CFD Modeling Of Entrained Flow Gasifiers

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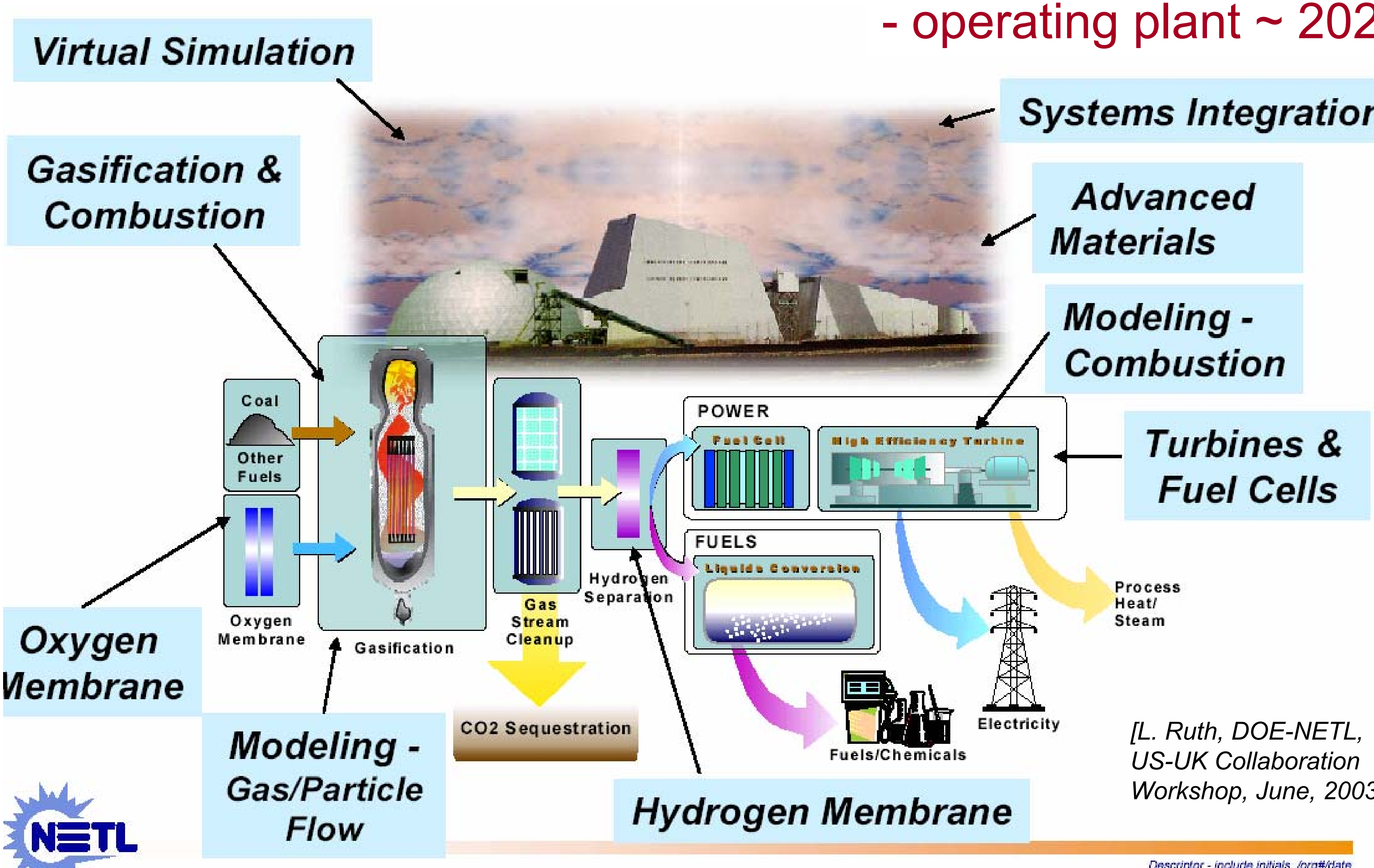
DOE Vision 21 Program
Cost Shared Agreement DE-FC26-00FNT41047

Advanced Power Systems

- power, multi-product
- CO2 capture ready
- operating plant ~ 2020



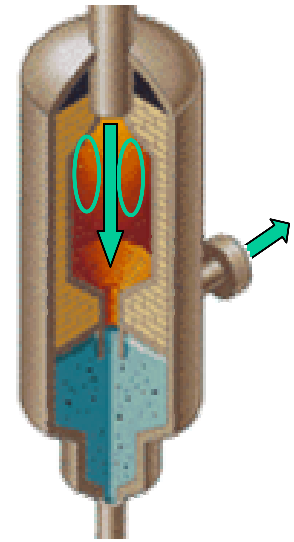
[L. Ruth, DOE-NETL, US-UK Collaboration Workshop, June, 2003]

DOE Techline - http://www.netl.doe.gov/publications/press/2000/tl_vis21sel2.html

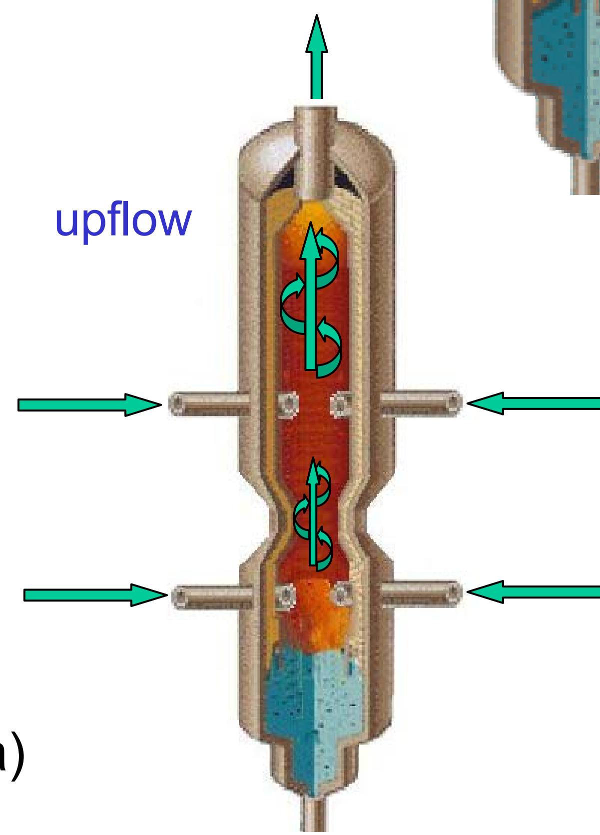
Entrained Flow Gasifier Model

- 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
    - reaction kinetics
      - high pressure and gasification
    - slag, ash, soot, tar
    - air toxics (metals, PM2.5)
- Collaboration
  - N. Holt (EPRI)
  - T.Wall,.. (Black Coal CCSD, Australia)
  - K.Hein (IVD, U. of Stuttgart)

downflow



upflow



Challenges / Opportunities….

