Modeling Entrained Flow Gasifiers

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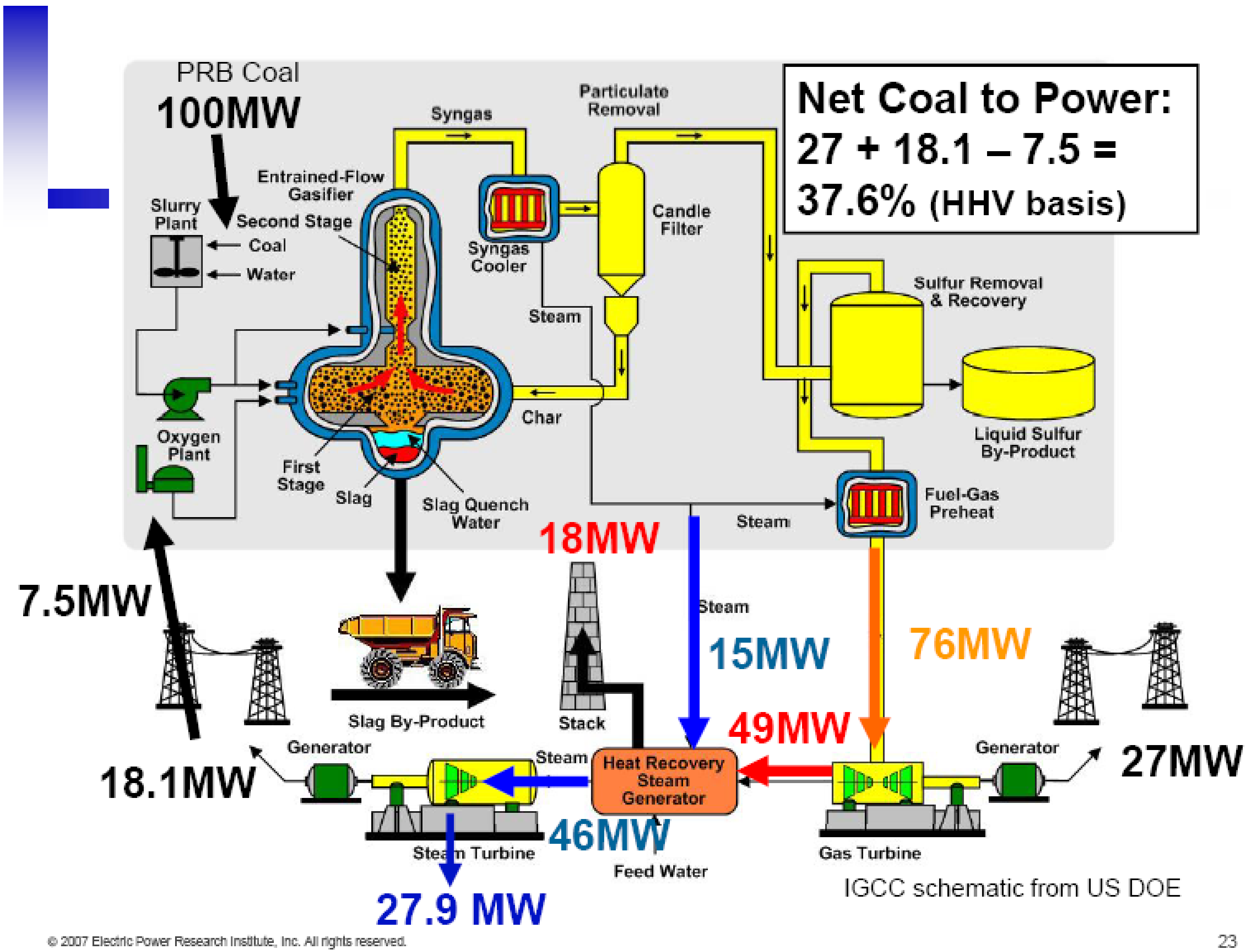
Vision 21 Program
“Computational Workbench Environment for Virtual Power Plant Simulation”
DOE NETL (COR=John Wimer, Bill Rogers, DE-FC26-00FNT41047)

Clean Coal R+D Project
“A Virtual Engineering Framework for Simulating Advanced Power Systems”
DOE NETL (COR=Ron Breault, DE-FC26-05NT42444)

Advanced Power Systems



[J. Phillips, "IGCC 101", GTC 2009] http://www.gasification.org/library/overview.aspx

Why Use Modeling?

Cost effective approach for evaluating performance, operational impacts & emissions

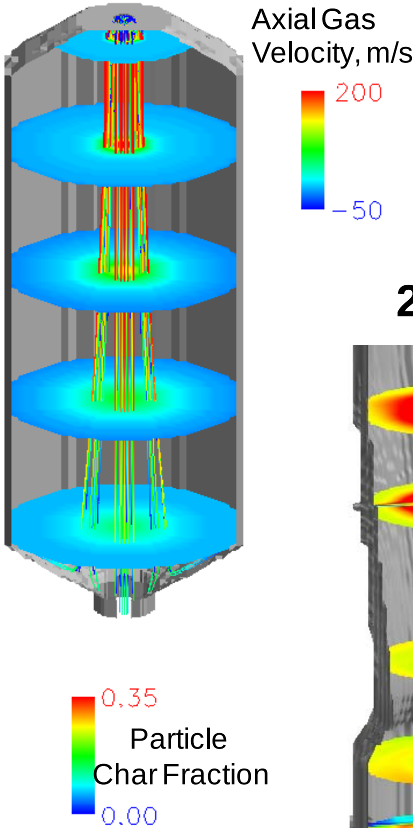
- Improve understanding
- Estimate performance
- Assist with conceptual design
- Identify operational problems
- Cheaper than testing
- More detailed information than testing
- Helps engineers make better, more informed decisions

Entrained Flow Gasifier Model

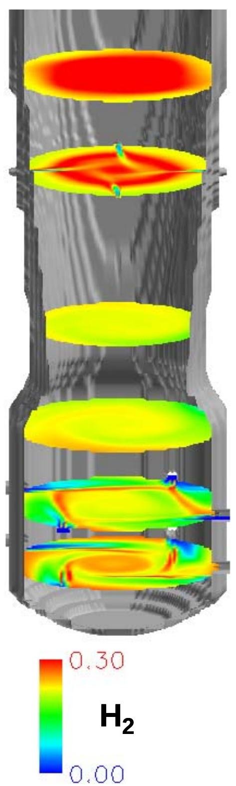
- Model Development
  - CFD + Process models
    - Allows modification of
      - Process conditions, burner characteristics
      - Fuel type, slurry composition
      - gross geometry
    - Generic Configurations:
      - downflow / upflow
      - 1 stage / 2 stage
      - based on public information
    - Define Parameters with DOE
  - Improved physical models
    - pressure effects on radiation heat transfer
    - reaction kinetics
      - high pressure, gasification w / inhibition
    - slag, ash (vaporization), tar, soot
- Collaboration
  - N. Holt (EPRI)
  - T.Wall,.. (Black Coal CCSD, Australia)
  - K.Hein (IVD, U. of Stuttgart)

[Clearwater 2001-2008], [PCC 2002-2009],

1 stage



2 stage

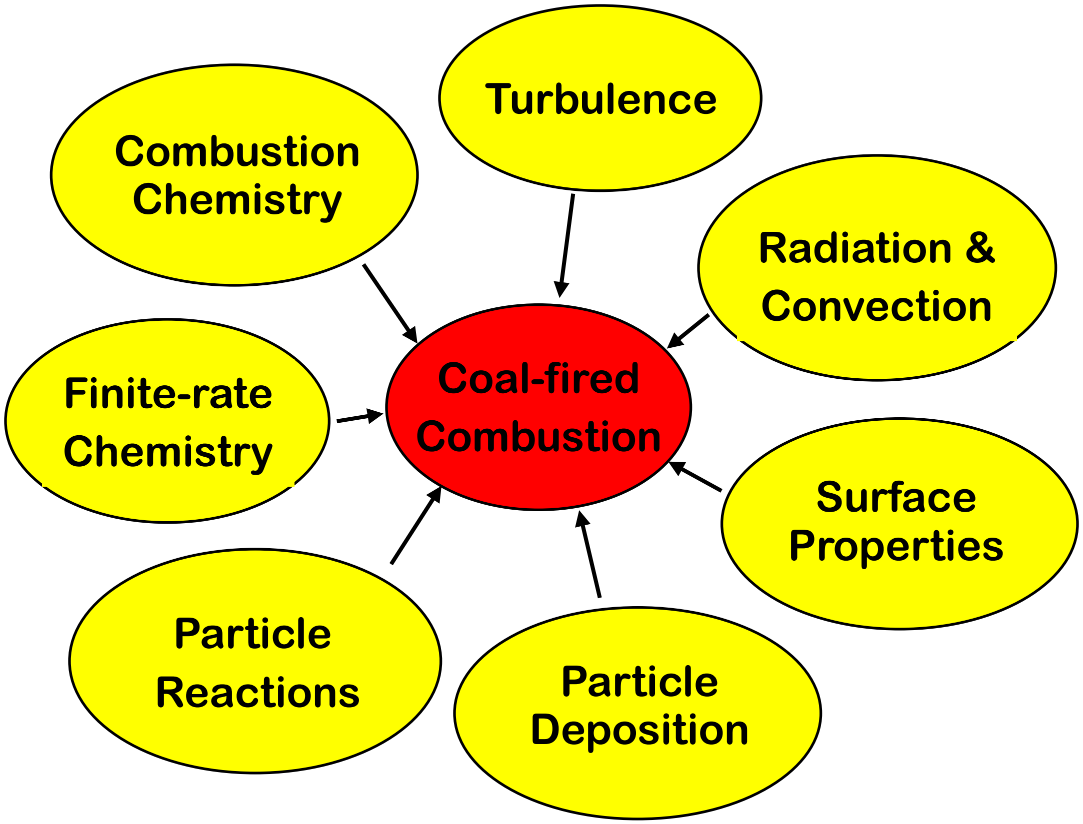


Glacier Software

- *Glacier* is REI’s in-house, CFD-based combustion simulation software
- Over 30 years of development
- Over 15 years of industrial application
- Designed to handle “real-world” applications
  - Judicious choice of sub-models & numerics
  - Qualified modelers

