Process/Equipment Co-Simulation for Gasification and Combustion-based Energy Applications

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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)

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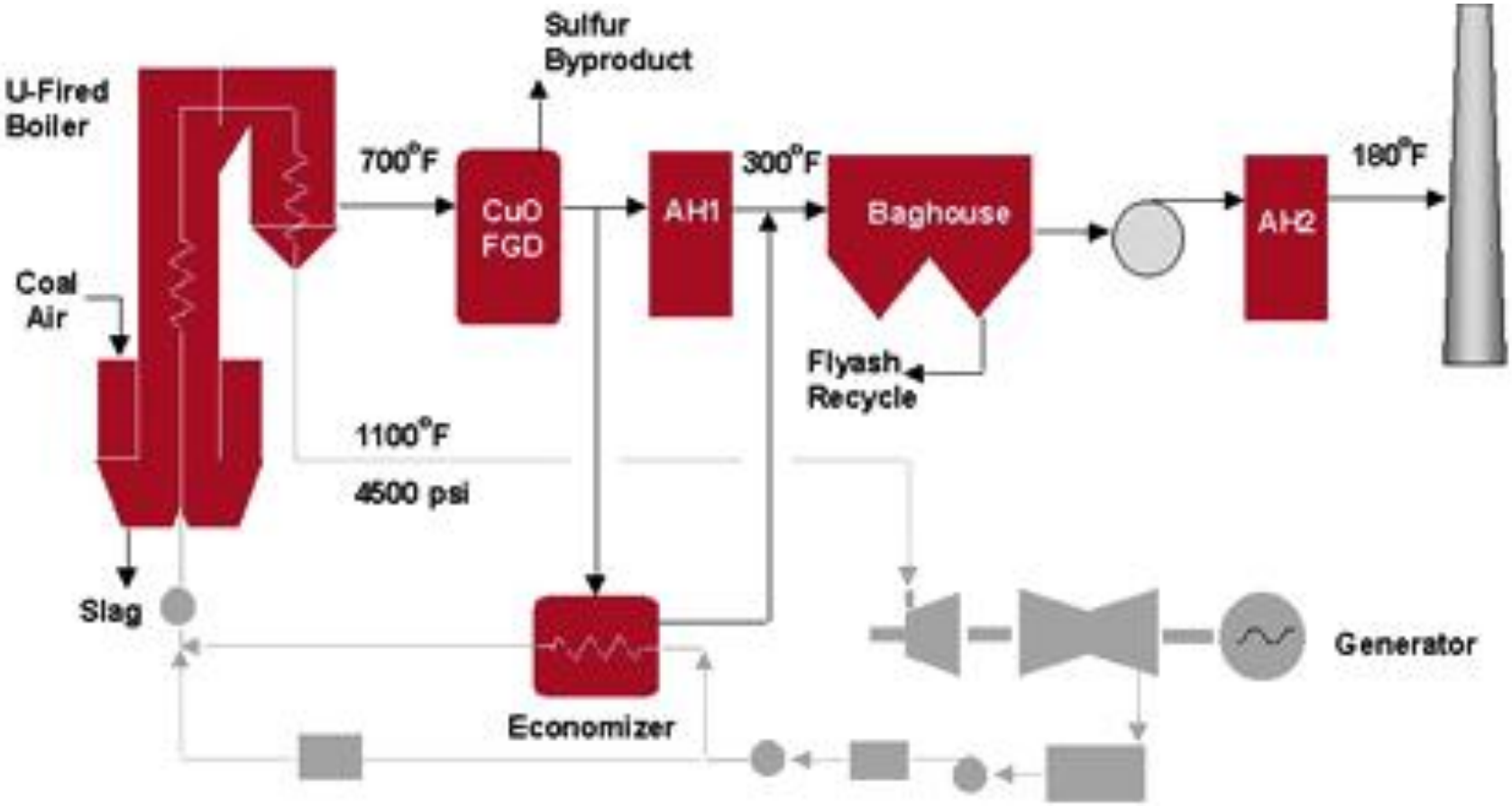
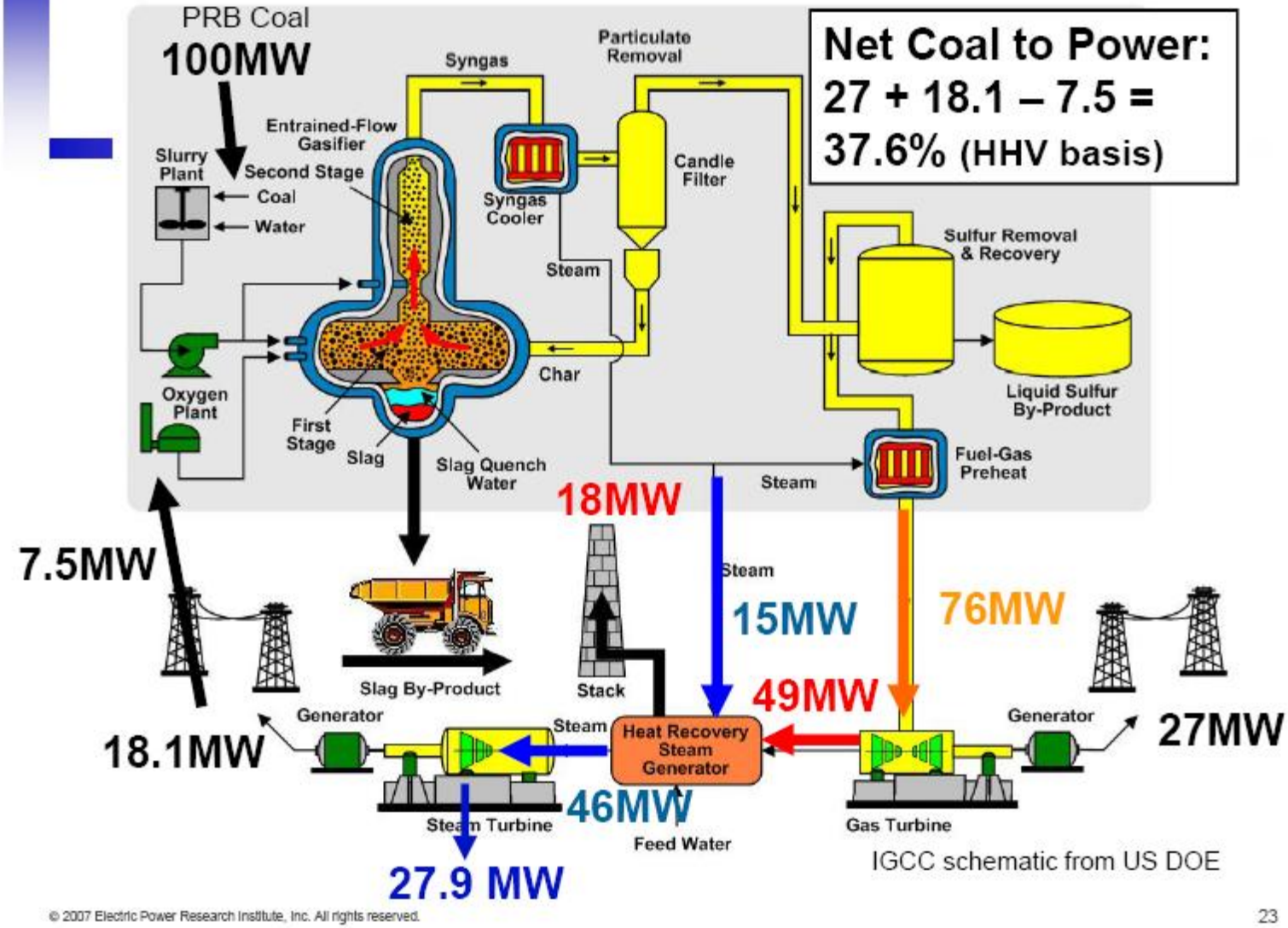
Co-Simulation and Power Systems

- Coal combustion ➔ CO_2 + Q (heat)
  - Use heat to generate electricity in steam turbine
  - Conventional, SuperCritical , UltraSuperCritical
    - Relatively Simple plant layout
  - Oxy-fire boiler
    - Recycle of CO_2 complicates plant and operation
  - Flue gas conditioning
    - Reagents, sorbents for pollution control
  - Water consumption, heat integration
- Natural Gas combustion ➔ CO_2 + Q (heat)
  - Use natural gas to generate electricity in combustion turbine
  - Combined cycle (NGCC) system
  - Performance monitoring, Flue gas conditioning
- Coal Gasification ➔ Syngas (CO, H_2, CO_2, H_2O, CH_4)
  - Use syngas to generate electricity in combustion turbine
  - Combined cycle (IGCC) system
    - More complicated plant layout ~ “chemical plant”
    - Many “recycle” loops and coupling for gas, liquid, solids streams

Conventional Power Plant



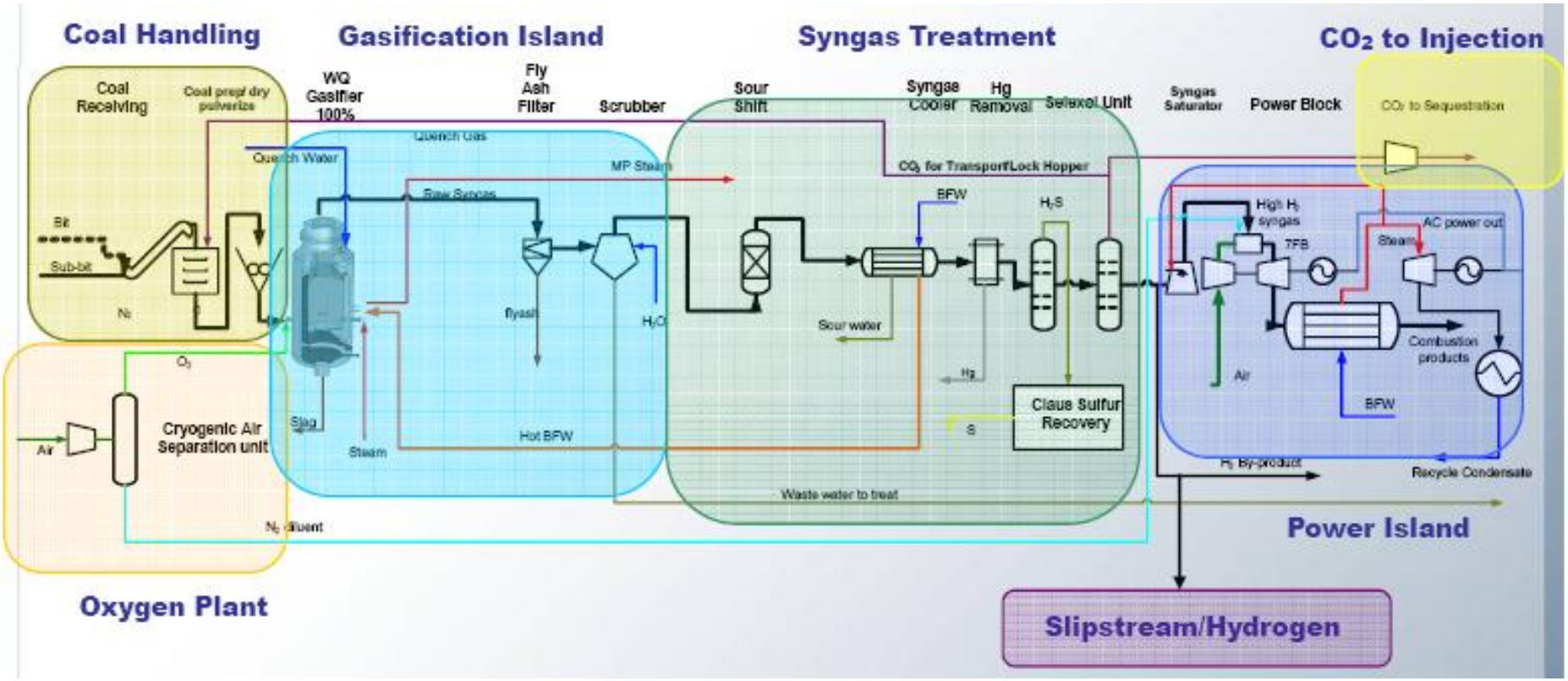
Advanced Power Systems



[J. Phillips, "IGCC 101", GTC 2009]