- RAM = Reliability, Availability & Maintainability
- Carbon Conversion & Syngas Quality
  - Fuel Switching
    - Coal, Petcoke, Wastes, Oil, Biomass, Dirt, Blends
  - Fuel Feed System
    - Dry (N2, CO2); Wet (H2O); Pre-heat; Grind
    - Oxidant: Air vs O2
  - System Modifications / Scale Up
    - Injectors (location, quantity, orientation, spray)
    - Volume (L/D ratio)
    - System pressure
- Slag and Ash Management
  - Viscosity, composition, flux mat'l
  - Carbon content: slag vs flyash
- Refractory Wear
  - Heat extraction
- Transient Operation
  - start-up / shutdown / switching

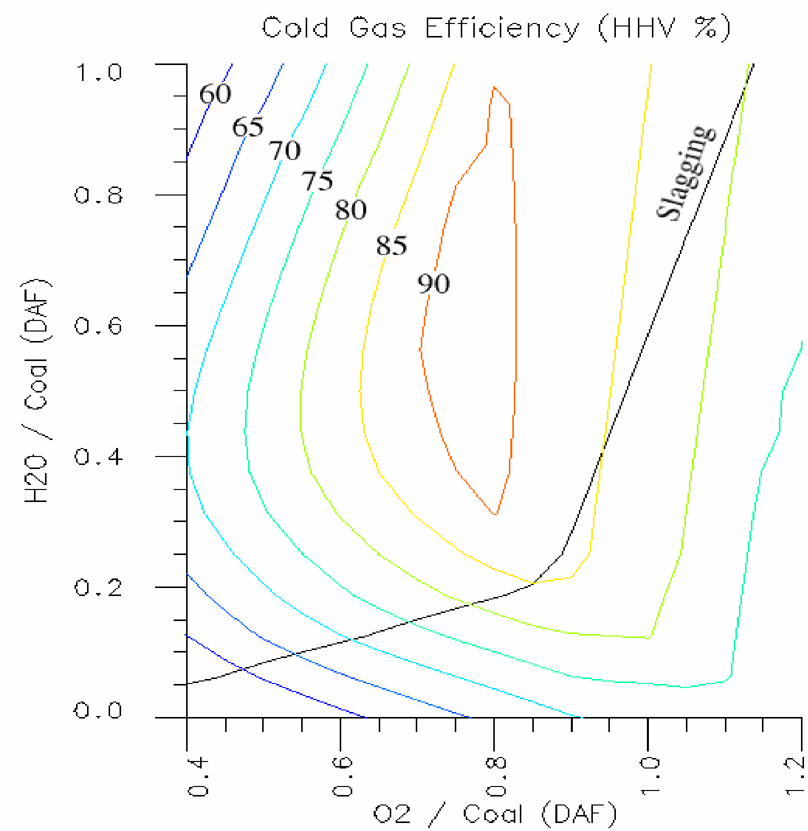
See Gasification Technologies
- Stiegel, Clayton and Wimer [2001]
- Holt et al [2001], [Holt, 2004]
- Dogan et al [2002]
- Mudd et al [2003]

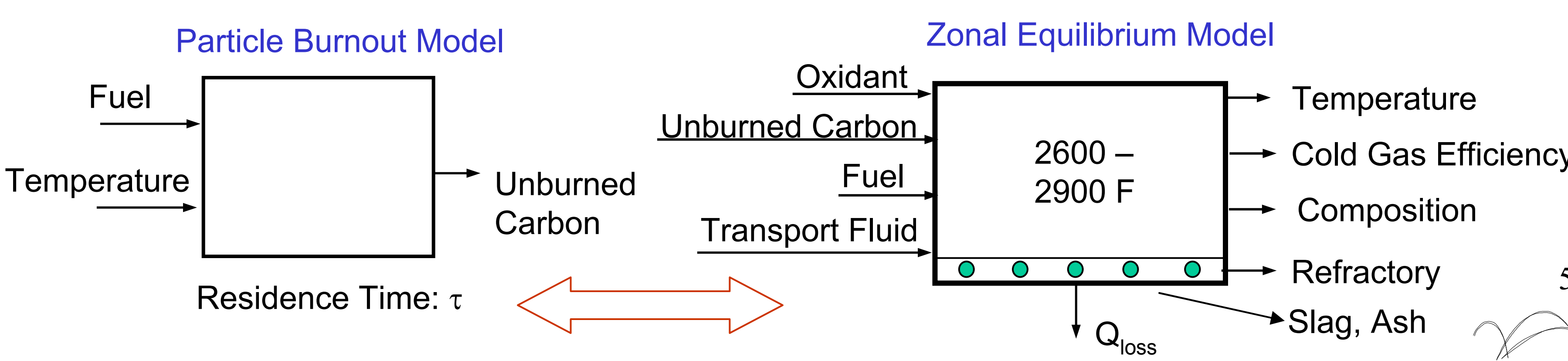
See DOE Gasification Tech. Report
- Clayton, Stiegel, and Wimer

See Clearwater Confernce
- Dogan et al [2002], [2003]

Gasifier – Flow Sheet / Process Model

- fast running model to asses operating conditions
  - 1 & 2 Stage designs
- mass & energy balance
  - particle burnout + equilibrium chemistry
  - heat transfer
- slag flow indicator
- Includes impacts of:
  - Fuel type, Unburned carbon, recycled char, incomplete burnout
  - Oxidant conditions
  - Wet vs Dry feed
  - Fuel particle size

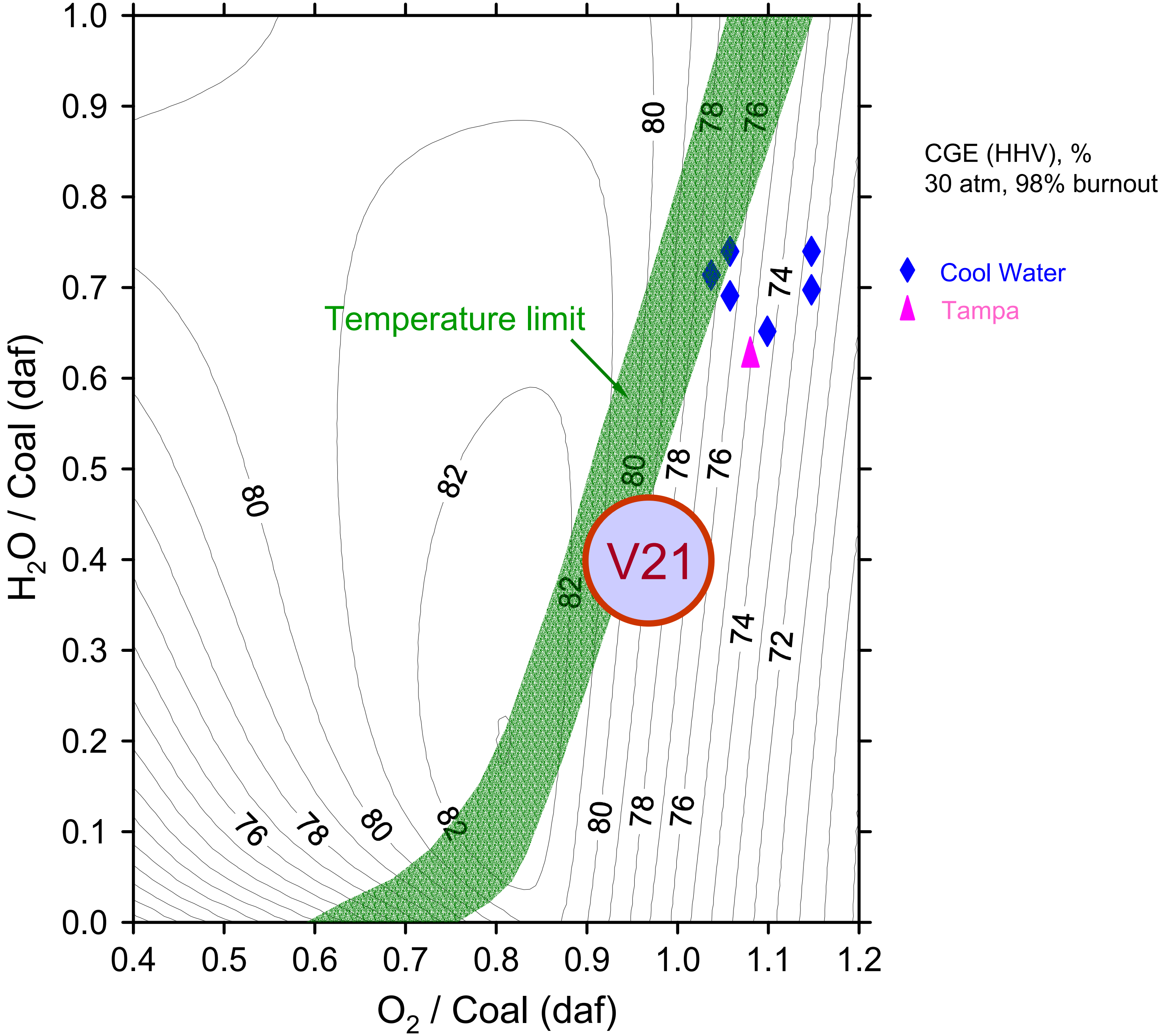




Effect of Operating Conditions on Cold Gas Efficiency

1 stage

(slurry-feed)