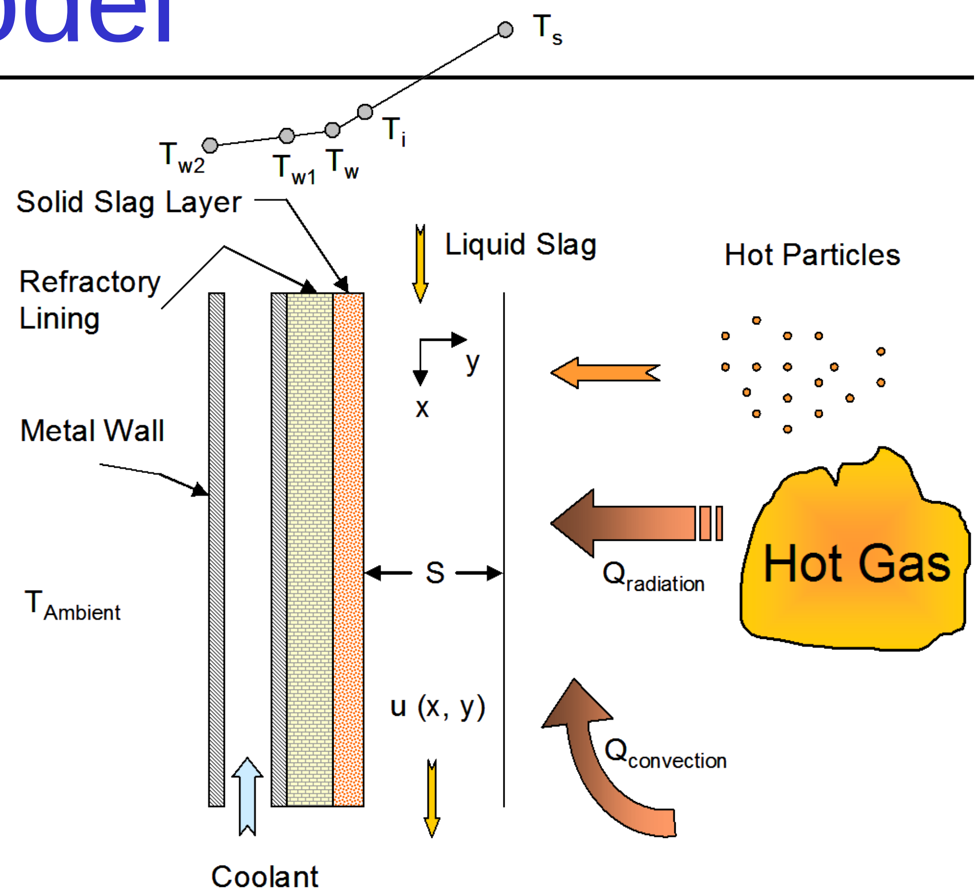
Modeling Coal Combustion

- **Computer model represents**
  - Furnace geometry
  - Operating conditions
  - Combustion processes
  - Pollutant formation
- **Accuracy depends on**
  - Input accuracy
  - Numerics
  - Representation of physics & chemistry



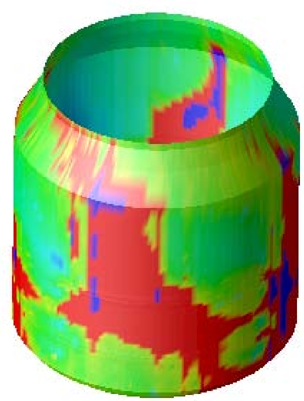
Flowing Slag Model

- Model accounts for:
  - Wall refractory properties
  - Back side cooling
  - Fire side flow field + heat transfer
  - Particle deposition on wall
    - Local Deposition Rate
    - Fuel ash properties
    - Composition (ash, carbon)
    - Burning on wall
- Slag model computes
  - Slag viscosity
    - Tcv = critical viscosity
    - ash composition
  - Slag surface temperature
  - Liquid & frozen slag layer thickness
  - Heat transfer through wall



Based on work by [Benyon], [CCSD], [Senior], [Seggiani]

[Dogan et al, GTC2002]



For model details see
- Pittsburgh Coal Conference 2002

Gasifier Slag Viscosity Model

- *Derived for a range of coal ashes*
- *Curve fit as a function of SiO2, TiO2, Al2O3, Fe2O3, CaO, FeO, MgO, Na2O, K2O and temperature.*
- *References:*

Kalmanovitch , D.P. And Frank, M., “An Effective Model of Viscosity of Ash Deposition Phenomena,” in Proceedings of the Engineering Foundation Conference on Mineral Matter and Ash Deposition from Coal, ed., Bryers, R.W. And Vorres, K.S.,Feb. 22-26, 1988.

Urbain, G., Cambier, F., Deletter, M., and Anseau, M.R., Trans. J. Gr. Ceram. Soc., Vol. 80, p. 139, 1981.

Based on mole fractions:

1. Calculate $M = CaO + MgO + Na_2O + K_2O + FeO + 2TiO$
2. Calculate $\alpha = M/(M + Al_2O_3 + Fe_2O_3)$
3. Calculate $B = B_0 + B_1 SiO_2 + B_2(SiO_2)^2 + B_3(SiO_2)^3$, where

$$B_0 = 13.8 + 39.9355\alpha - 44.049\alpha^2$$

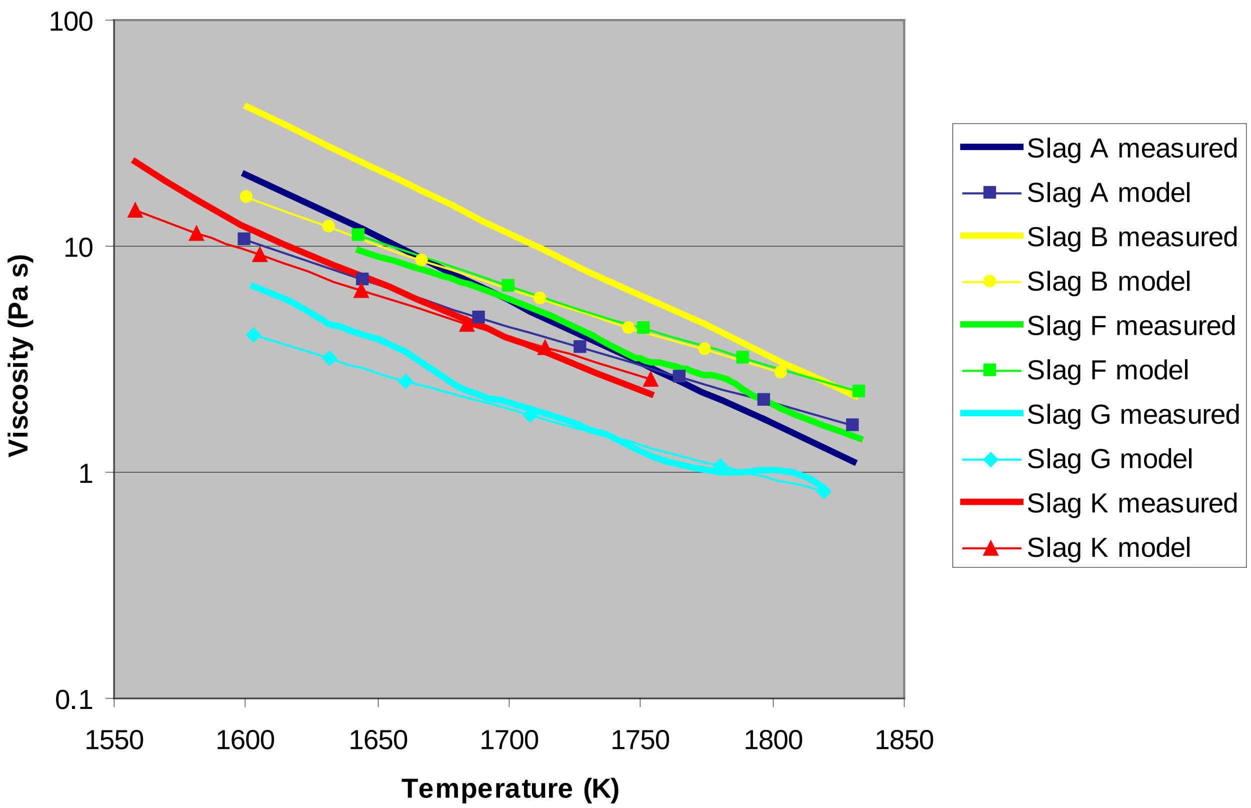
$$B_1 = 30.481 - 117.1505\alpha + 129.9978\alpha^2$$

$$B_2 = -40.9429 + 234.0486\alpha - 300.04\alpha^2$$

$$B_3 = 60.7619 - 153.9276\alpha + 211.1616\alpha^2$$

4. Calculate $A = -0.2812B - 11.8279$
5. Calculate $C = 0.43429*(A + \ln(T) + 1000B/T)$, T is temperature in K
6. Finally: $\mu = 10^{C-1}$, μ is the viscosity in Pa·s.