http://www.gasification.org/library/overview.aspx

Advanced Power Systems – FutureGen

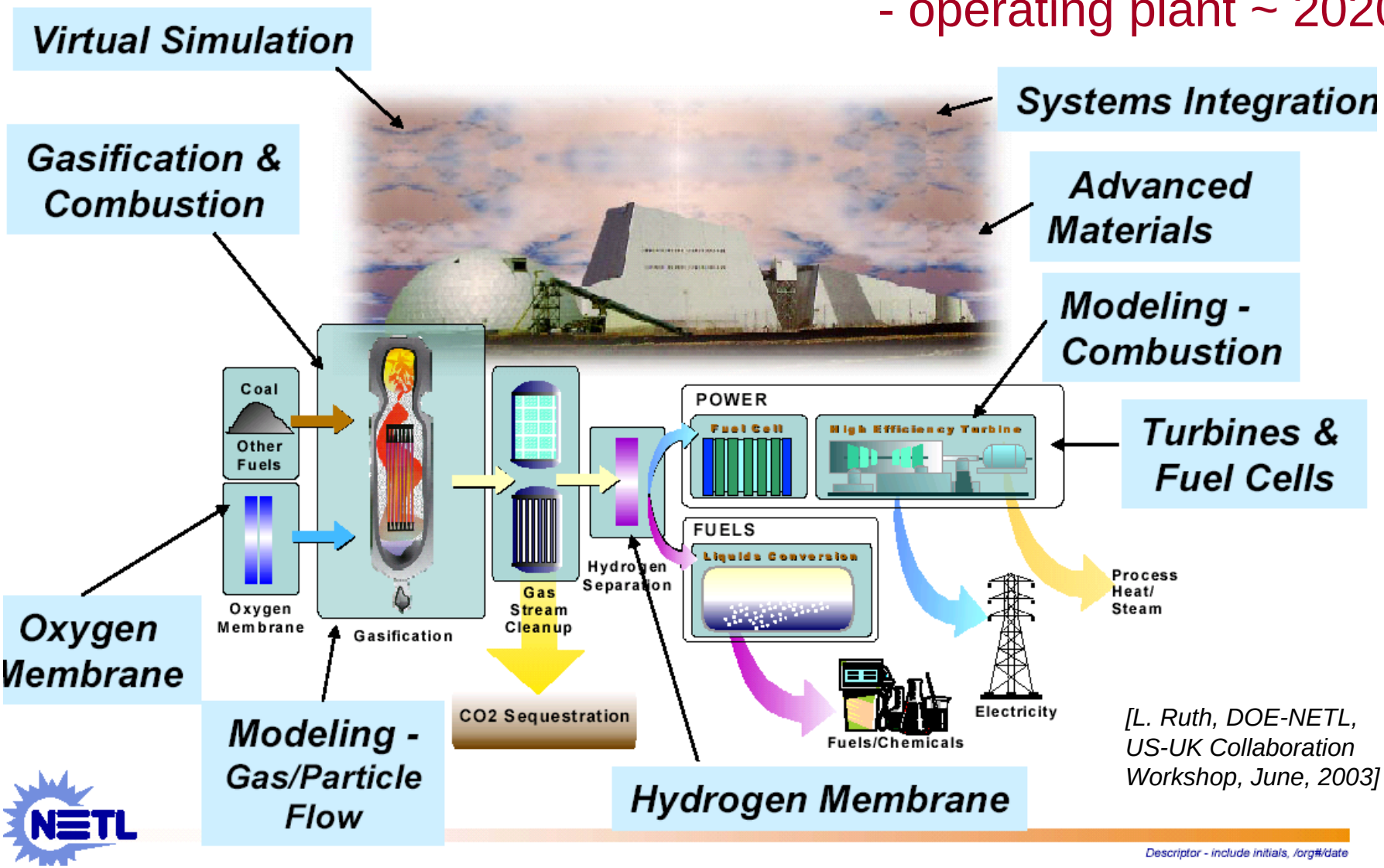


[D. Brown, “Rebirth of FutureGen at Mattoon,” GTC 2009]

http://www.gasification.org/library/overview.aspx

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

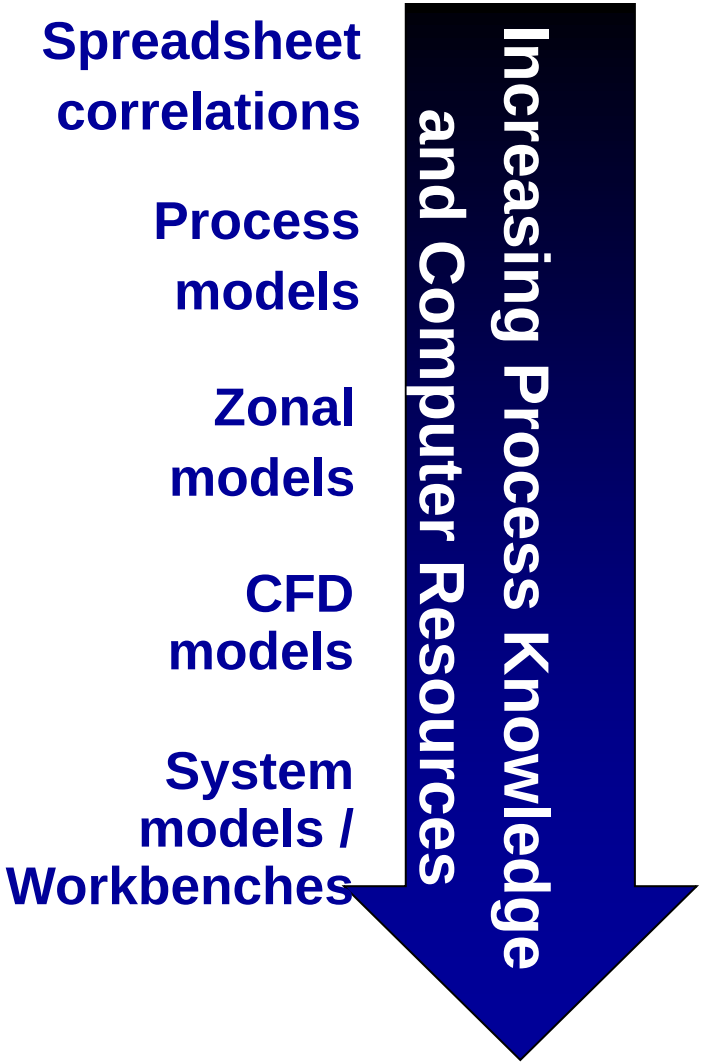
Why Use Modeling?

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**
- **Does NOT make decisions for engineers, but does help them be more informed**

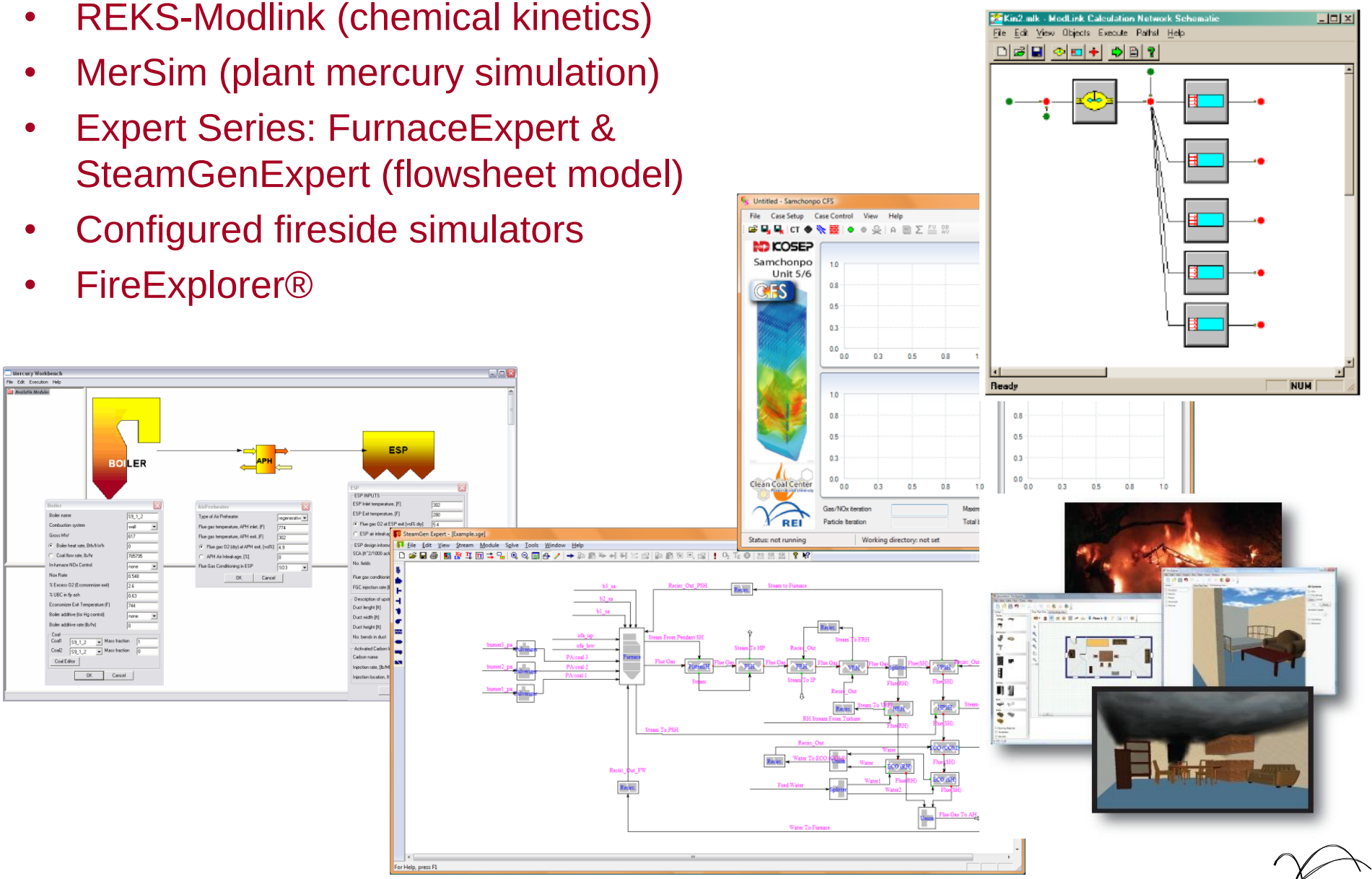
Simulation Capabilities

- Many types of simulation tools – each serves a different purpose
- Model development and use are correlated with:
  - Process knowledge
  - Modeling techniques
  - Computational resources
  - Value to market