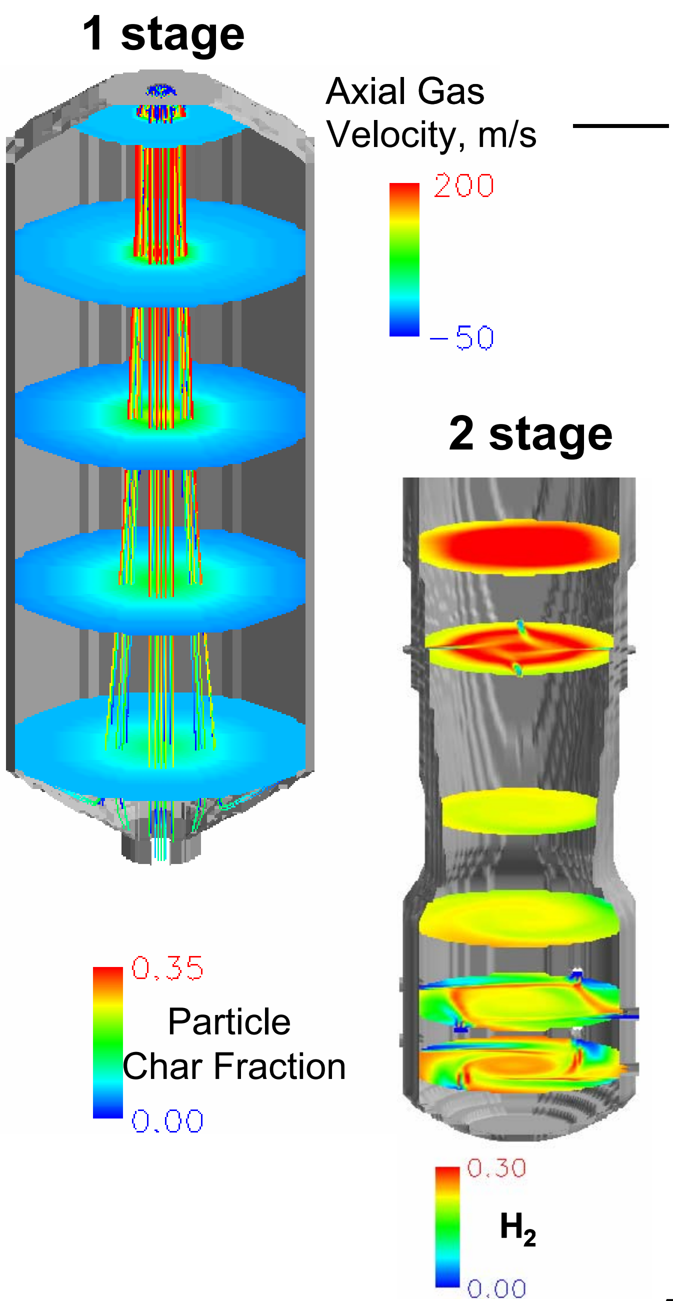


Gasifier - CFD Model

- 1 & 2 stage gasifier designs
  - Based on dominant commercial systems
- provides details on
  - gas flow field
    - temperature, velocity, species
  - wall conditions:
    - temperature, heat flux
    - critical viscosity, slag flow
  - carbon conversion, cold gas efficiency
  - unburned carbon in slag and flyash
  - generated syngas
    - species, temperature, particle loading,…
- evaluate impact on
  - carbon conversion, slag and ash properties, refractory

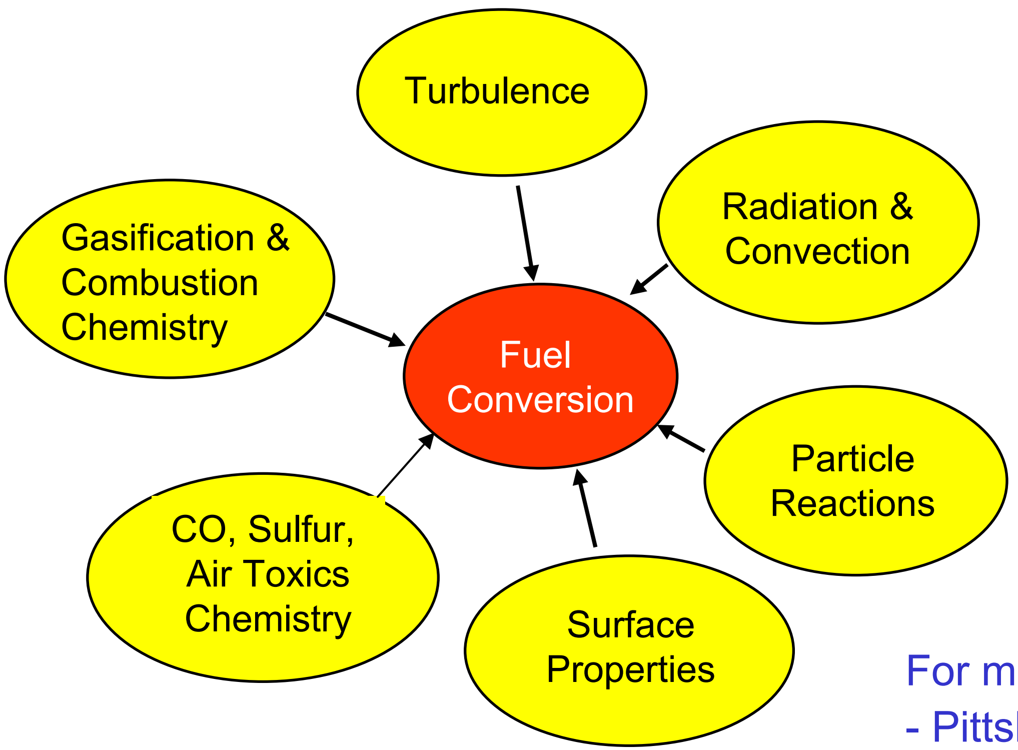
due to:

- fuel change or co-firing:
  - coal / char-recycle / petcoke / waste / biomass
- oxidant: oxygen concentration, pre-heat
- feed: wet vs dry, solids loading, pre-heat



CFD Model

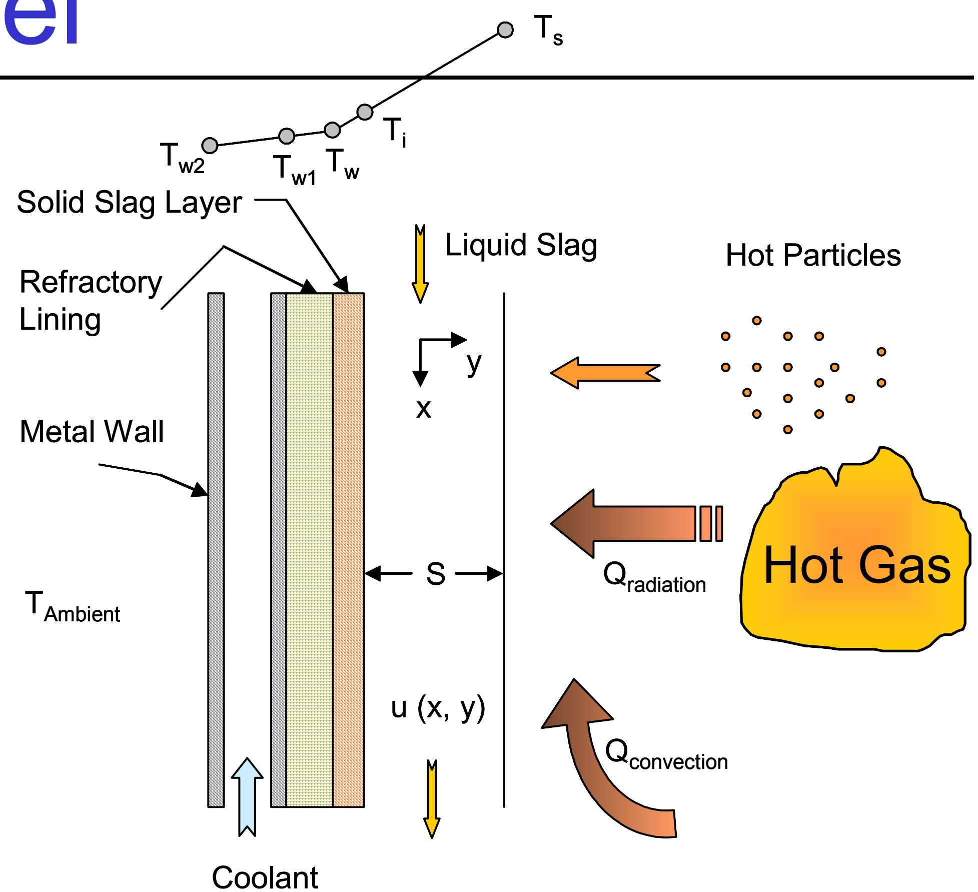
- **Computer model represents**
  - **Gasifier geometry**
  - **Operating conditions**
  - **Gasification processes**
- **Accuracy depends on**
  - **Input accuracy**
  - **Numerics**
  - **Representation of physics & chemistry**