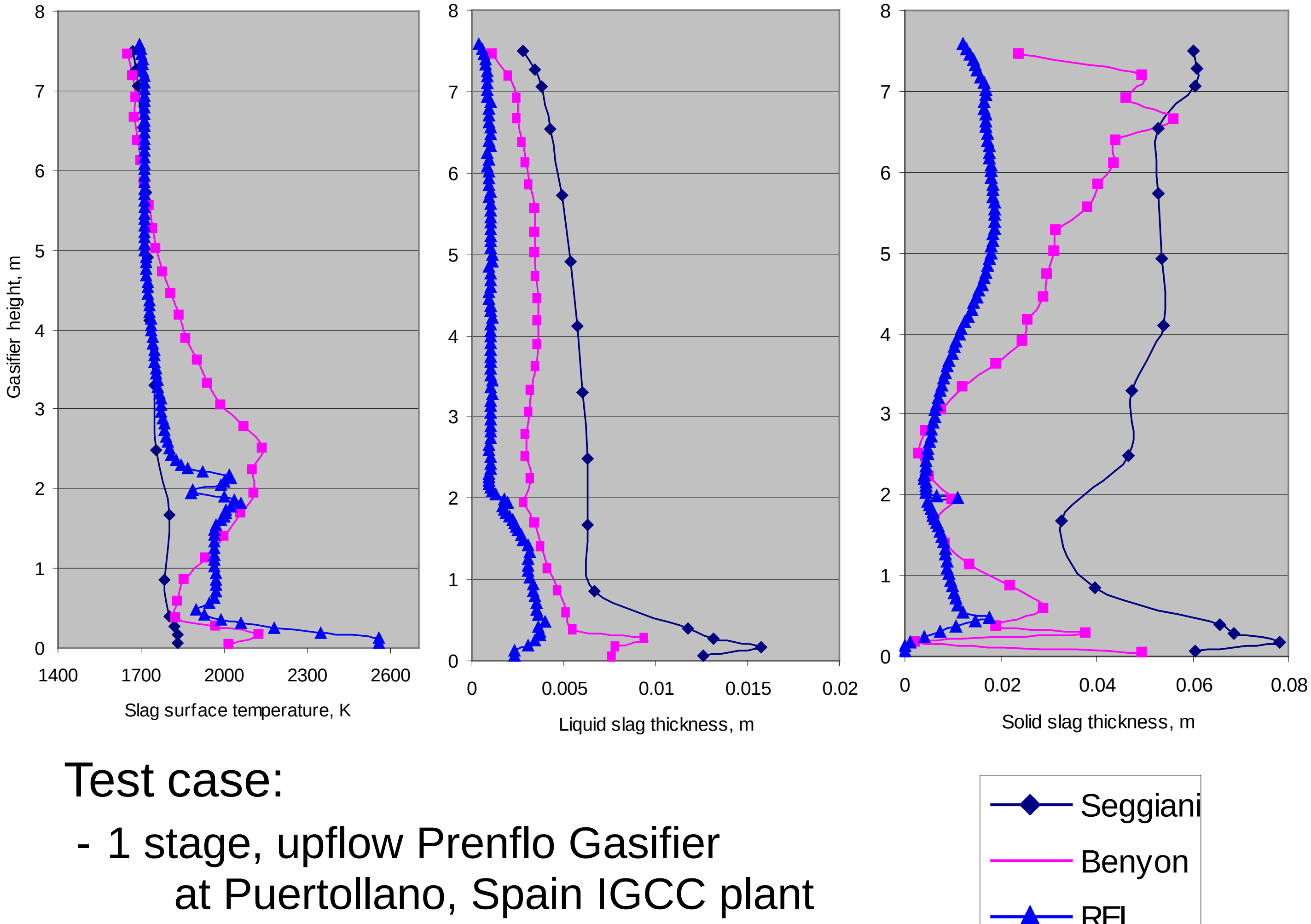
Viscosity Model



Gasifier slag data from Mills, K.C., and Rhine, J.M., “The measurement and estimation of the physical properties of slags formed during coal gasification 1. Properties relevant to fluid flow.,” *Fuel* vol. 68, pp. 193-198, 1989.

Flowing Slag Model

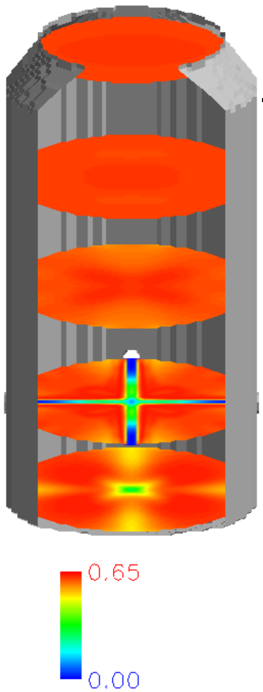
Slag Surface Temperature | Liquid Slag Thickness | Solid Slag Thickness



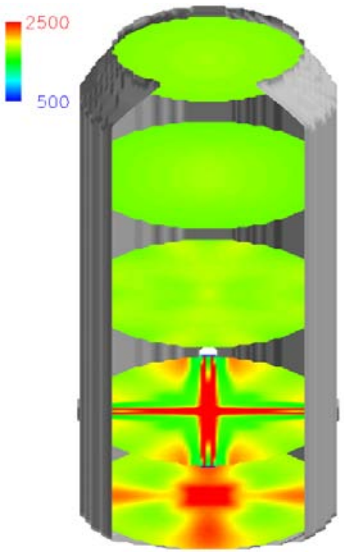
Test case:

- 1 stage, upflow Prenflo Gasifier at Puertollano, Spain IGCC plant
- 2600 tpd, dry feed, opposed fired
- water jacket to cool refractory

CO



Gas temperature, K



Carbon Conversion

- Carbon Conversion vs Time in PFR
- Contributions of Volatile Release and Gasification Rxns
  - ➢ [Roberts, Tinney, & Harris, CCSD, 2005]
  - ➢ symbols refer to different coals

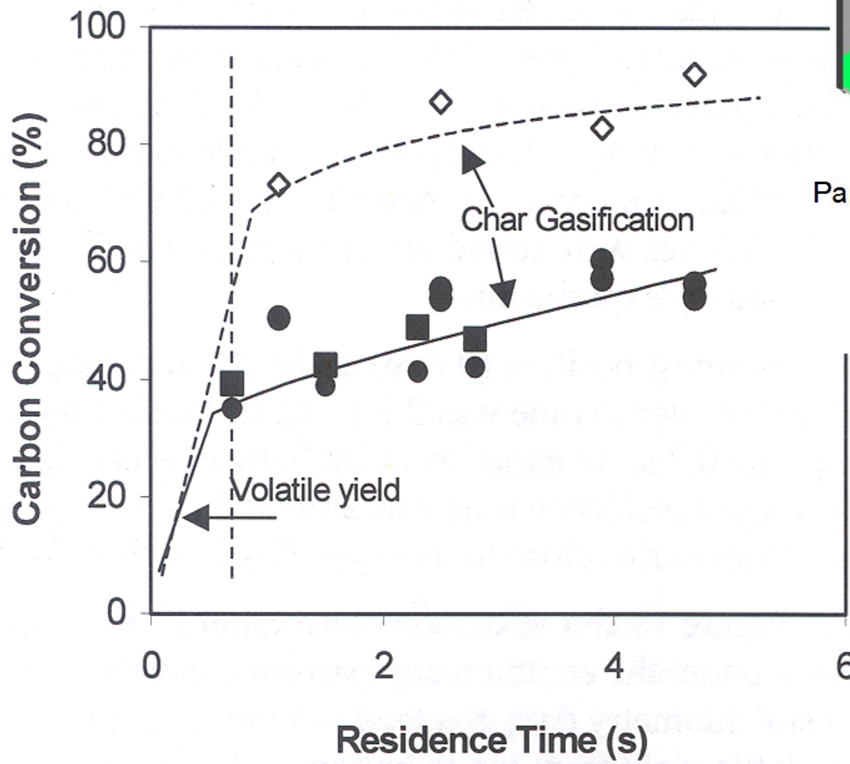
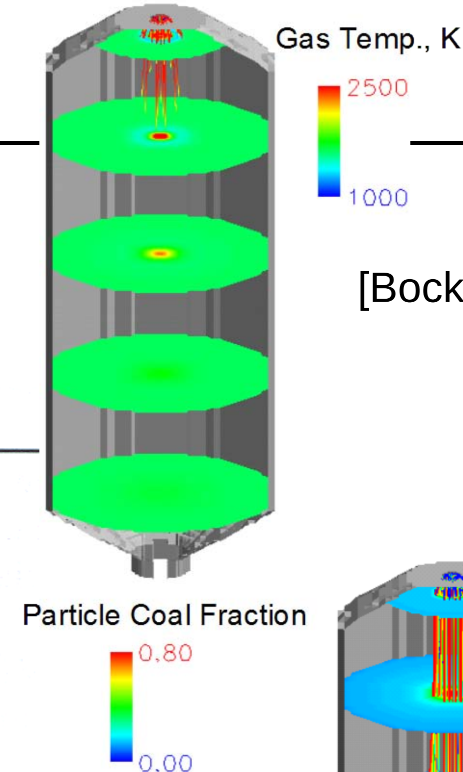
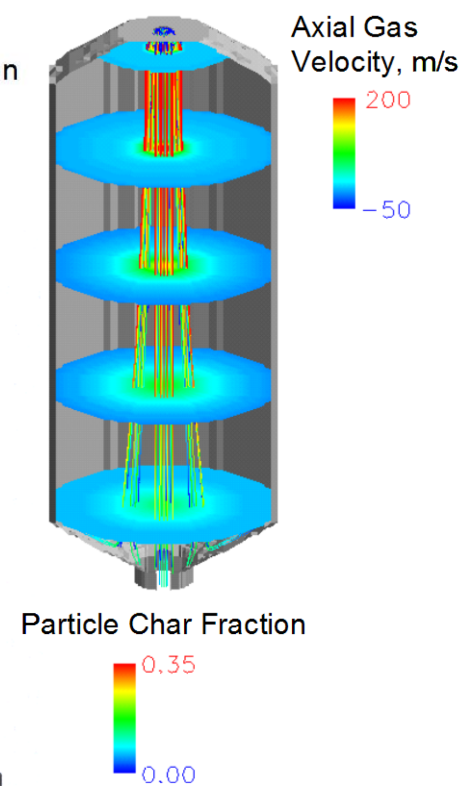


Figure 20: The stages of coal conversion highlighted using data generated in the PEFR. Up to approximately 0.5 s coal conversion is achieved by volatile release. The slower char conversion processes are then apparent at residence times above about 1 s.