Specialized Software Systems

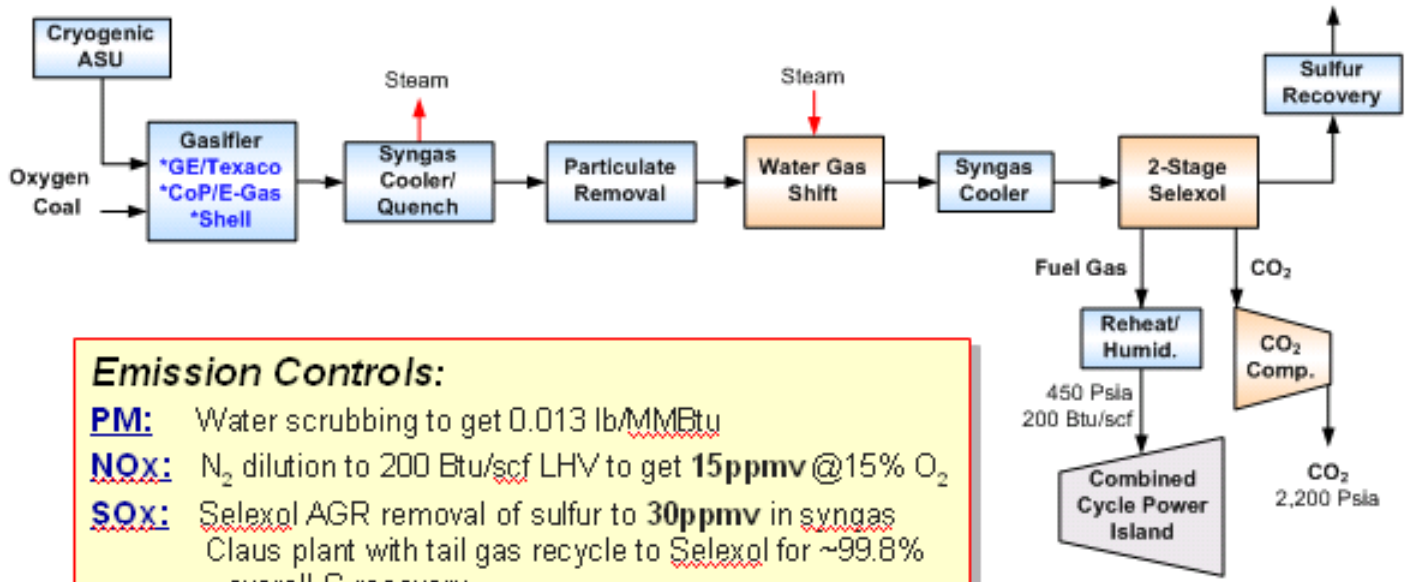
- REKS-Modlink (chemical kinetics)
- MerSim (plant mercury simulation)
- Expert Series: FurnaceExpert & SteamGenExpert (flowsheet model)
- Configured fireside simulators
- FireExplorer®



AspenPlus IGCC Flowsheet*

Pre-Combustion Current Technology

IGCC Power Plant with CO_2 Scrubbing



Emission Controls:

PM: Water scrubbing to get 0.013 lb/MMBtu

NOx: N_2 dilution to 200 Btu/scf LHV to get **15ppmv** @15% O_2

SOx: Selexol AGR removal of sulfur to **30ppmv** in syngas
Claus plant with tail gas recycle to Selexol for ~99.8% overall S recovery

Hg: Activated Carbon beds for ~90% removal

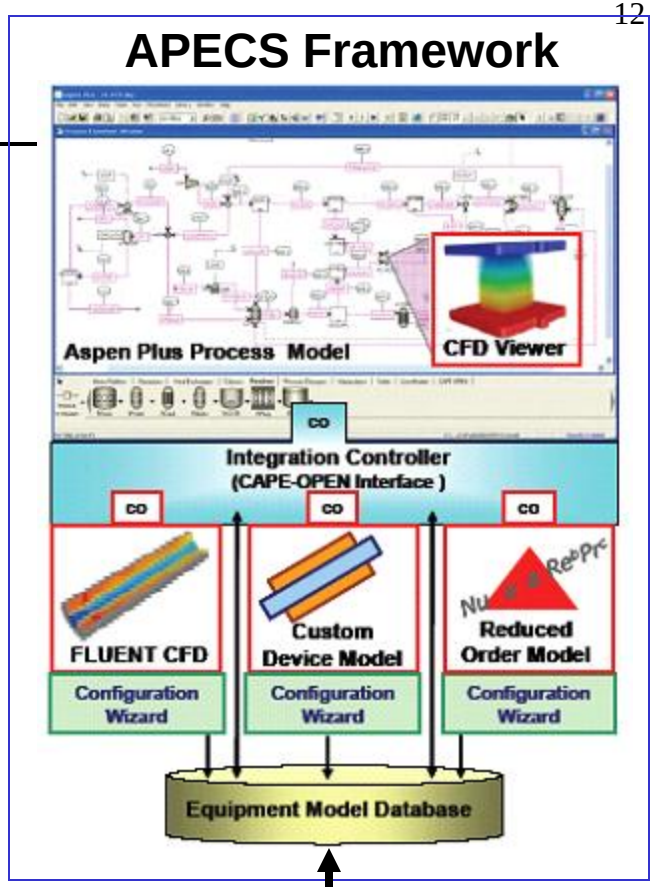
Advanced F-Class Turbine - 232MWe (42% LHV)

Steam Conditions - 1800psig/1050°F/1050°F

* Ciferno, J. and Klara, J., "2006 Cost & Performance Comparison of Fossil Energy Power Plants," Pittsburgh Coal Conf., 2006b
* Ciferno, J., "2006 Cost & Performance Comparison of Fossil Energy Power Plants," Clearwater Conf. 2006a

Equipment Models*

- Gasifiers
  - entrained flow (slurry, dry, 1 stage, 2 stage)
  - transport reactor
- Heat Exchangers
  - syngas cooler, HRSG, recuperator
- Air Separation Unit (ASU)
- Gas Clean Up (cold, warm, hot)
  - cyclone, chlorine guard, bulk desulfurizer,
  - sulfur polisher, SCR,
  - AGR, Carbon Bed
- Gas Turbine Equipment
  - turbine, compressors,
- expanders, combustors
- Solid Oxide Fuel Cells (SOFC)
- Reactors with Kinetics
  - Perfectly Stirred Reactor (PSR), Plug Flow Reactors (PFR)
- SOFC Exhaust Gas Combustors
  - dump, catalytic
- Membrane Based Gas Separation Units
  - water gas shift membrane reactor
- Balance of Plant



CAPE-Open

REI Models

Project Team Models

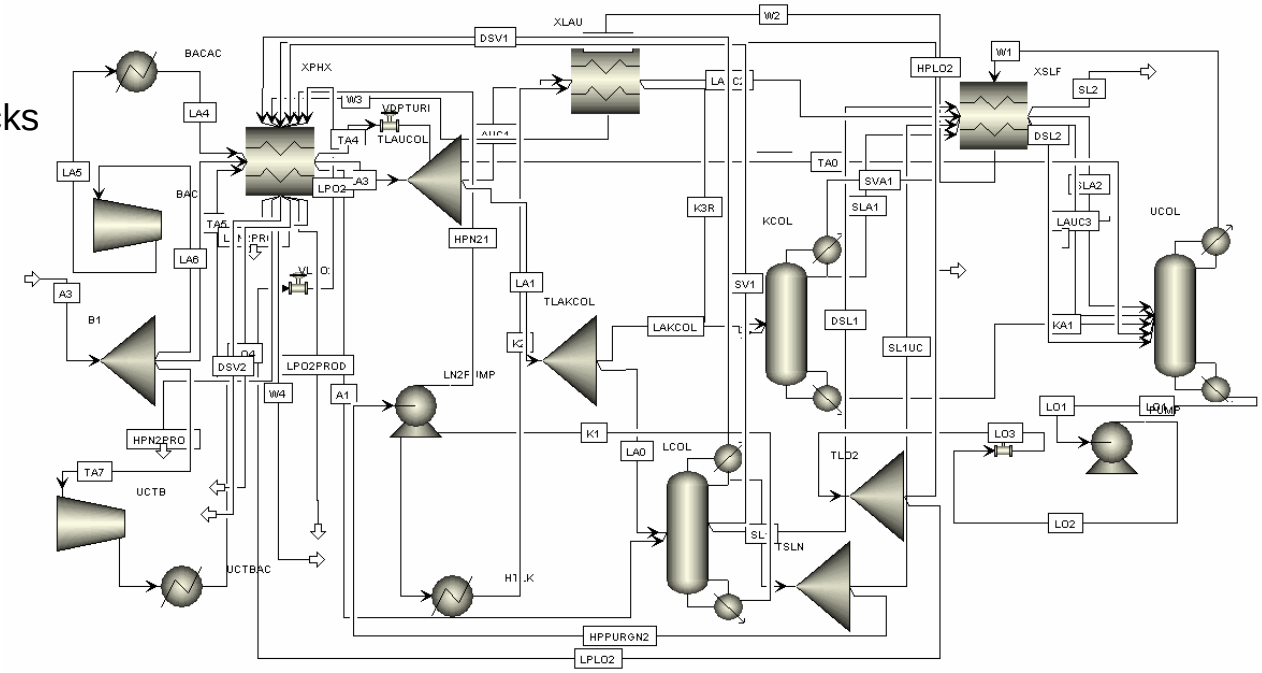
GE GateCycle

* Bockelie, M., Swensen, D.A., Denison, M.K., Maguire, M., Yang, C., Chen, Z., Sadler, B., Senior, C.L., Sarofim, A.F. "A Computational Workbench Environment for Virtual Power Plant Simulation", Contract DE-FC26-00NT41047, Final Report, December, 2004.