For model details see
- Pittsburgh Coal Conference 2002
- Gasification Technologies Conference 2002

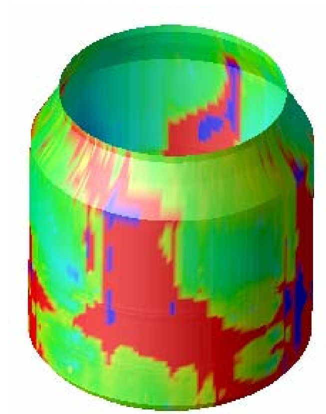
Flowing Slag Model

- 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
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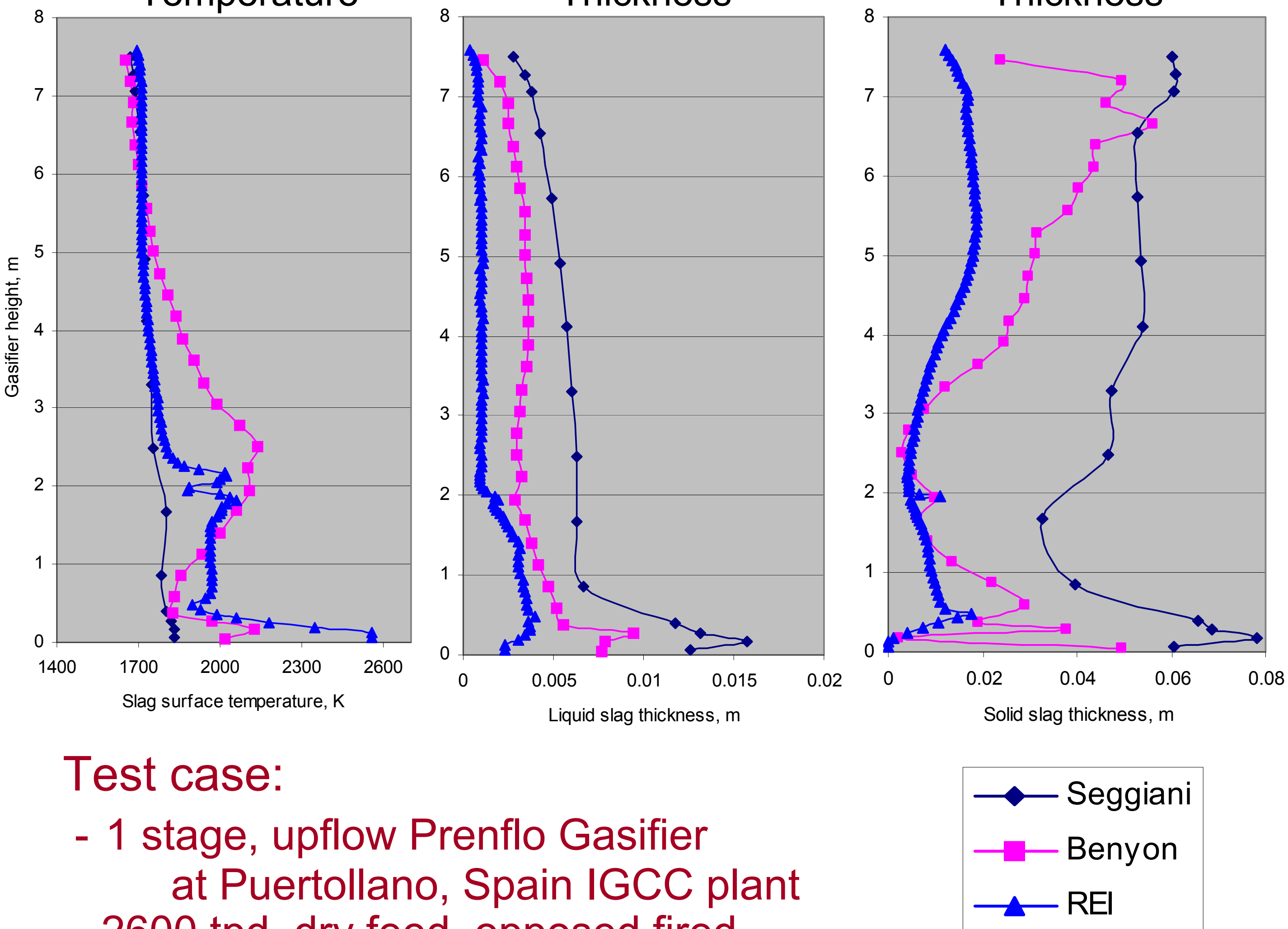
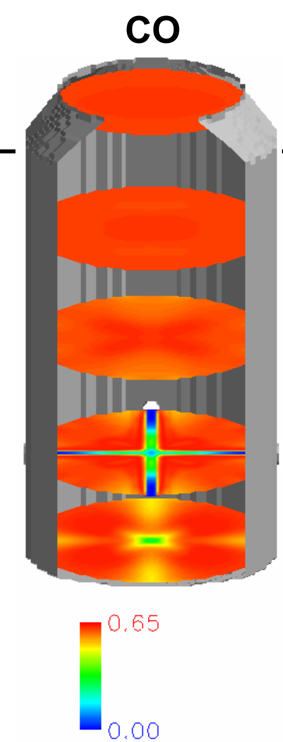
Flowing Slag Model

Slag Surface Temperature	Liquid Slag Thickness	Solid Slag Thickness

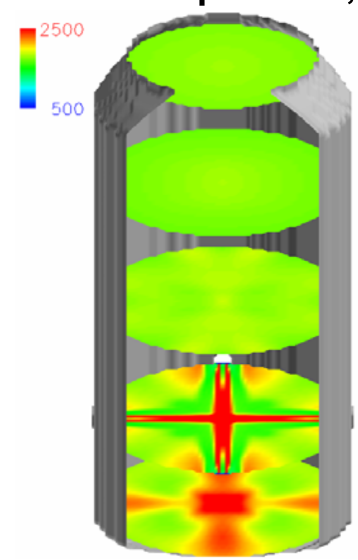


Test case:

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



Gas temperature, K



PREKIN → kinetics pre-processor for solid fuel oxidation/gasification

Inputs:

- Fuel properties: C, H, O, Ash, Volatile matter
- Particle size distribution
- Intrinsic rate parameters in:
  - Power law kinetics
  - Langmuir-Hinshelwood kinetics
- Reaction Conditions: temperature, partial pressure

Outputs:

A_G, E_G, & n

For given range of reaction conditions

PREKIN

Kinetic pre-processor

- Generate gasification rate based on input temperature and pressure
- Combination of various sub-models: devolatilization, porosity development, thermal annealing, ash inhibition, diffusion, CO/CO_2, and gasification rate
- Fit and Optimize results with the equation