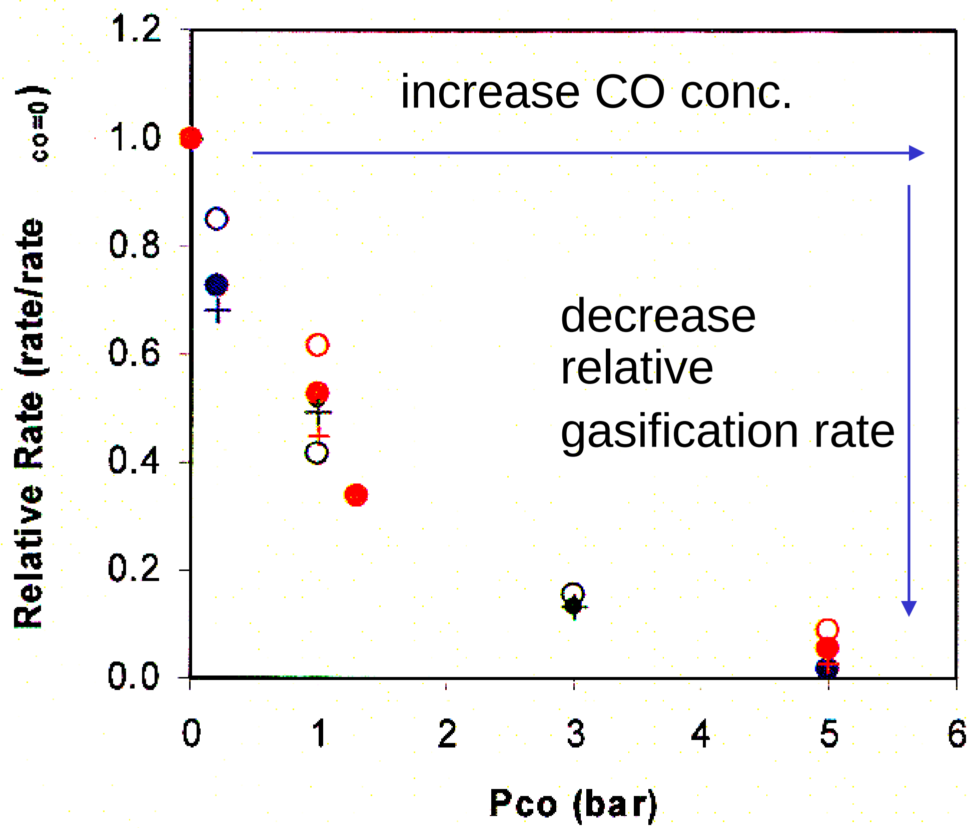


[Bockelie et al, 2002]



Effect of CO Inhibition on Carbon Gasification Rate

- [Roberts, Tinney, & Harris, CCSD, 2005]
- symbols refer to different coals



CO reduces gasification rate

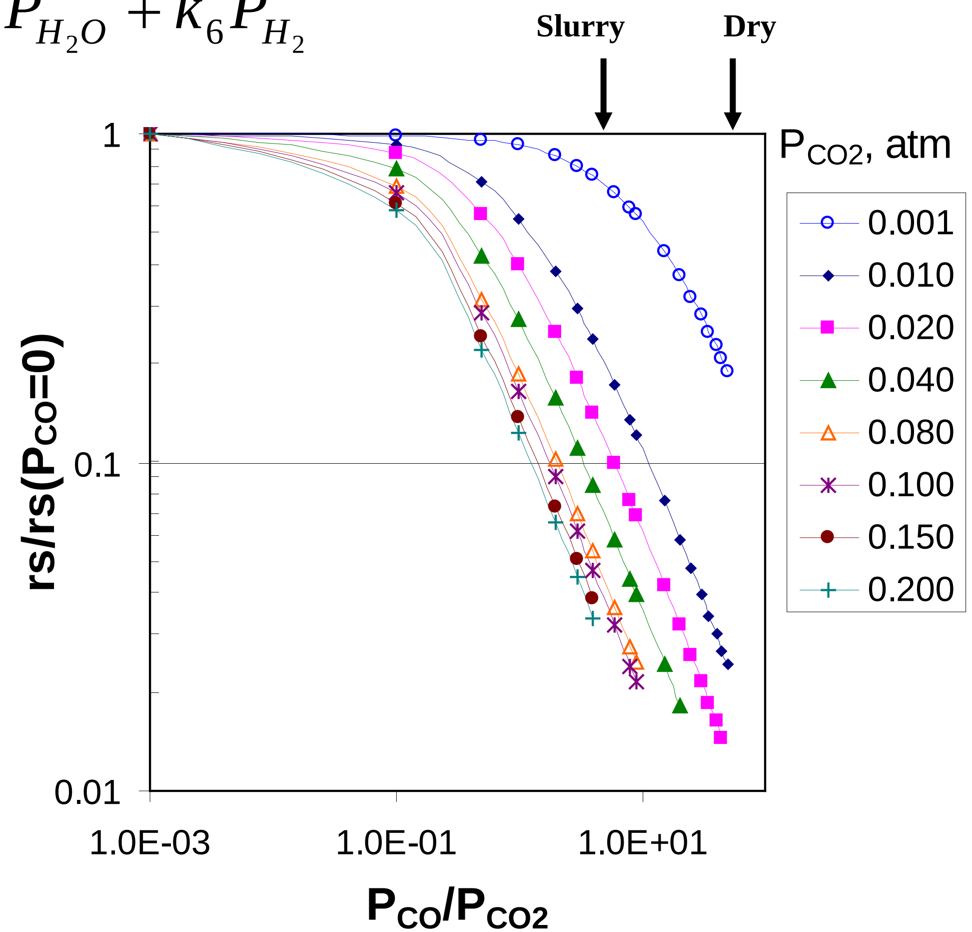
Figure 8: Relative rate data for all chars and CO_2 pressures combined. Blue data = 5 bar CO_2, green data = 10 bar CO_2, red data = 15 bar CO_2. • = CRC272, ○ = CRC252, and + = CRC281

Gasification Kinetics – with inhibition

- *CO, CO_2, H_2, H_2O*

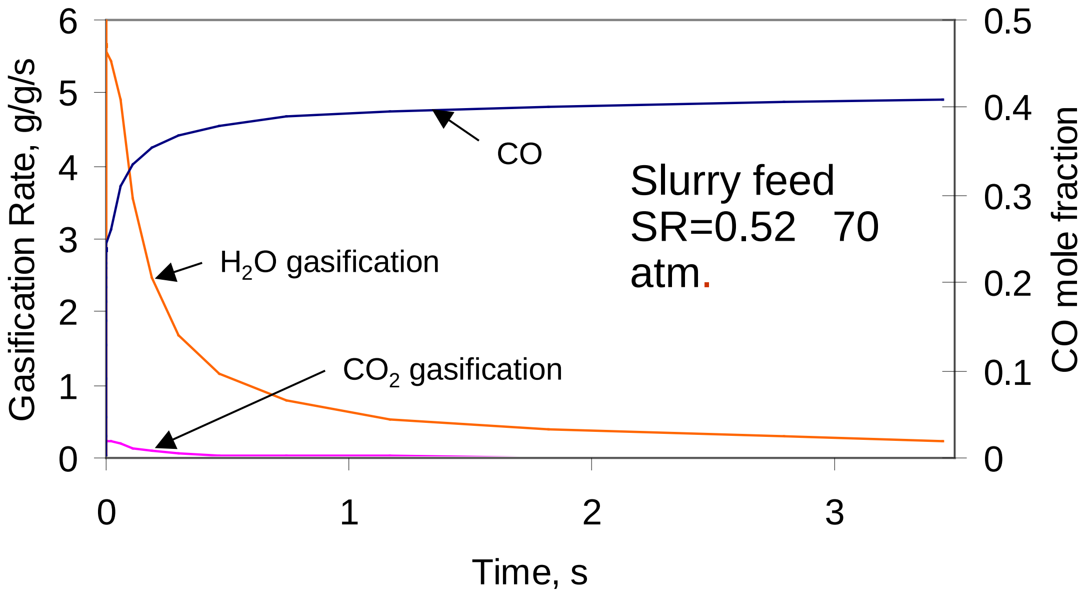
$$r_s(1/s) = \frac{k_1 P_{CO_2} + k_2 P_{H_2O}}{1 + k_3 P_{CO_2} + k_4 P_{CO} + k_5 P_{H_2O} + k_6 P_{H_2}}$$

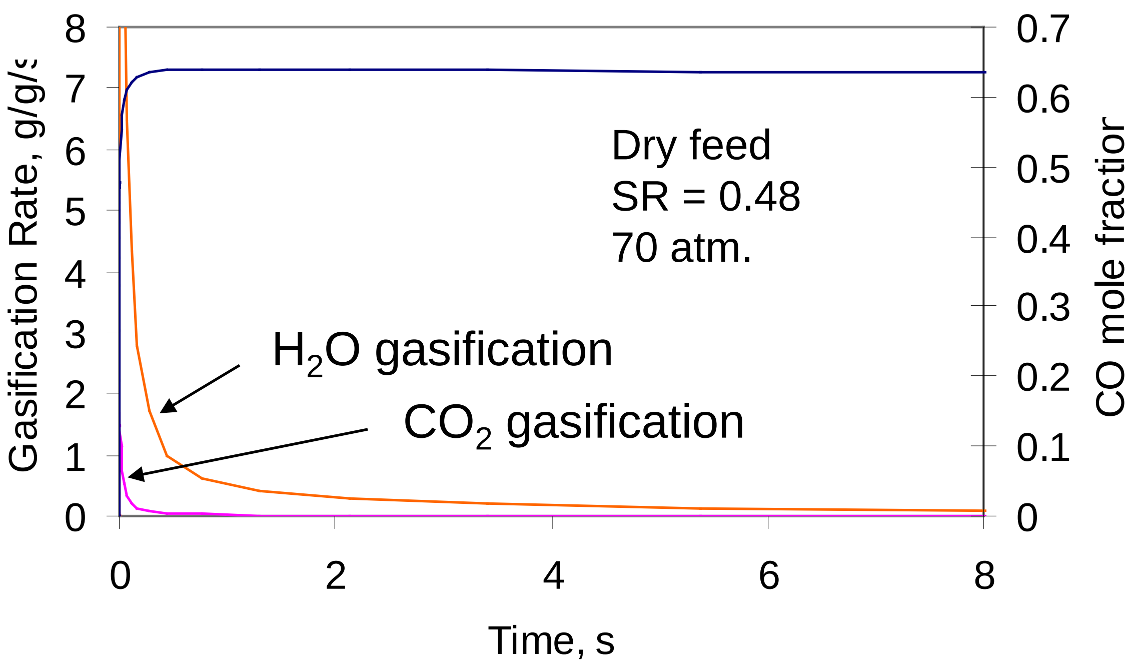
$$k_i = k_{i0} \cdot \exp\left(-\frac{E_i}{RT}\right)$$



[van Heek & Muhlen, 1991]