Cryogenic ASU Model

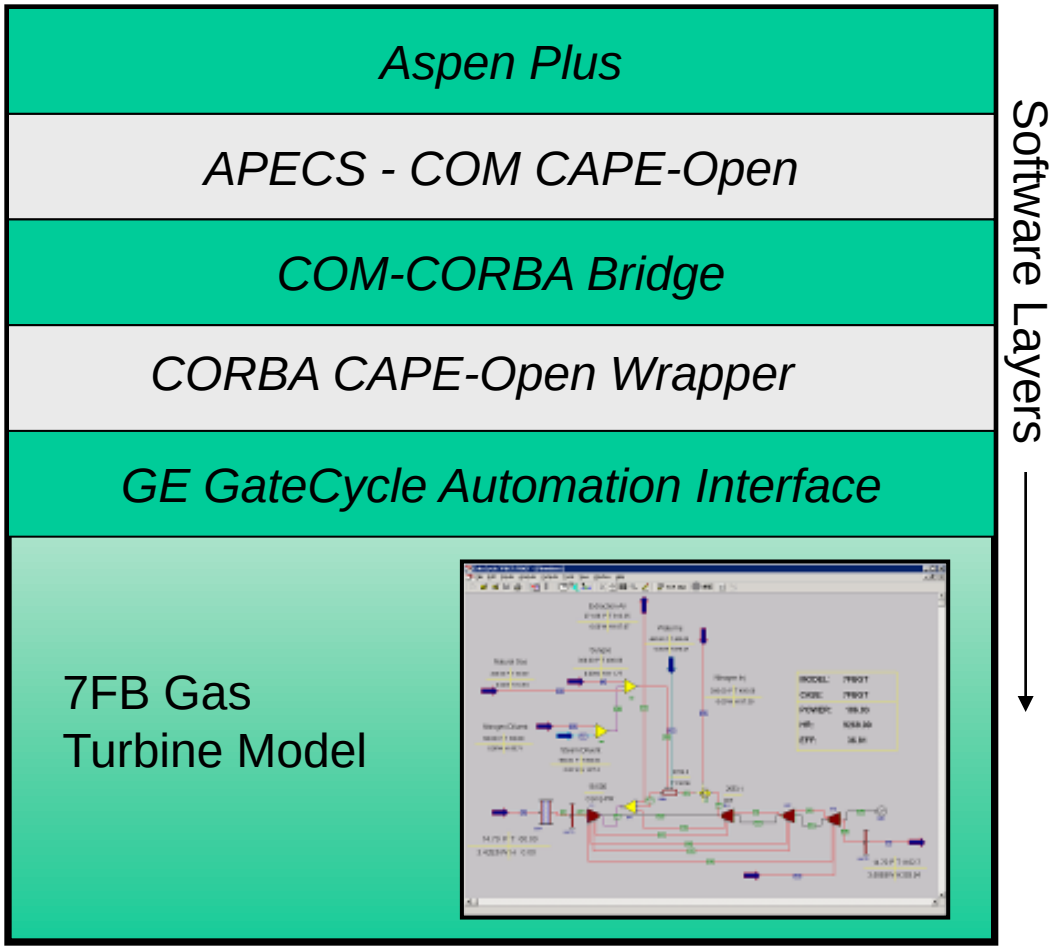
- PRAXAIR provided ASU model as a HYSYS network
- REI replicated HYSYS model with AspenPlus network
  - Benchmarked AspenPlus and HYSYS versions of model
    - good agreement obtained
    - must use comparable Eqn. of State for properties (Peng-Robinson)

AspenPlus network consists of
- 3 Distillation Column (RadFrac) blocks
- 3 Heat exchanger (MHeatX) blocks
- 3 Heater (Heater) blocks
- 5 Splitter (FSplit) blocks
- 2 Compressors (Compr) blocks
- 2 Pump blocks
- 3 Valve blocks



Models – GE GateCycle

- Create CAPE-Open Coupling to GE GateCycle
  - Access selected equipment models from APECS
  - 7FB Gas Turbine is first model chosen
  - Prototype of APECS 7FB model is being tested
    - ~60 model inputs
    - ~65 model outputs
- REI + Enginomix



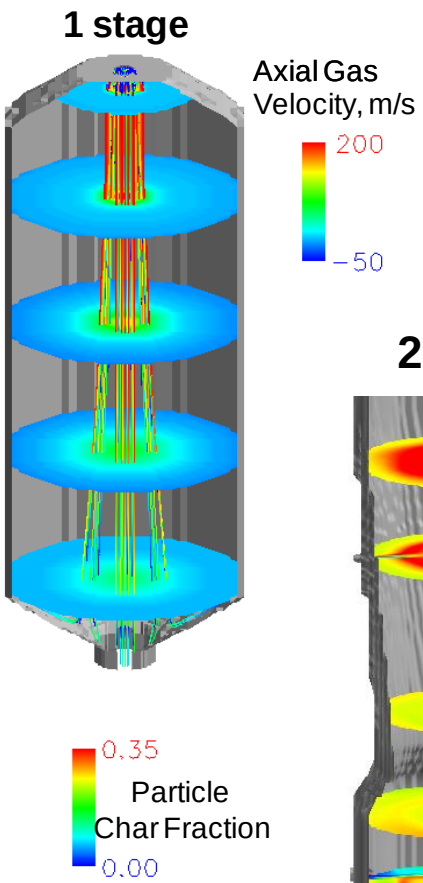
note: user must have a valid GE GateCycle license to exercise this capability

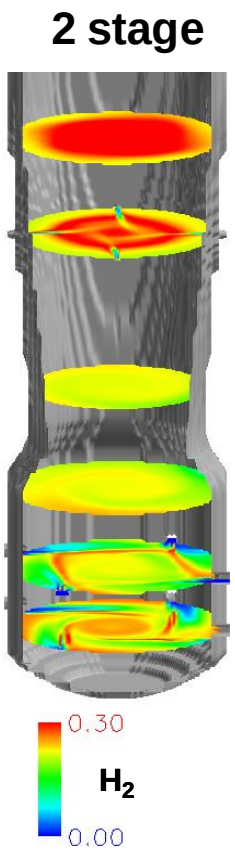
[AIChE 2006]

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 2006], [PCC 2006], [Clearwater, 2008]