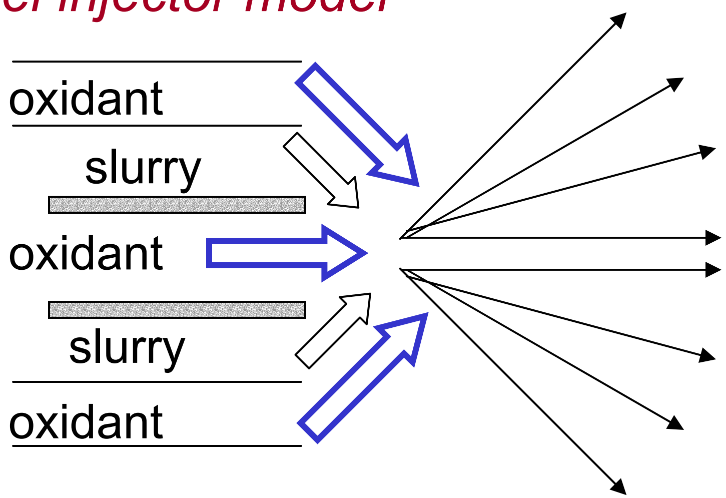
$$q_{rxn} = A_G \cdot \exp\left(-\frac{E_G}{R \cdot T_P}\right) \cdot (P_s)^n$$

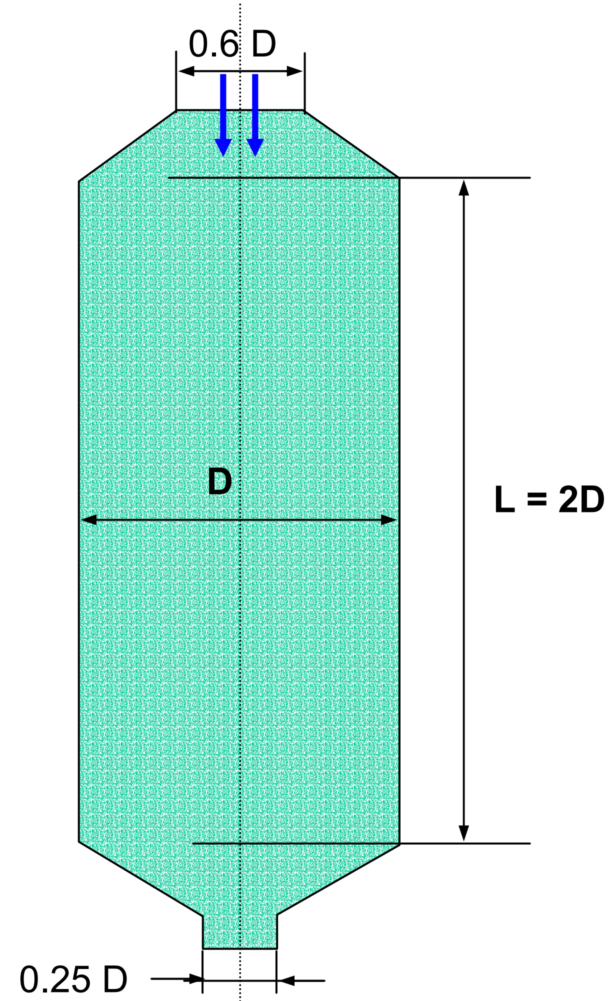
- sub-models
  - devolatilization: Two-step & CPD
  - pore structure: Power law & random pore
  - intrinsic rates: Power law & Langmuir-Hinshelwood (CO inhibition)
  - thermal annealing & ash inhibition

Single Stage – Down Flow

- Vision 21 Firing Conditions
  - Pressure = 32 atm.
  - 3000 tpd Illinois #6
    - H_2O 11%, Ash 10%
  - Slurry: 74% solids (wt.)
  - Oxidant
    - 95% O_2, 5% N_2
    - O_2:C (molar) = 0.46
    - Inlet Stoichiometry ~ 0.51