Gasification Kinetics – CO effects



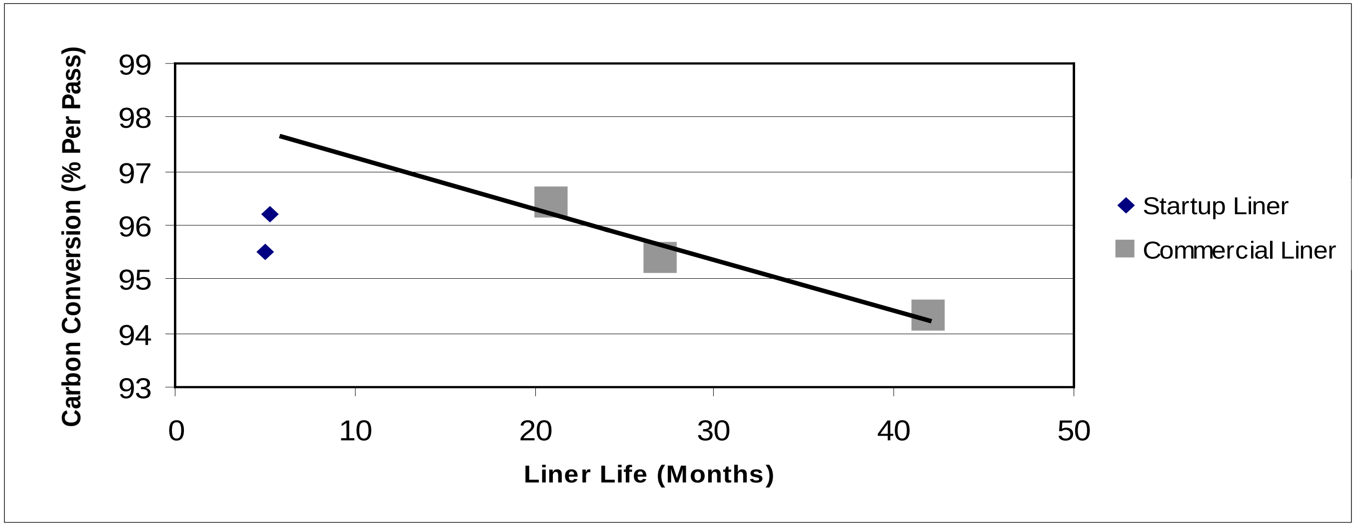


Presence of CO reduces gasification rate

Gasification rate for H2O is greater than for CO2

Gasifier Issues

Reduce carbon conversion → increase refractory liner Life (Tampa Electric Polk Plant)

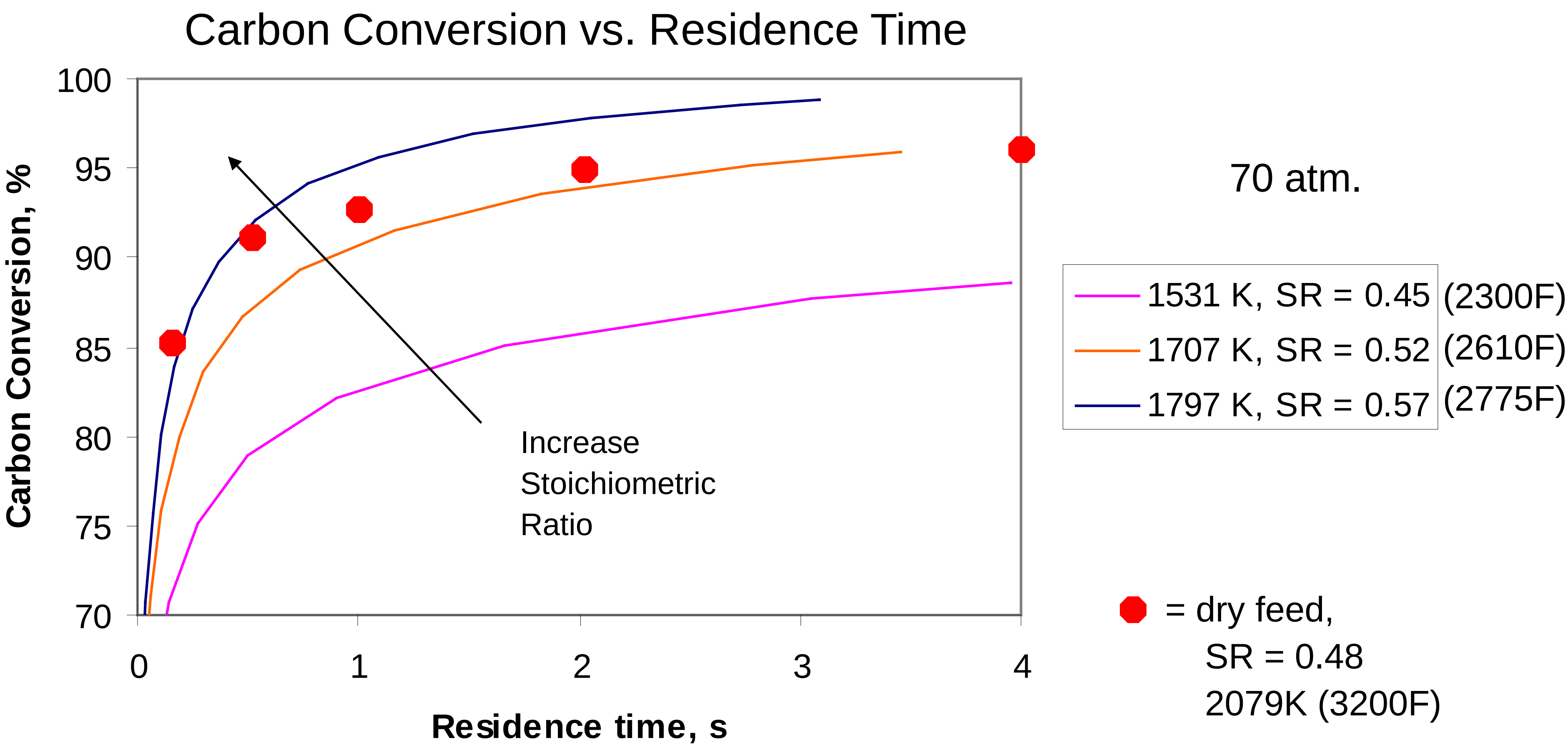


Humphrey Pittsburg #8

[TECO, July 2000]

Effect of Temp. on Carbon Conversion

- Increase gasifier volume (residence time) ➔ small benefit
- Increase temperature ➔ increase carbon conversion
  BUT can reduce refractory life



Tar & Soot Model

- Semiempirical model*
  – Coal-derived soot is assumed to form from only tar.
  – Tar yields is calculated by CPD model† based on measured coal characteristics.
  – Three equations for conservation of the mass of soot and tar, and the number of soot particles.

** Brown, A.L.; Fletcher, T.H. Energy Fuels 1998, 12, 745-757.*

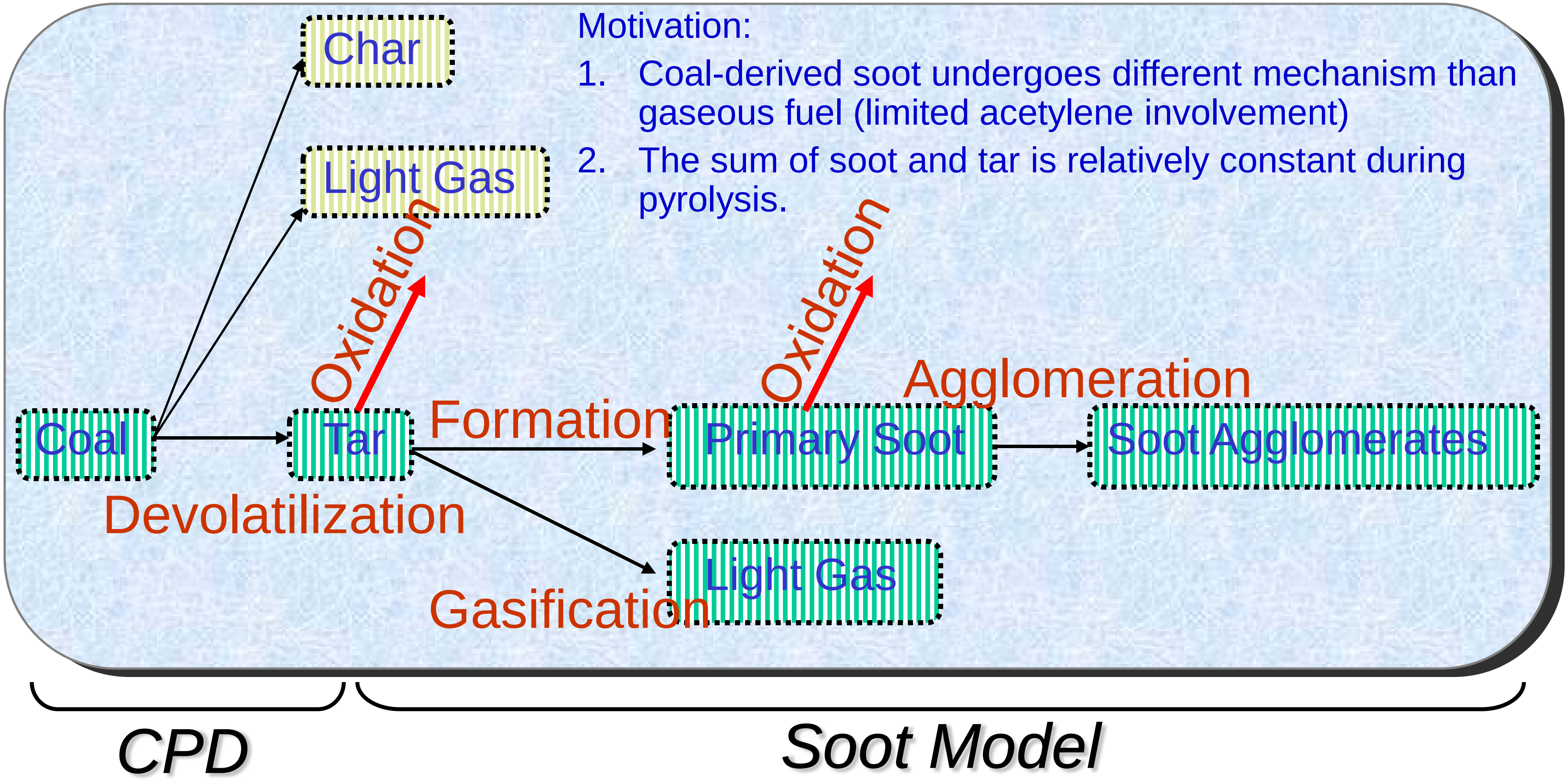
† Fletcher, T.H.; Kerstein, A. R.; Pugmire, R. J.; Solum, M. S.; Grant, D. M. Energy Fuels 1992, 6, 414-431.