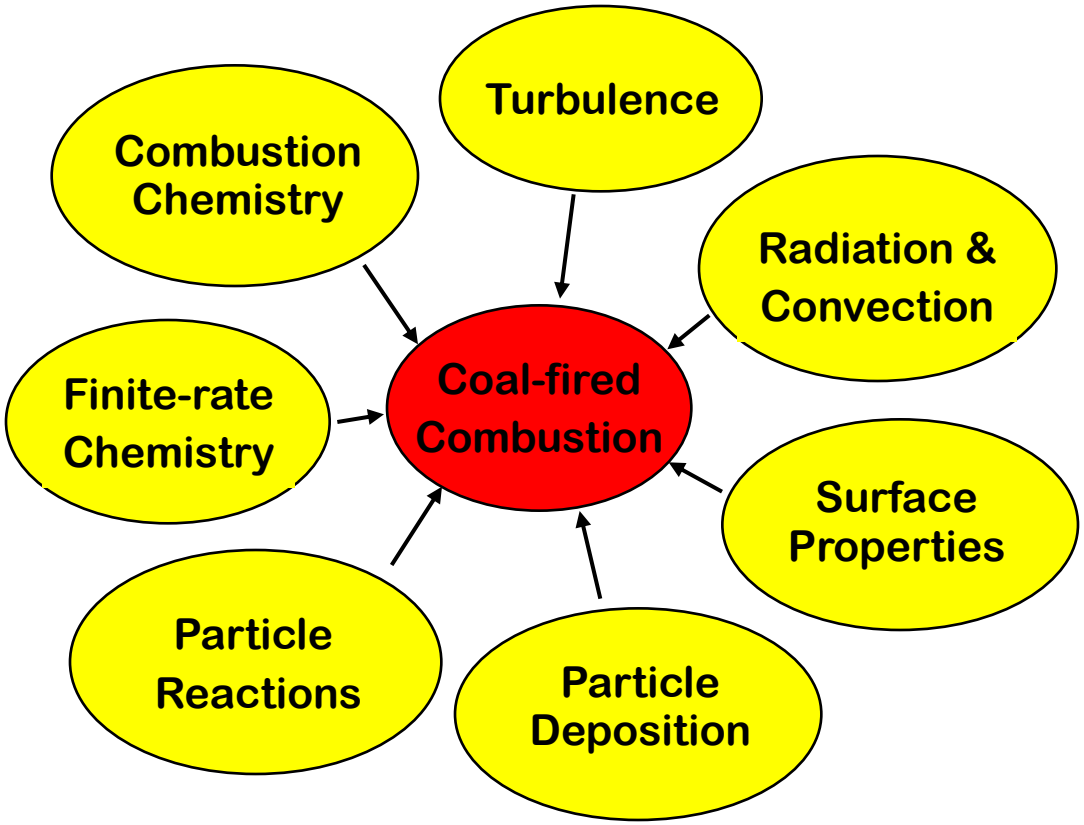


Glacier Software

- *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

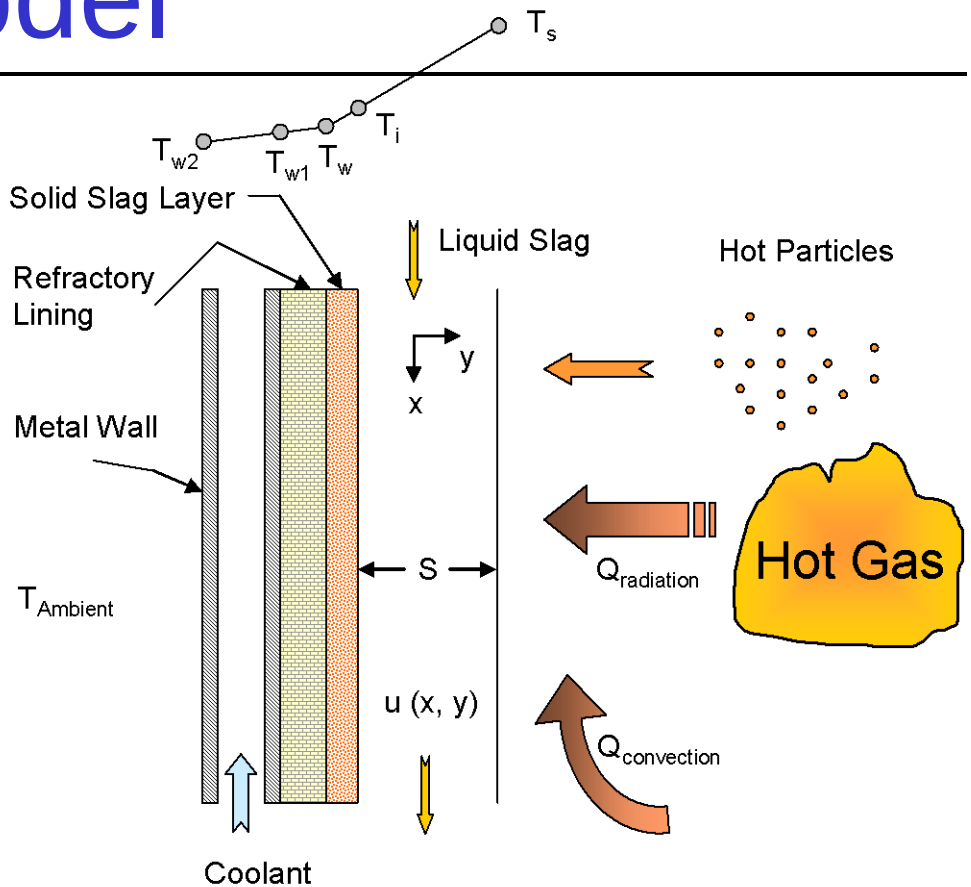
Modeling Coal Combustion

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



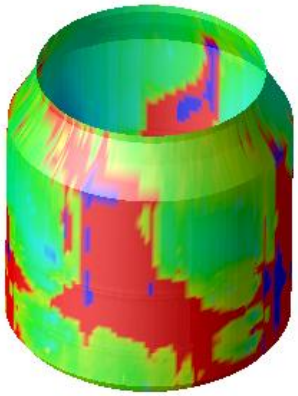
Flowing Slag Model

- 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

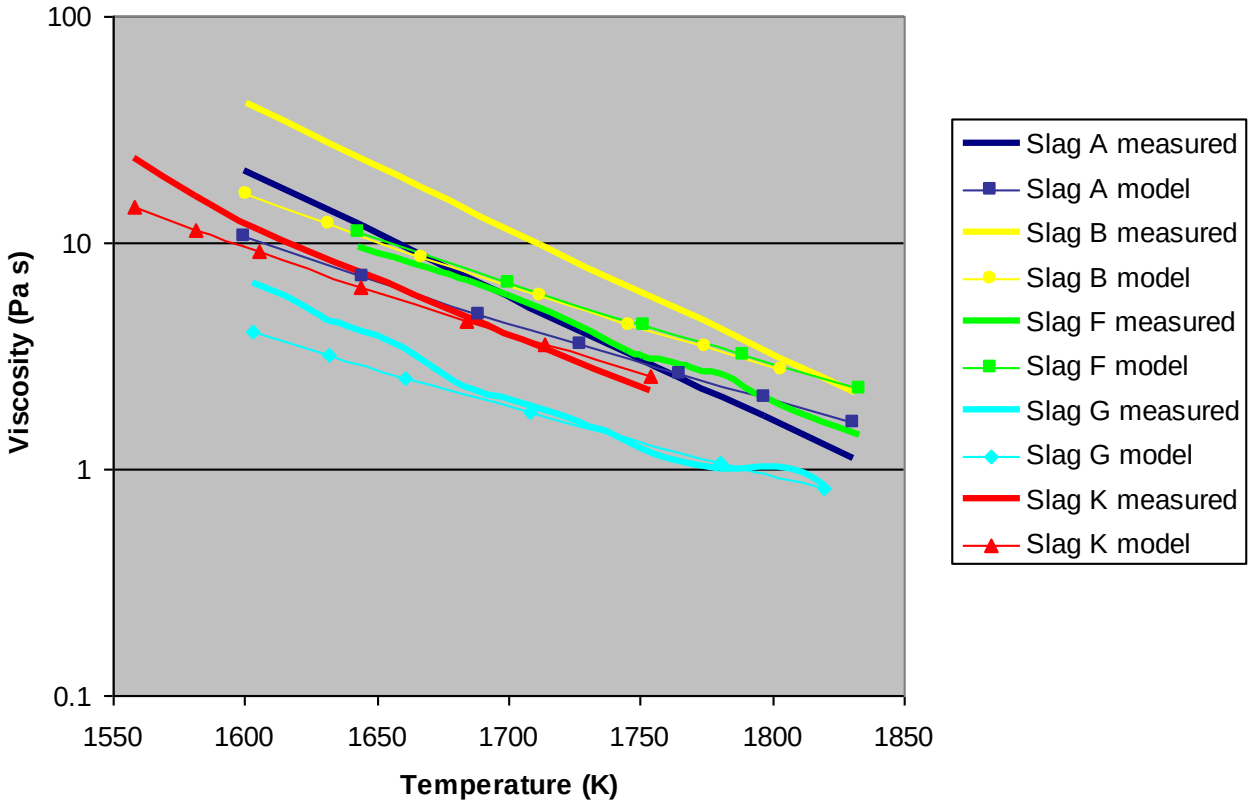
Gasifier Slag Viscosity Model

- *Derived for a range of coal ashes*
- *Curve fit as a function of SiO_2, TiO_2, Al_2O_3, Fe_2O_3, CaO, FeO, MgO, Na_2O, K_2O 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.

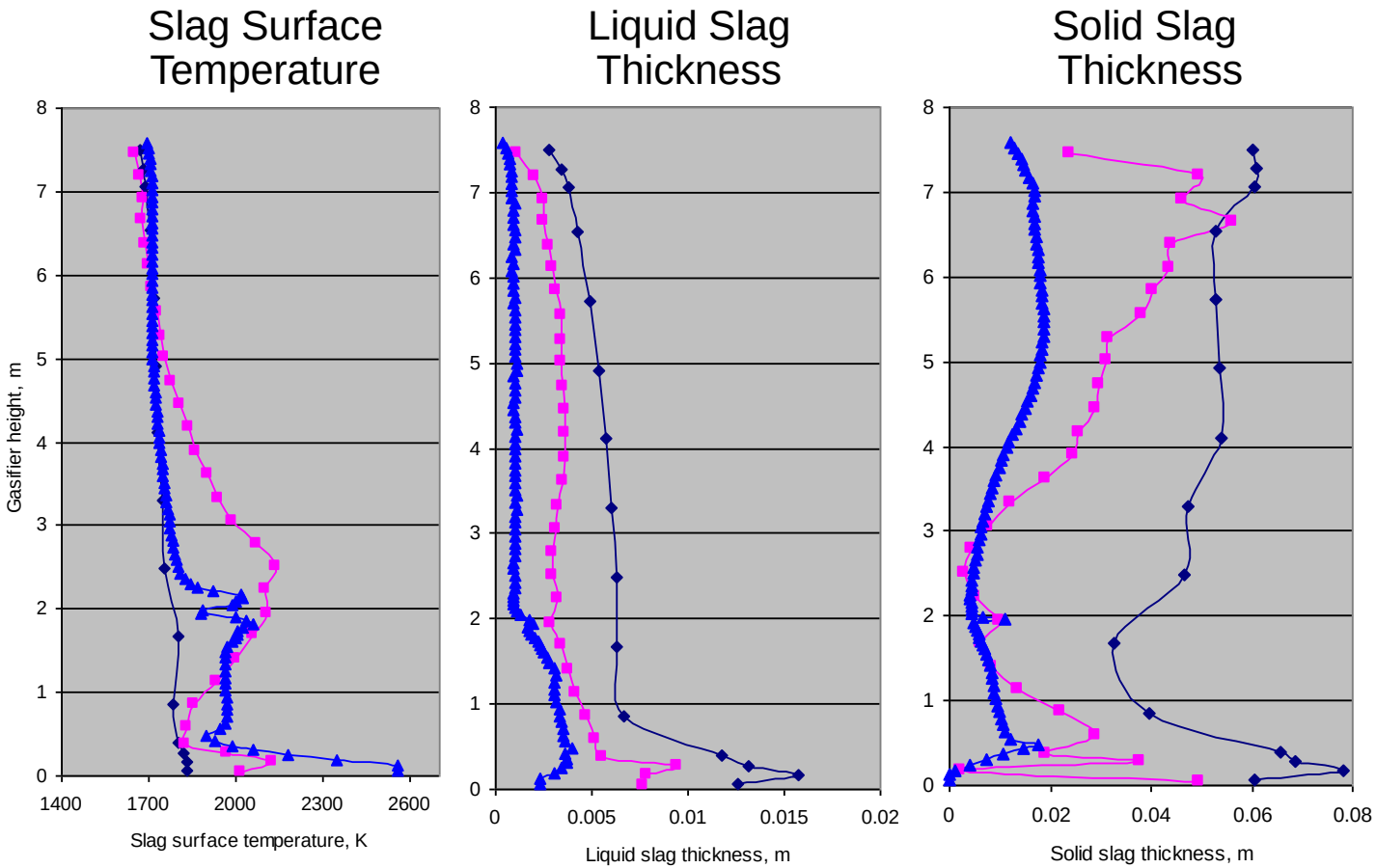
Urbain, G., Cambier, F., Deletter, M., and Anseau, M.R., Trans. J. Gr. Ceram. Soc., Vol. 80, p. 139, 1981.

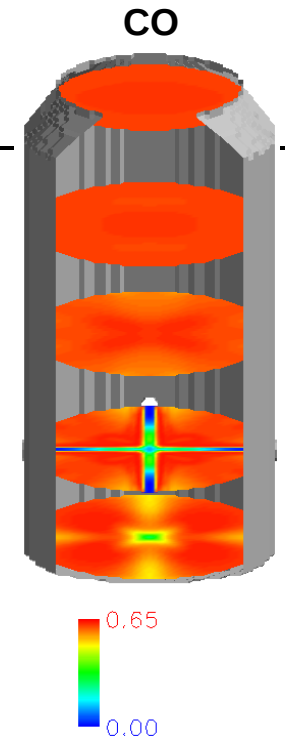
Viscosity Model

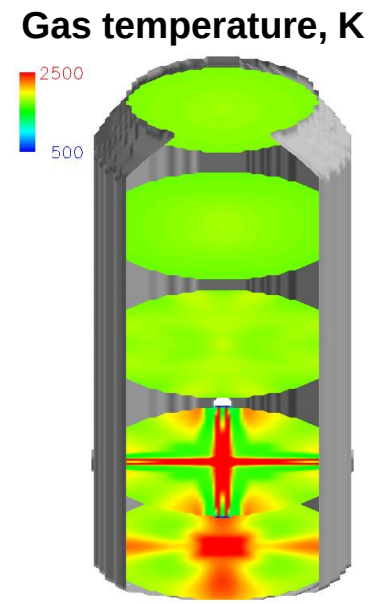


Gasifier slag data from Mills, K.C., and Rhine, J.M., "The measurement and estimation of the physical properties of slags formed during coal gasification 1. Properties relevant to fluid flow.," *Fuel* vol. 68, pp. 193-198, 1989.

