coal chemical fractionation database

Thank You