Assumed Soot Formation Mechanism

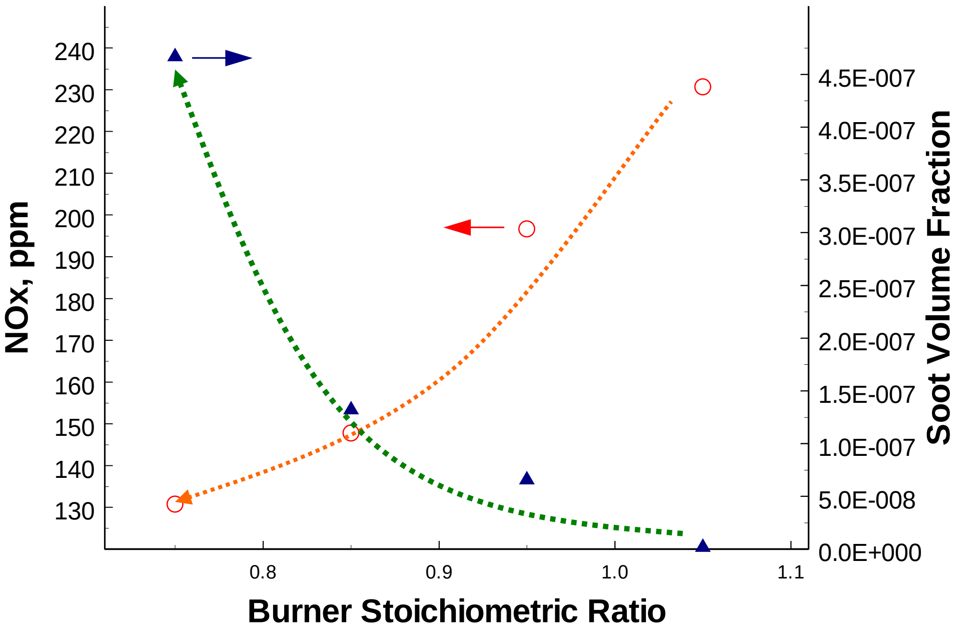
Brown, A.L.; Fletcher, T.H. Energy Fuels 1998, 12, 745-757.

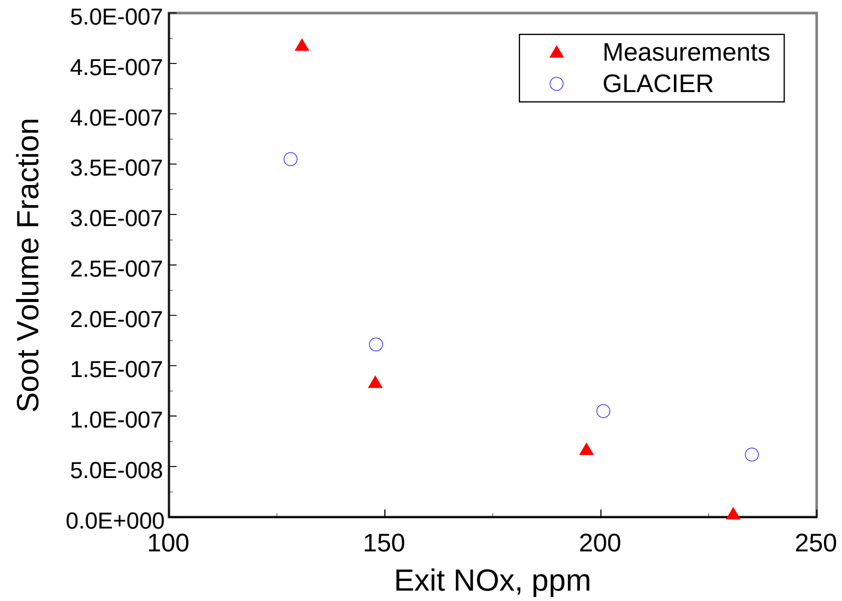
Motivation:

1. Coal-derived soot undergoes different mechanism than gaseous fuel (limited acetylene involvement)
2. The sum of soot and tar is relatively constant during pyrolysis.