Flowing Slag Model





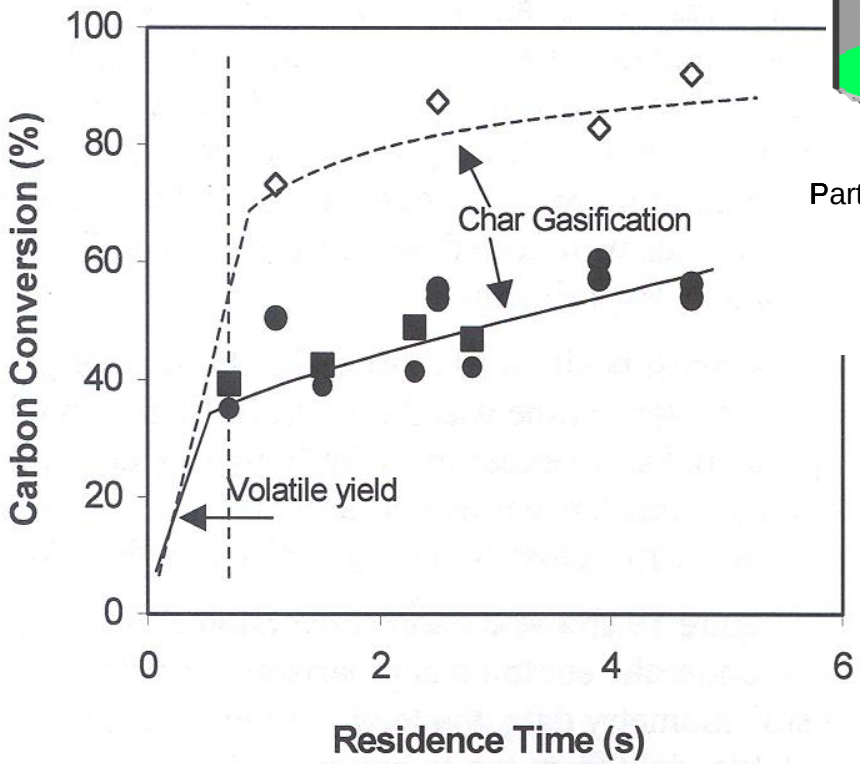


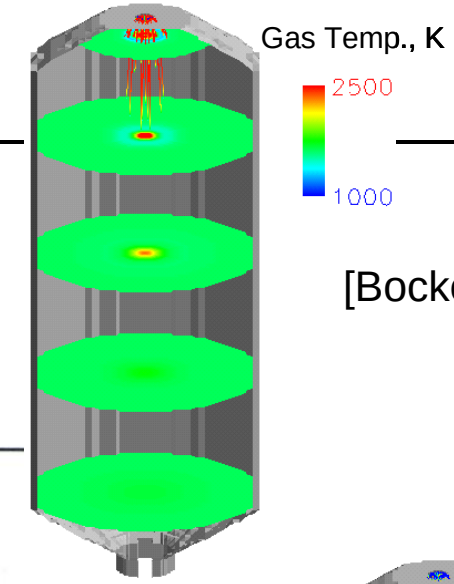
Test case:

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

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





[Bockelie et al, 2002]

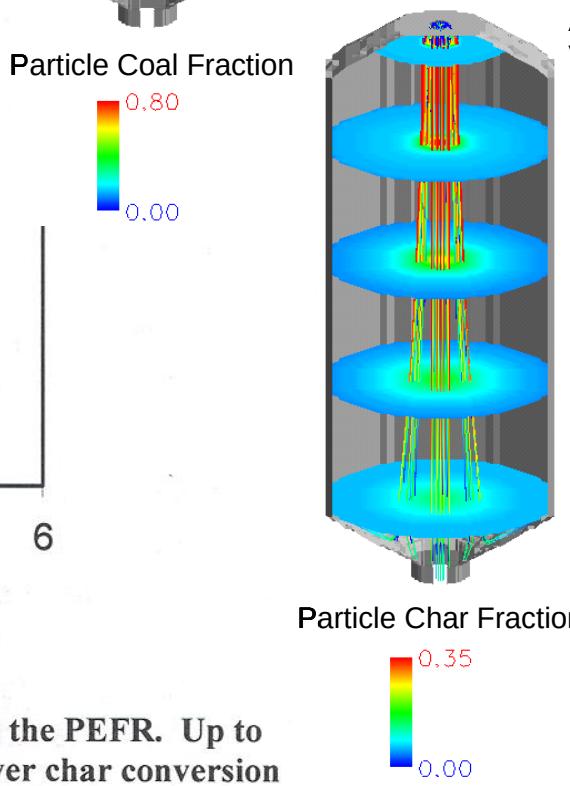
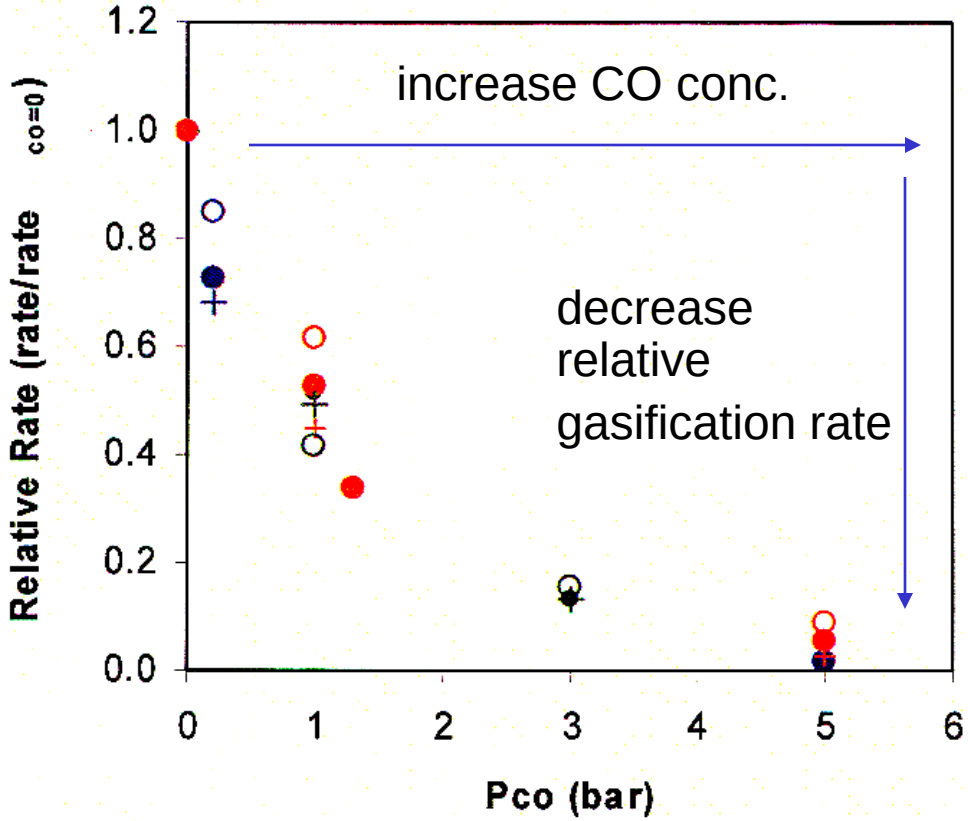


Figure 20: The stages of coal conversion highlighted using data generated in the PEFR. Up to approximately 0.5 s coal conversion is achieved by volatile release. The slower char conversion processes are then apparent at residence times above about 1 s.

Effect of CO Inhibition on Carbon Gasification Rate

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



CO reduces gasification rate

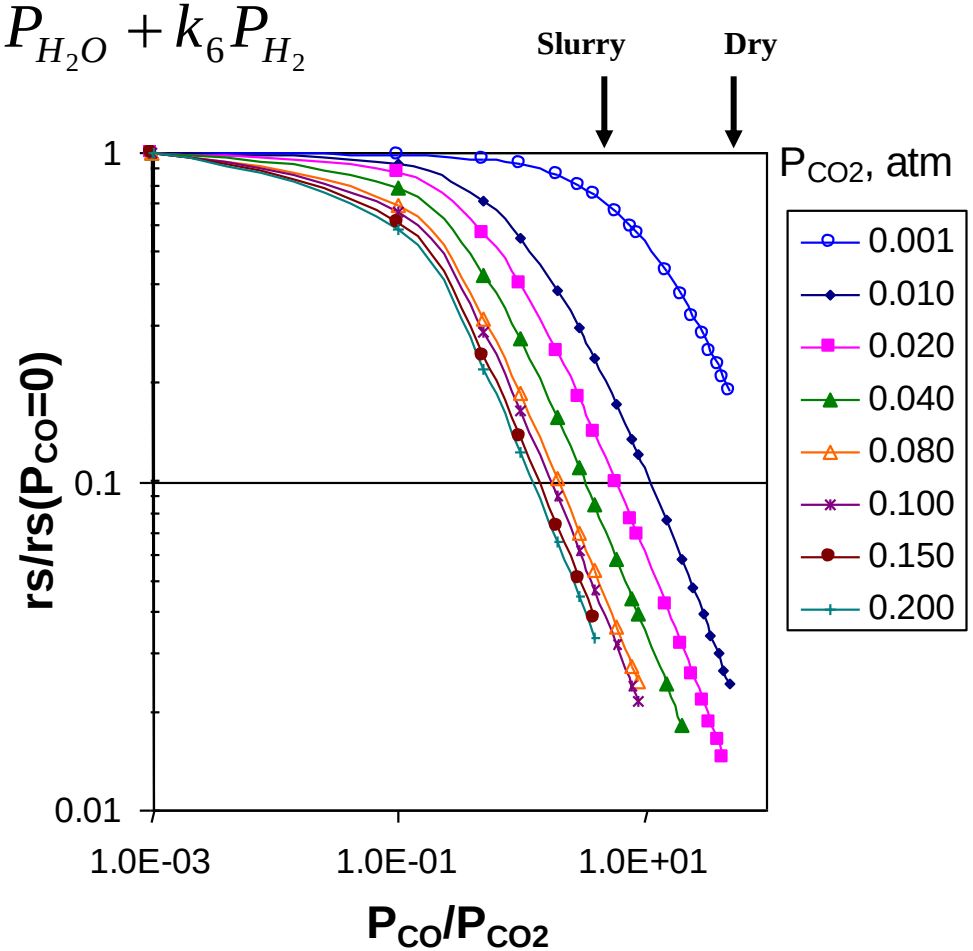
Figure 8: Relative rate data for all chars and CO_2 pressures combined. Blue data = 5 bar CO_2, green data = 10 bar CO_2, red data = 15 bar CO_2. • = CRC272, ○ = CRC252, and + = CRC281