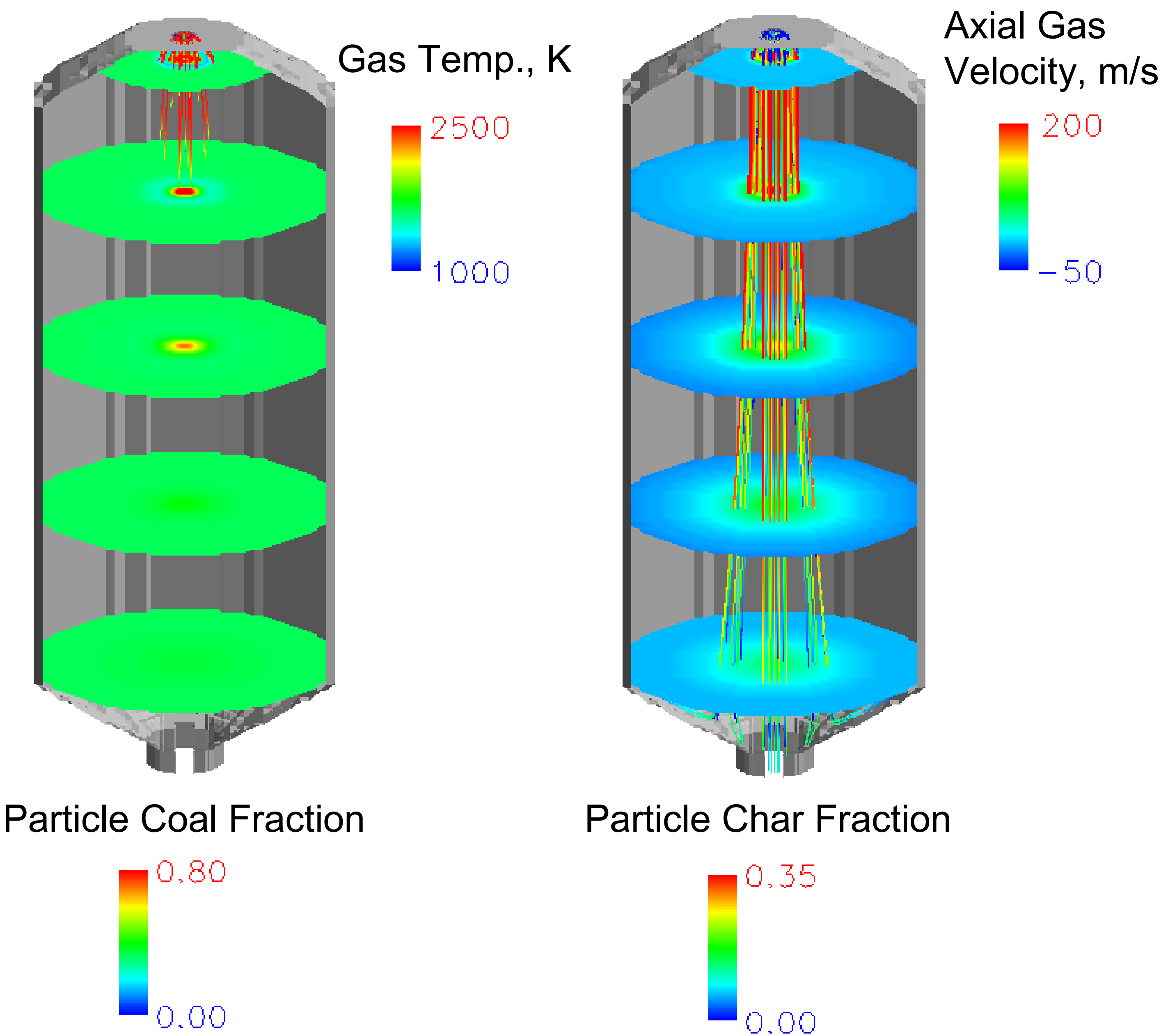
fuel injector model



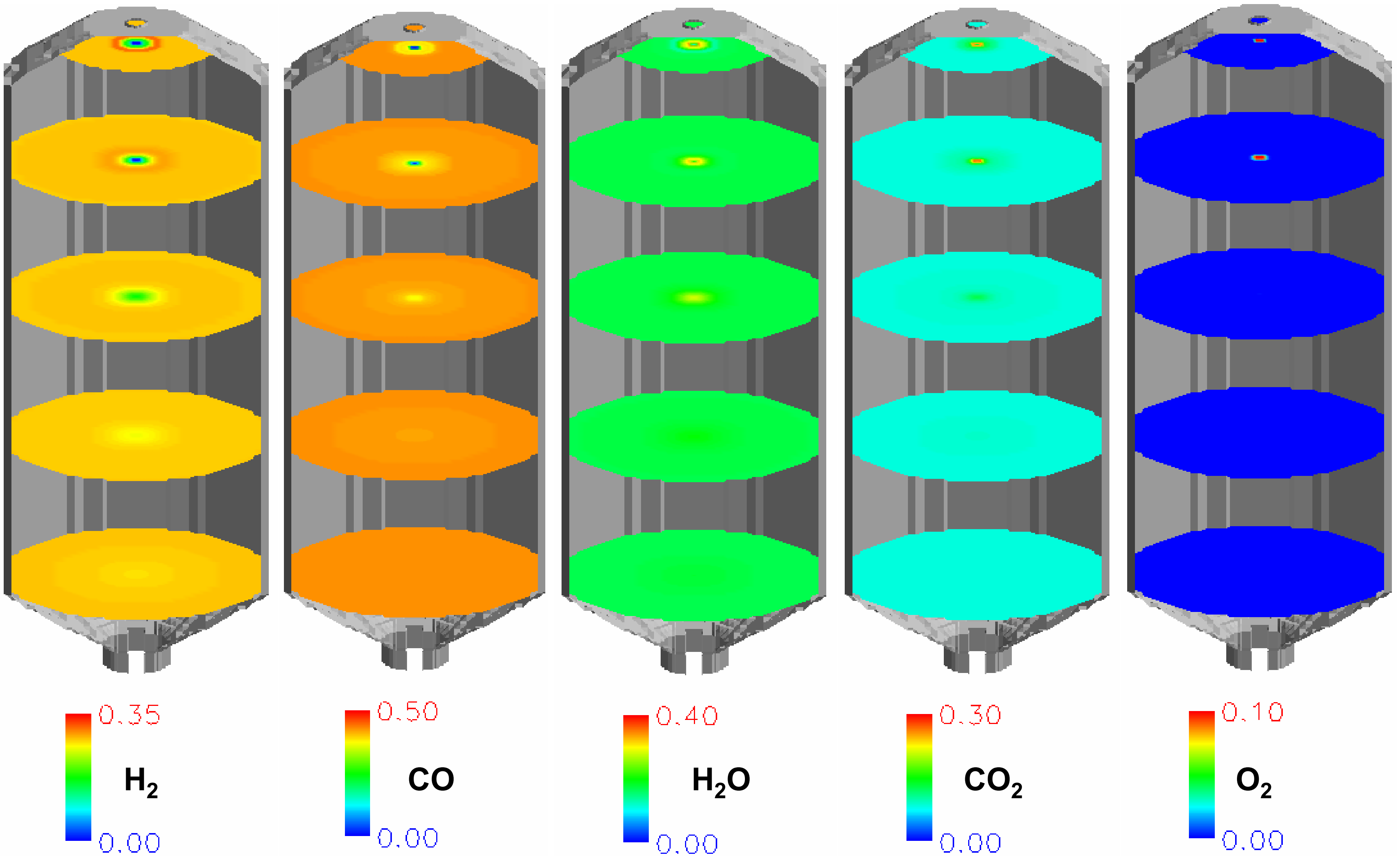


D = 2.2m

Gas and Particle Flow Field

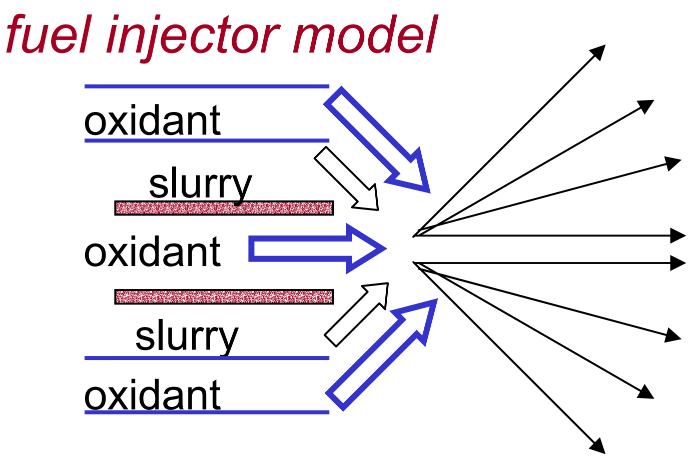


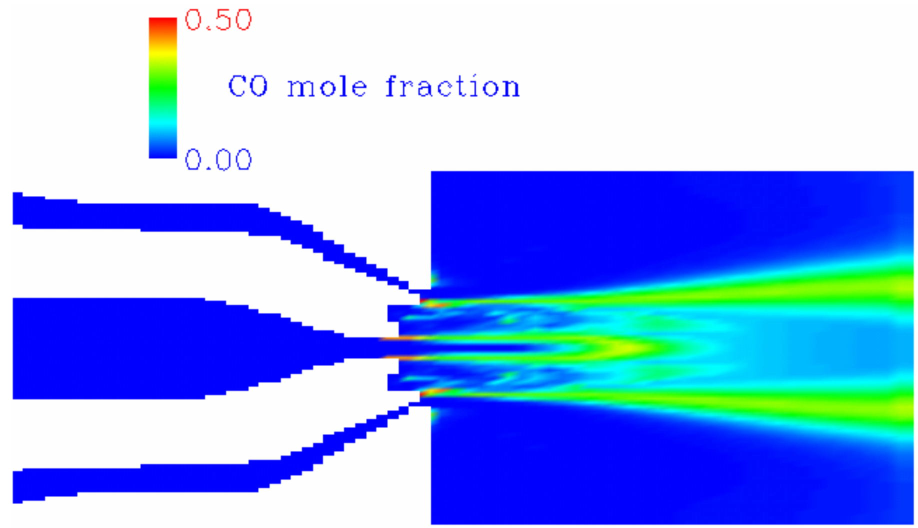
Gas Composition at Elevations

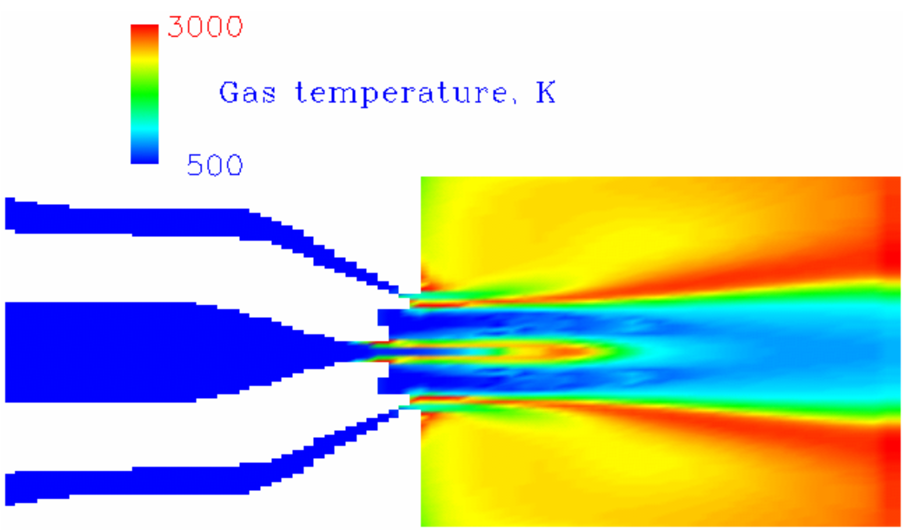


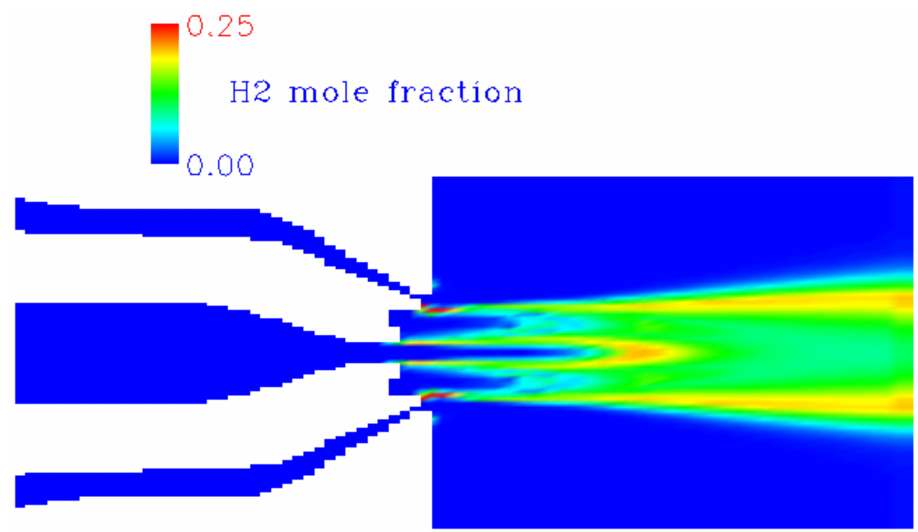
Fuel Injector Study

- Overheating ~ reduces injector life = a limiting item for IGCC