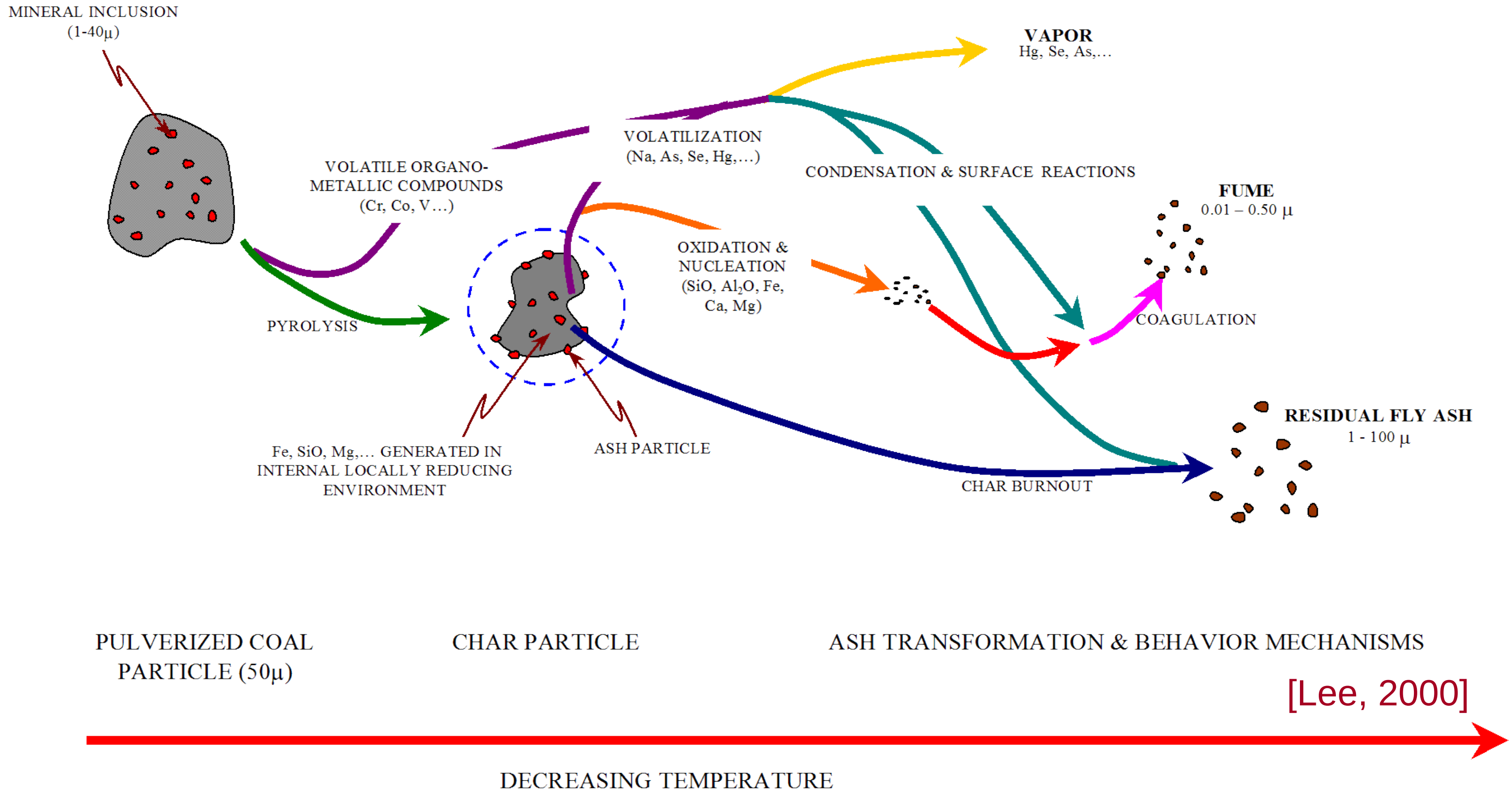


Soot Model Evaluation





Mineral Matter Transformation Pathways

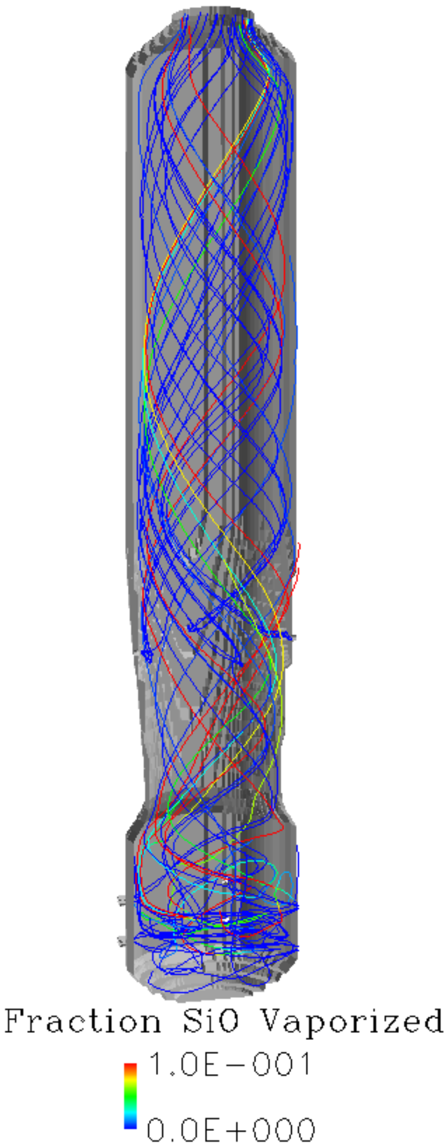


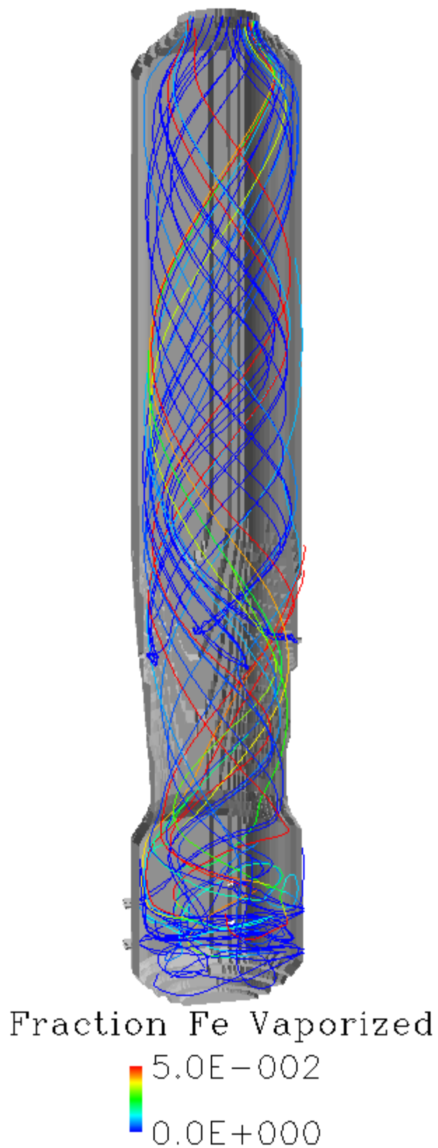
1) Fly ash (residual solid)
2) Organometallics (solid + vapor)
3) Vapor (fume) created by reduction of stable condensed metal oxide (SiO2, MgO, CaO, Al2O3, FeO) to more volatile suboxides (SiO, Al2O) or metals (Mg, Ca, Fe)

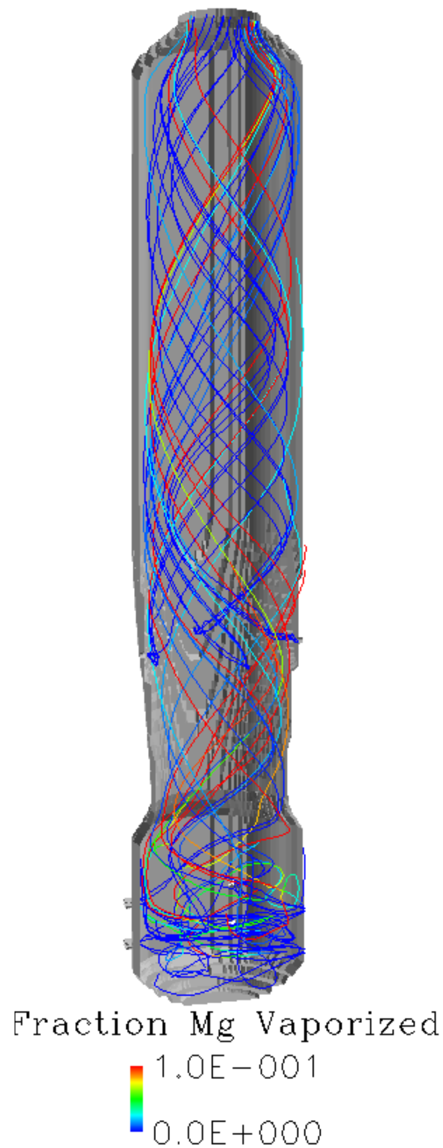
$$MO_n(c) + CO \Leftrightarrow MO_{n-1}(v) + CO_2$$

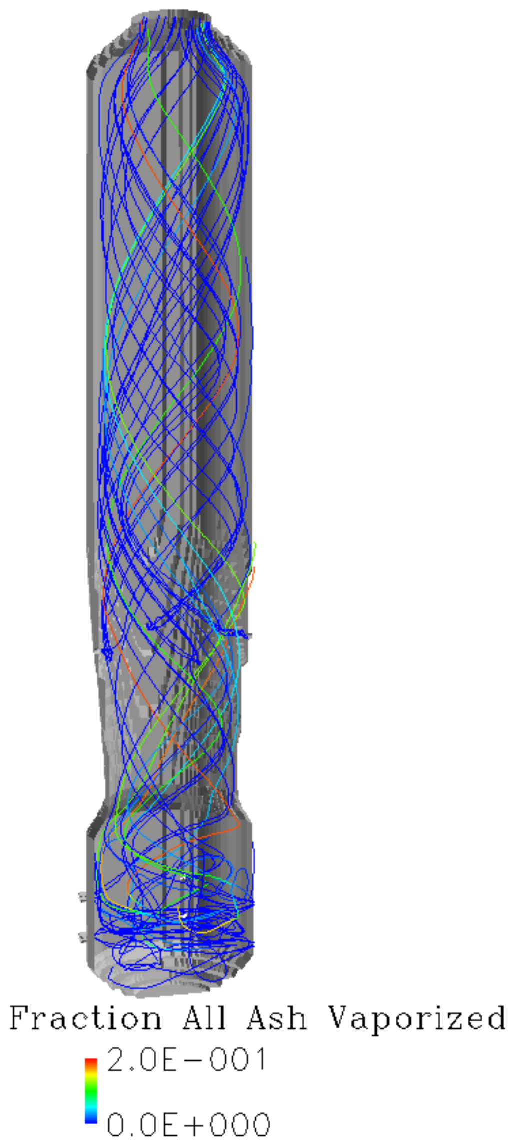
2 Stage Gasifier – Vaporization Along Representative Particle Trajectories

25 to 60 micron



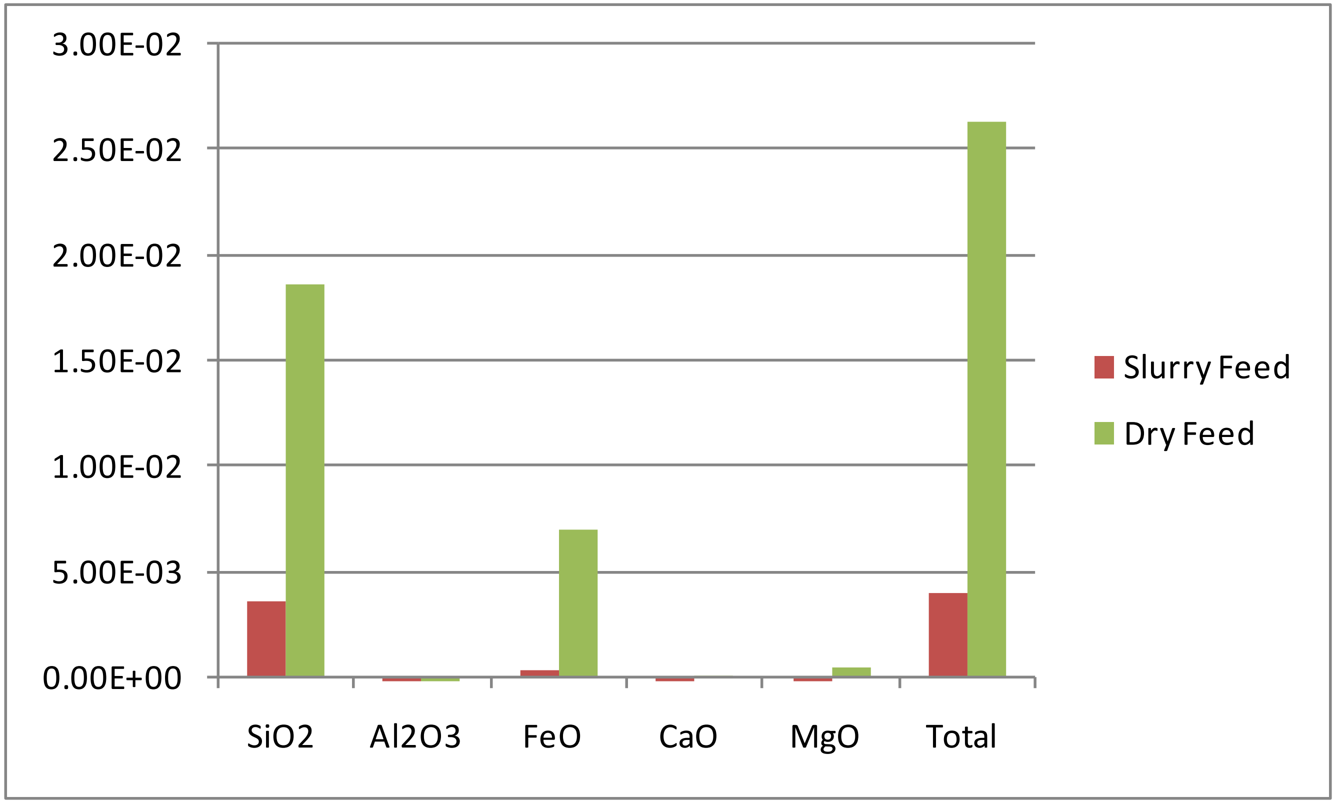






Ash Vaporization Summary

Mass Fraction of Inlet Ash Vaporized
(relative to initial total ash mass)



Syngas Cooler Fouling

- REI fouling model ➔ mechanistic model that includes impacts of
  - ash properties (individual particle composition, particle size, temperature, density, viscosity, surface tension),
  - included/excluded minerals (e.g., pyrite),
  - local conditions (gas composition, temperature, heat flux to surfaces)
  - properties of deposits (composition, temperature, density, viscosity, surface tension (if wet)).
  - refine model to account for data from NETL gasification studies [Gibson, 2009]
- Model predicts
  - properties of particles exiting furnace in-flight,
  - deposition rate (growth rate)
  - properties of sintered deposits on walls,
  - impacts of fouling on gas phase properties, overall heat transfer, etc.
  - emissions of Ca, Mg, Fe, SiO from ash that react in the gas phase to produce submicron aerosols (e.g., FeS) observed by Brooker [1993, 1995] which forms part of the glue for the sticking
- Model builds on work of many investigators
  - [Walsh et al., 1990, 1992], [Wall et al., 1979, 1993], [Gallagher et al., 1990, 1996], [Senior and Srinivaschar, 1995], [Wang et al., 1997, 1999], [Quann and Sarofim, 1982]

Figure 1. Example of plugged CSC inlet tubesheet [Polk, 2002].