Gasification Kinetics – with inhibition

- *CO, CO_2, H_2, H_2O*

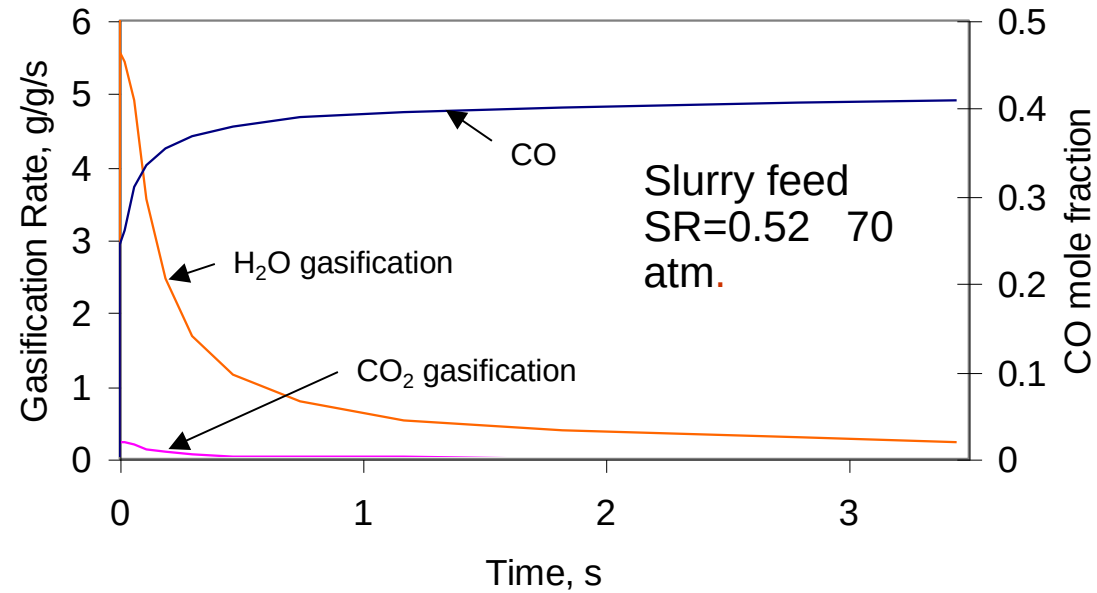
$$r_s(1/s) = \frac{k_1 P_{CO_2} + k_2 P_{H_2O}}{1 + k_3 P_{CO_2} + k_4 P_{CO} + k_5 P_{H_2O} + k_6 P_{H_2}}$$

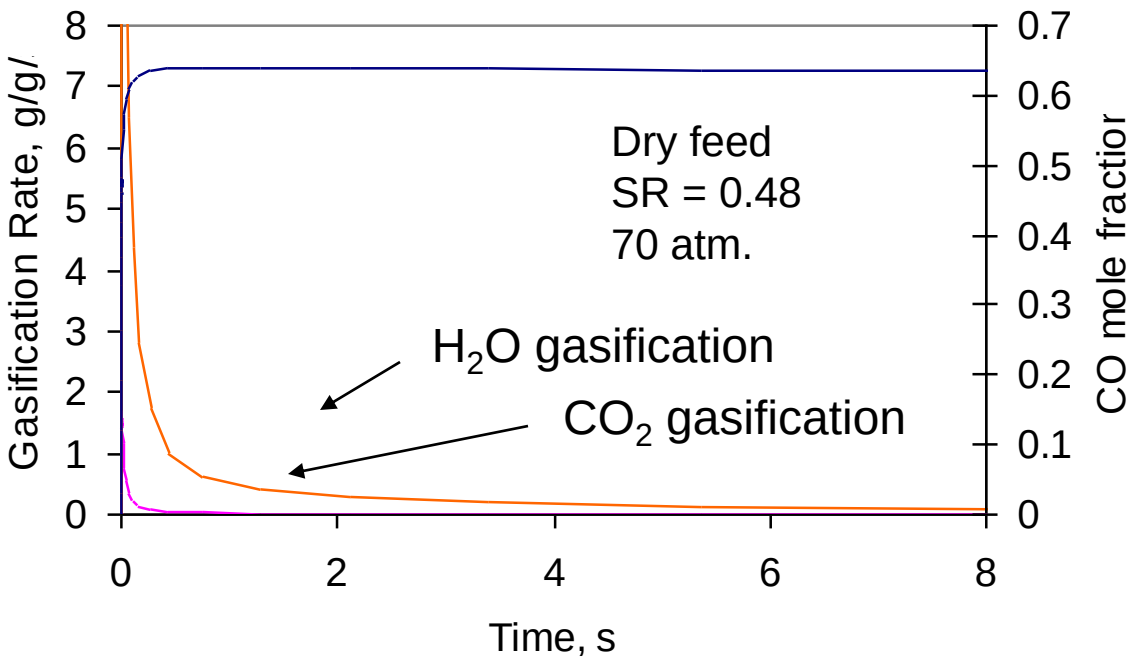
$$k_i = k_{i0} \cdot \exp\left(-\frac{E_i}{RT}\right)$$



[van Heek & Muhlen, 1991]