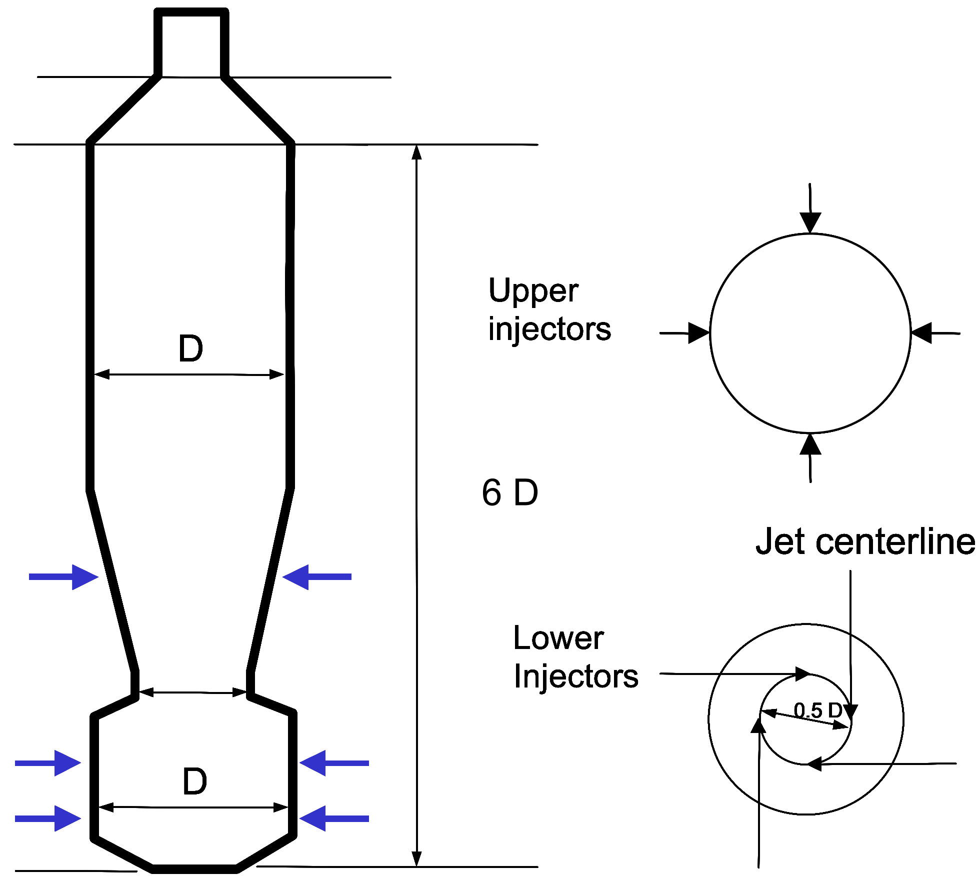




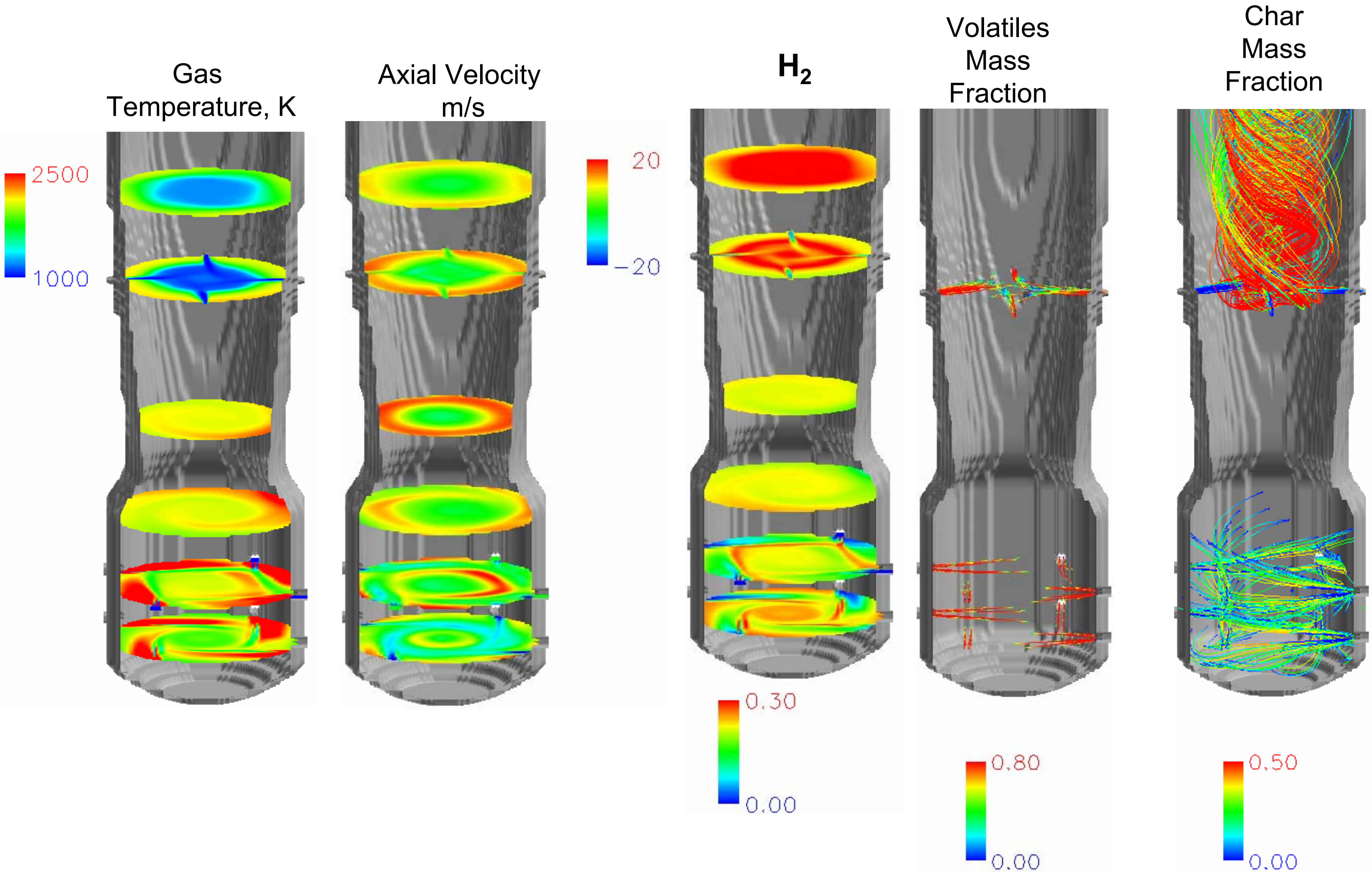
Example: Two Stage – Up Flow

- **Vision 21 Firing Conditions**
  - Pressure = 28 atm.
  - 3000 tpd Illinois #6
    - H_2O 11%, Ash 10%
  - Recycle 100 tpd char + ash
  - Slurry: 74% solids (wt.)
  - Slurry Distribution
    - 39%, 39%, 22% (upper)
  - Oxidant
    - 95% O_2, 5% N_2
    - O_2:C (molar) = 0.43
    - Inlet Stoichiometry ~ 0.50