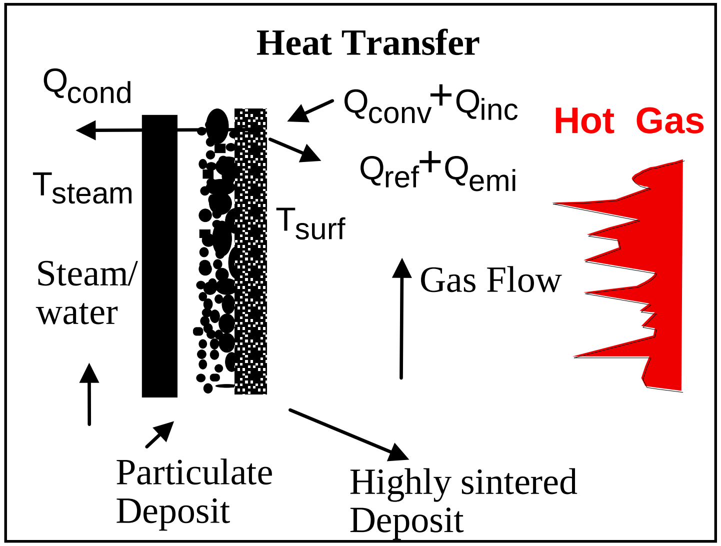


Figure 2. Schematic of REI Fouling Model.

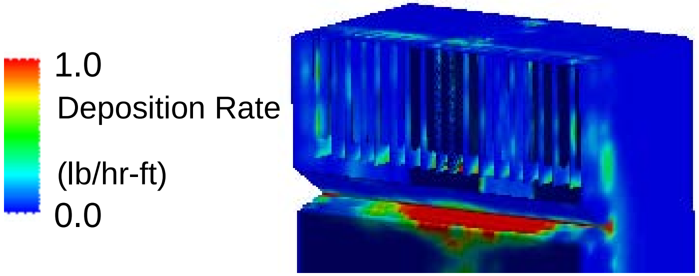
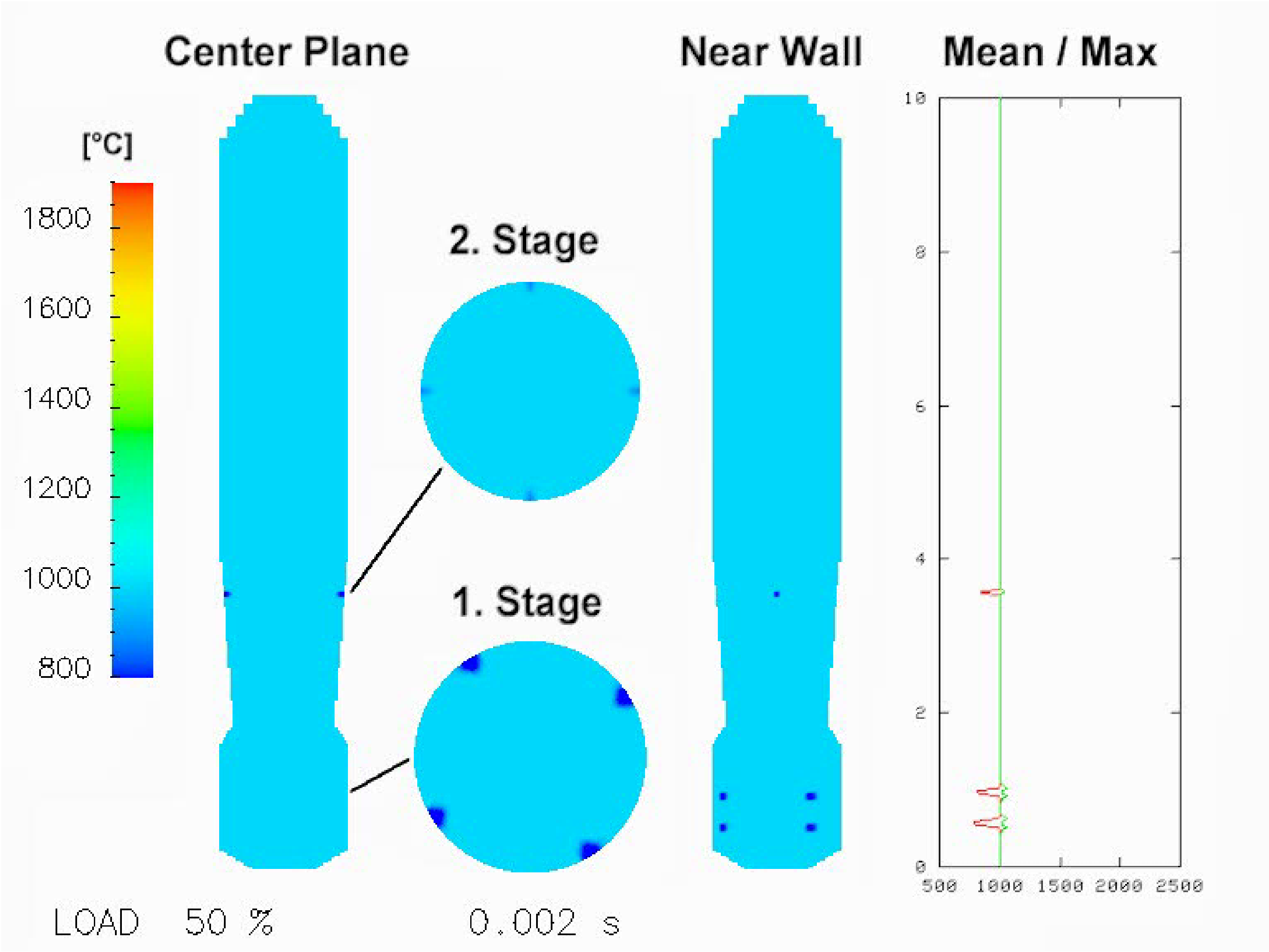


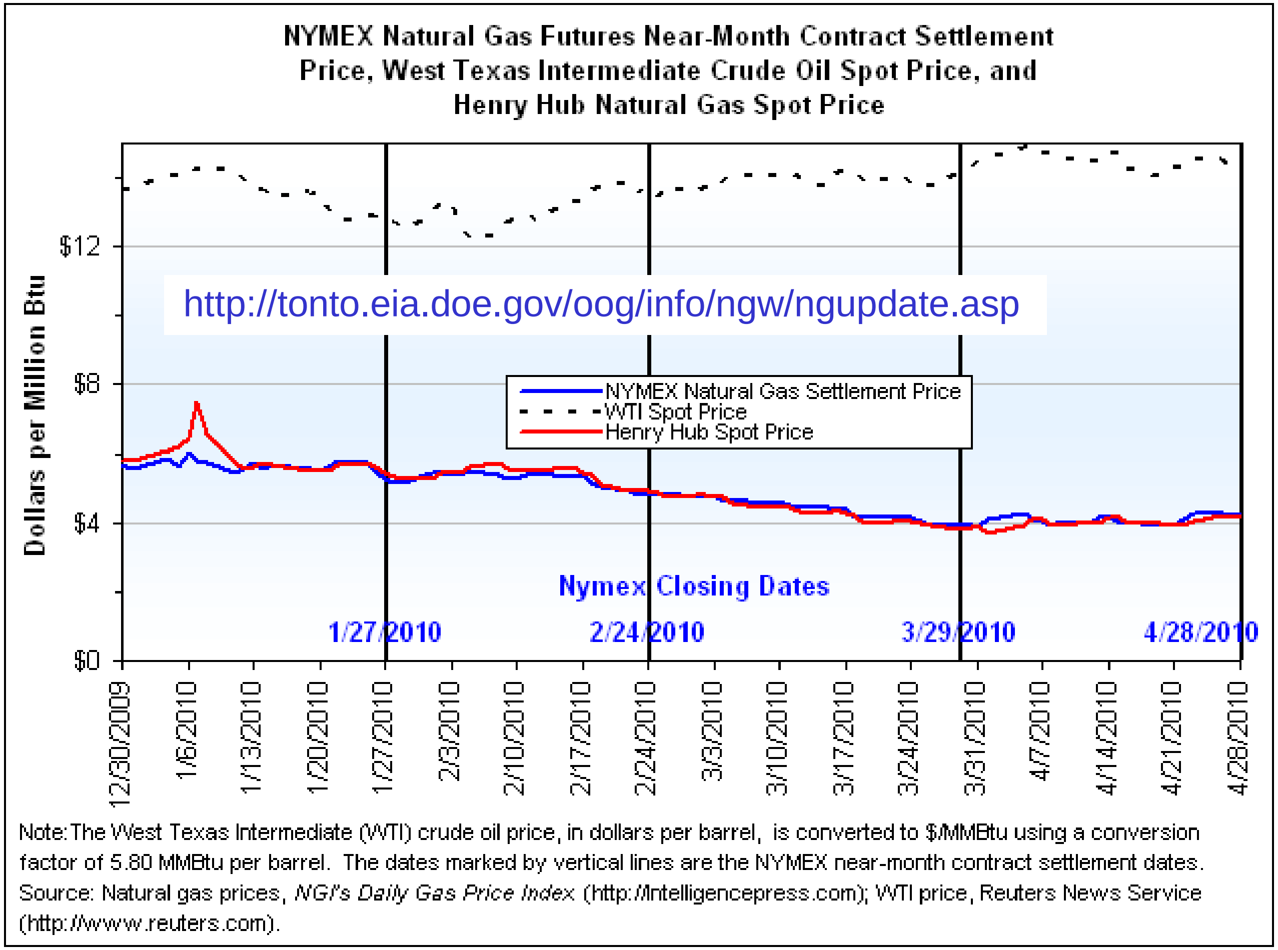
Figure 4. Predicted deposition rate on rear wall of 800 MWe coal fired boiler.

Gasifier - CFD Model - transient



Gas Temperature

Challenges for IGCC / Gasification



Coal-fired gasification power plant cost rises by $530 million

16 April 2010 – Duke Energy Indiana told regulators the cost of its 618 MW Edwardsport coal gasification plant under construction in southwest Indiana will rise from $2.35 billion (or $3,800/kW) to $2.88 billion (or **$4,660/kW**).
[http://www.duke-energy.com/indiana.asp]