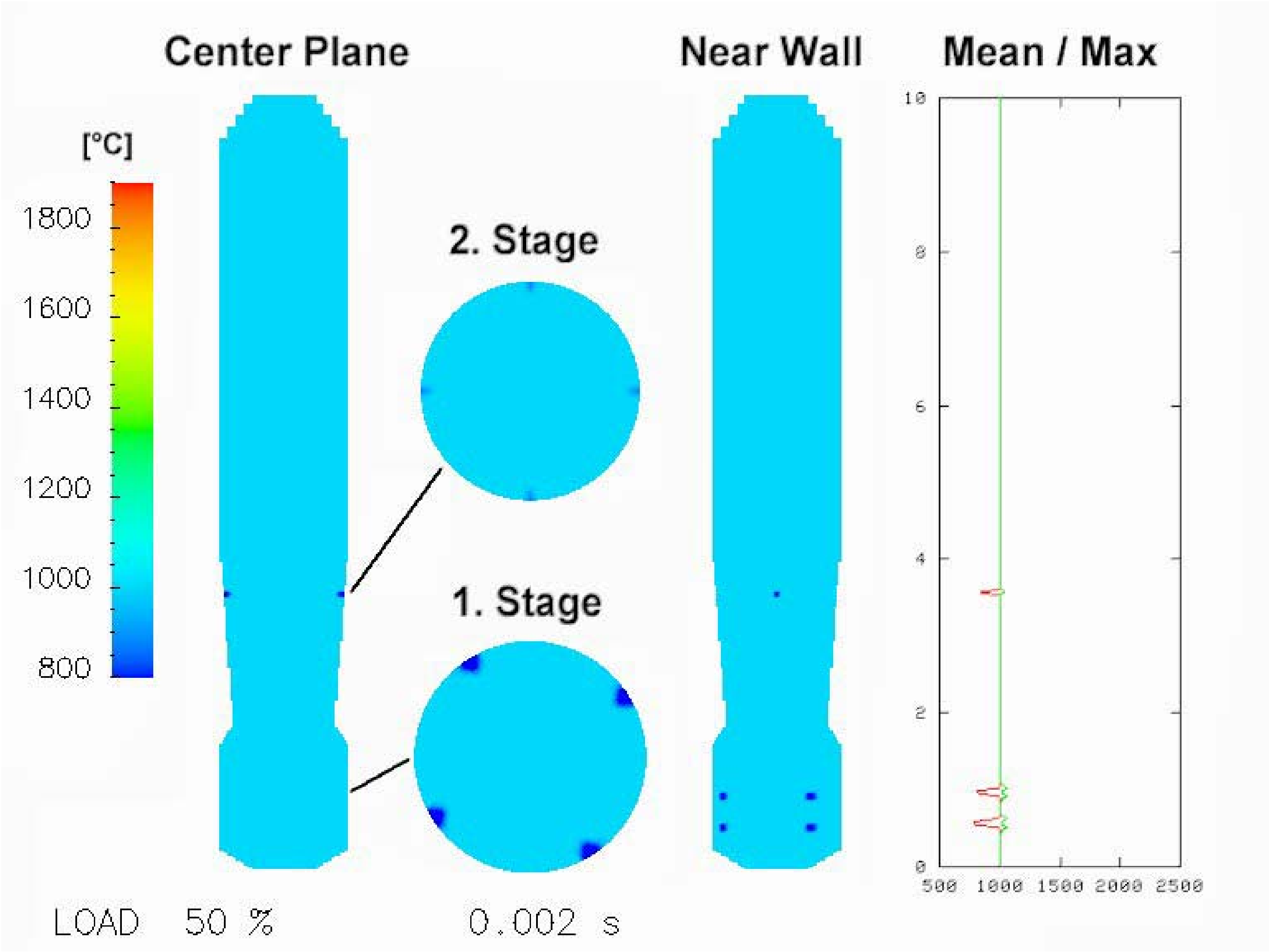
- **Firing System**
  - 4 fuel injectors / level
  - Fuel Injectors ~ pipes



Gas and Particle Flow Field



Gasifier - CFD Model - transient



Gas Temperature

Difficulty of Obtaining Data on Gasification Conditions

Ruprecht et al., Fuel (1988)

Table 6 Output data

Reactor temperature	(°C)
O/C-ratio	(–)
C-conversion	(%)
Dry gas production	($m^3 h^{-1}$)
Dry gas composition	(vol %)
CO_2	
CO	
H_2	
N_2	
H_2S	
COS	
CO/H_2-ratio	(–)
Water content of the wet gas	(vol %)
Spec. O_2-consumption	($m^3 t^{-1}$)
	($m^3 m^{-3}$)
Spec. syngas production	($m^3 t^{-1}$)
Cold gas efficiency	(%)
Spec. steam production	($t t^{-1}$)

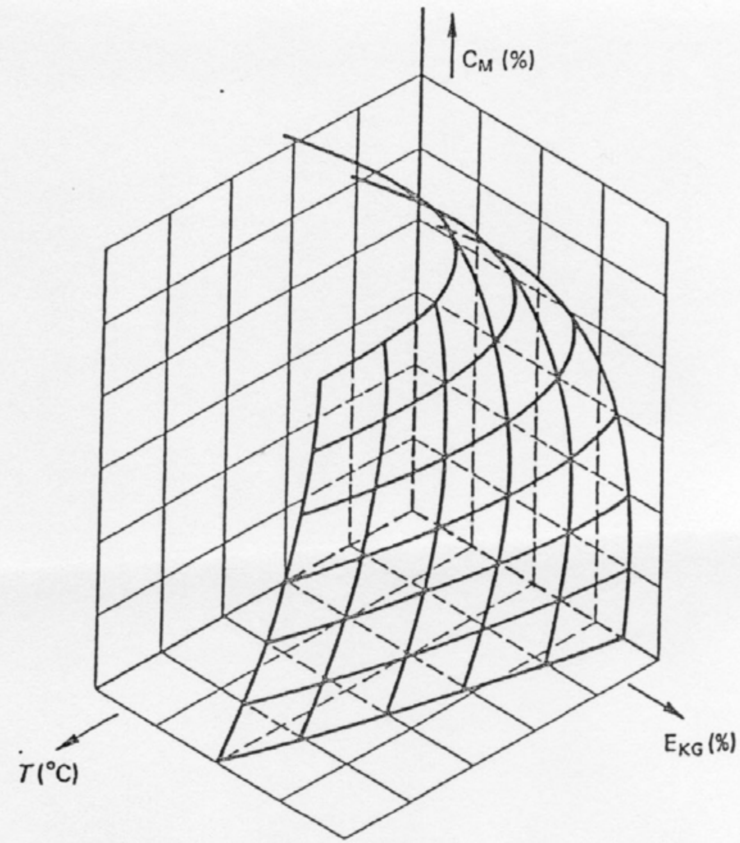


Figure 5 Relationship between cold gas efficiency, gasifier temperature and slurry concentration

Acknowledgements

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REI

Dave Swensen (Software Lead), **Martin Denison** (Modeling Lead)
Zumao Chen, Temi Linjewile, David Lignell, Connie Senior, Adel Sarofim, REI Technical Staff
- Develop component models, framework, ….

And

Neville Holt (EPRI)
Gasifier System Configurations & Validation

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Coal Gasification Data and Mineral Matter Sub-models

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Transient gasifier simulations, gasification in the EU

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