Gasification Kinetics – CO effects



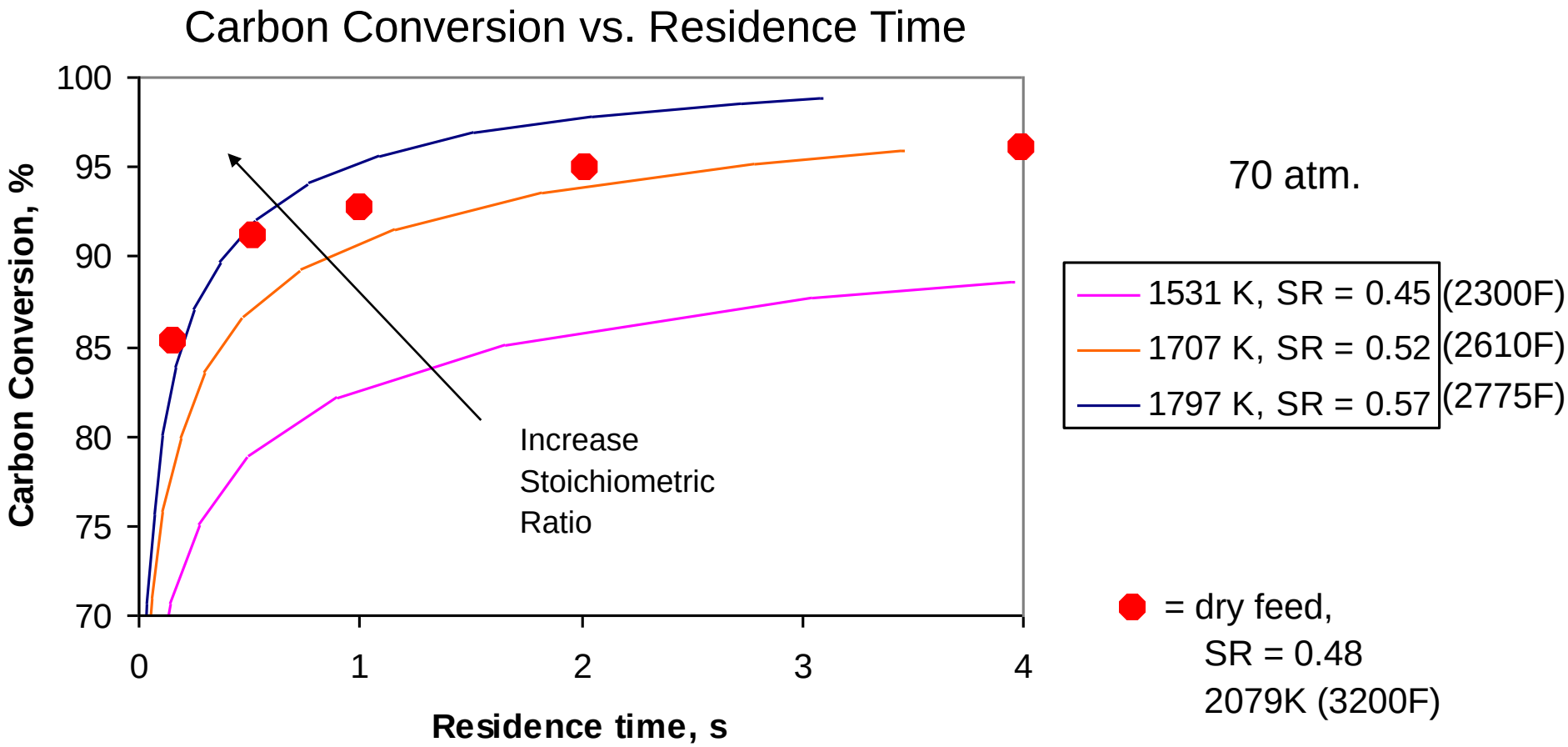


Presence of CO reduces gasification rate

Gasification rate for H2O is greater than for CO2

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

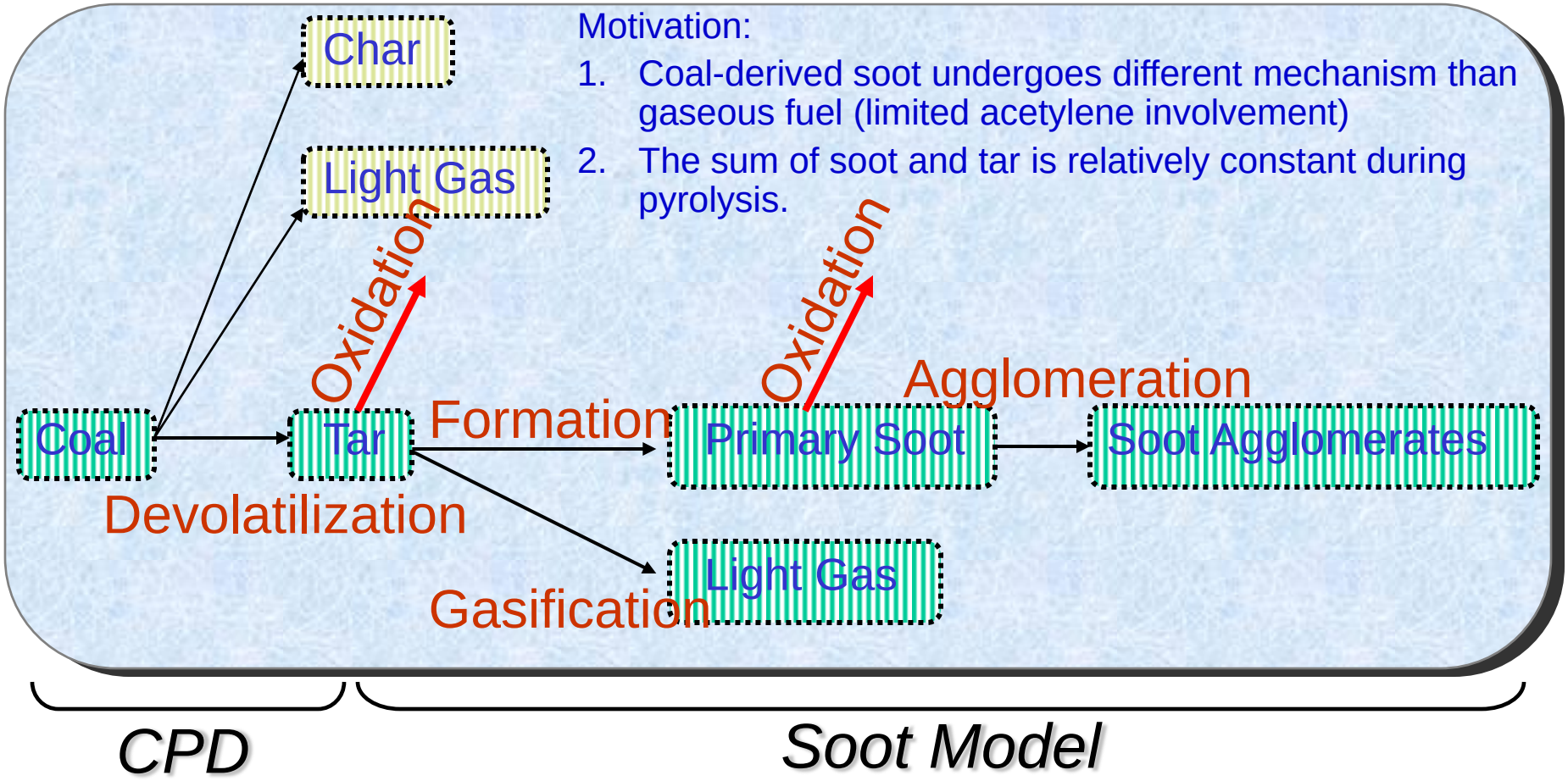
- Semiempirical model*
  - Coal-derived soot is assumed to form from only tar.
  - Tar yields is calculated by CPD model† based on measured coal characteristics.
  - Three equations for conservation of the mass of soot and tar, and the number of soot particles.

** 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

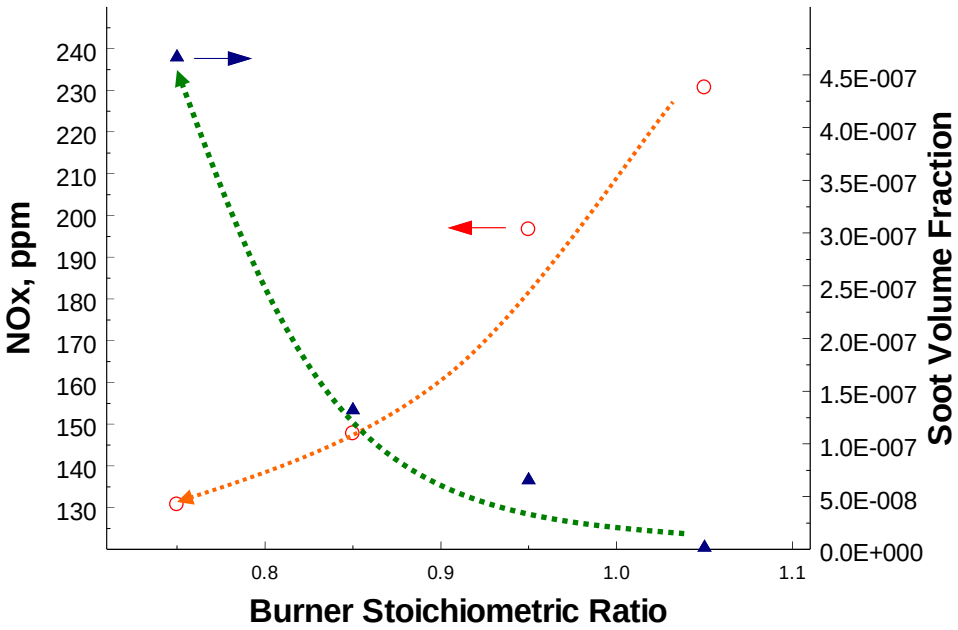
Brown, A.L.; Fletcher, T.H. Energy Fuels 1998, 12, 745-757.

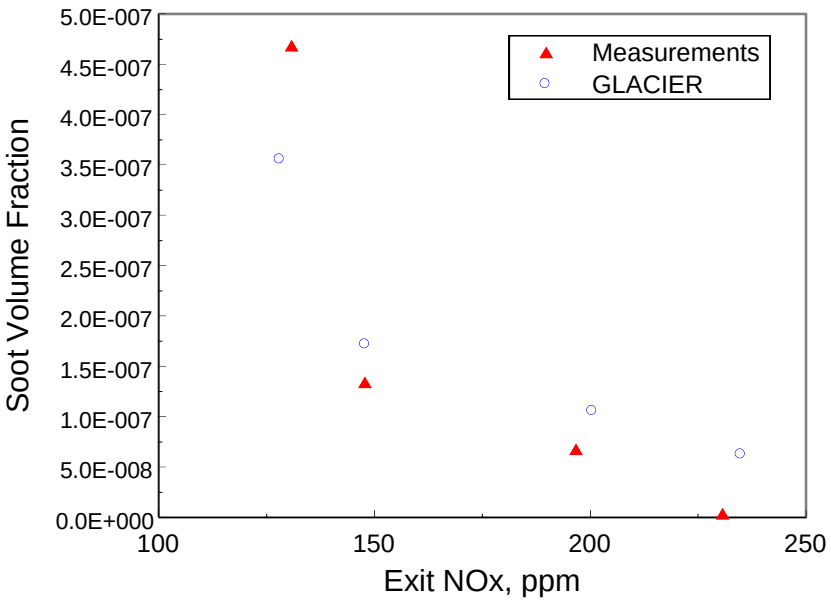


Motivation:

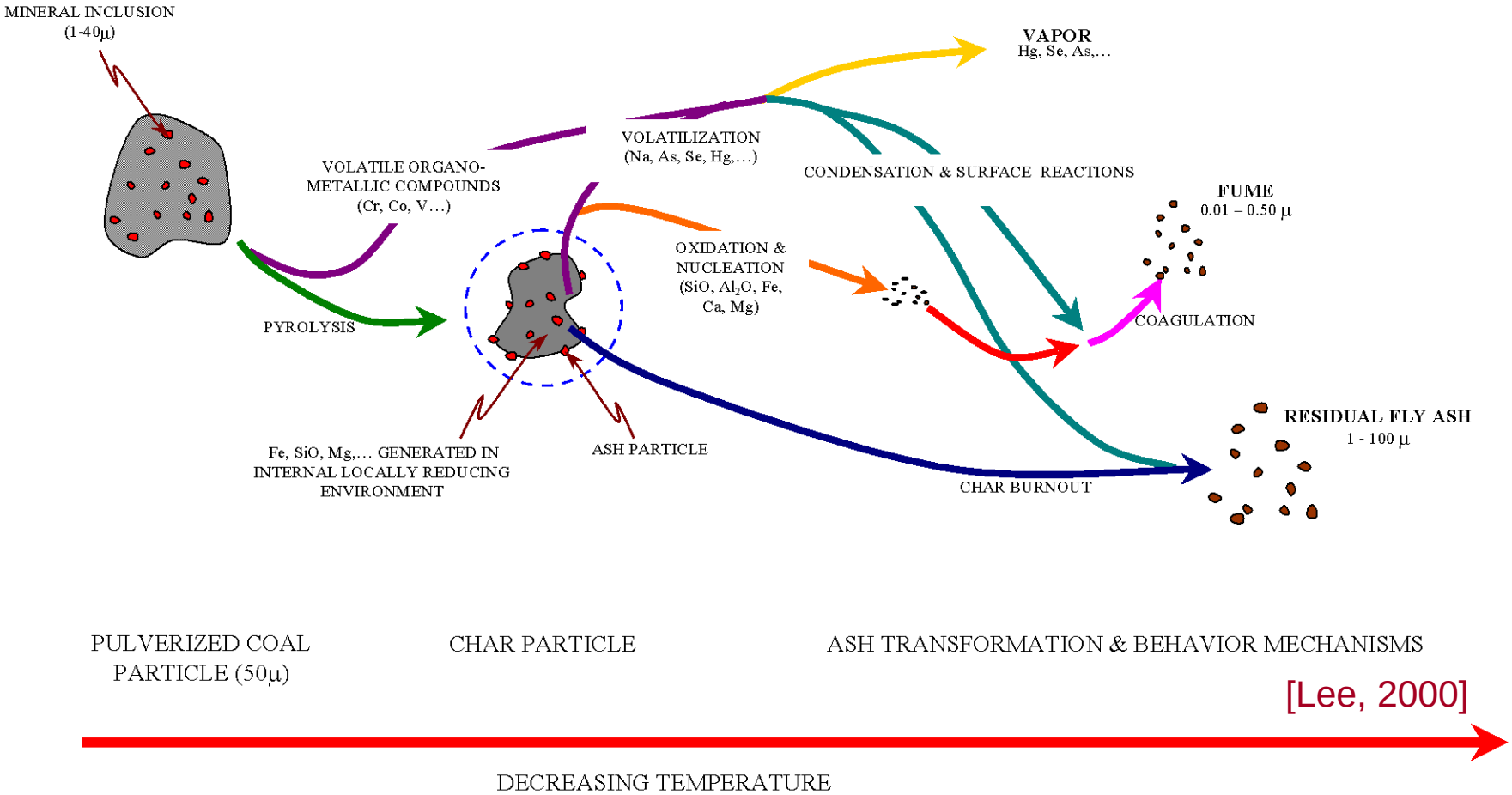
1. Coal-derived soot undergoes different mechanism than gaseous fuel (limited acetylene involvement)
2. The sum of soot and tar is relatively constant during pyrolysis.

Soot Model Evaluation





Mineral Matter Transformation Pathways



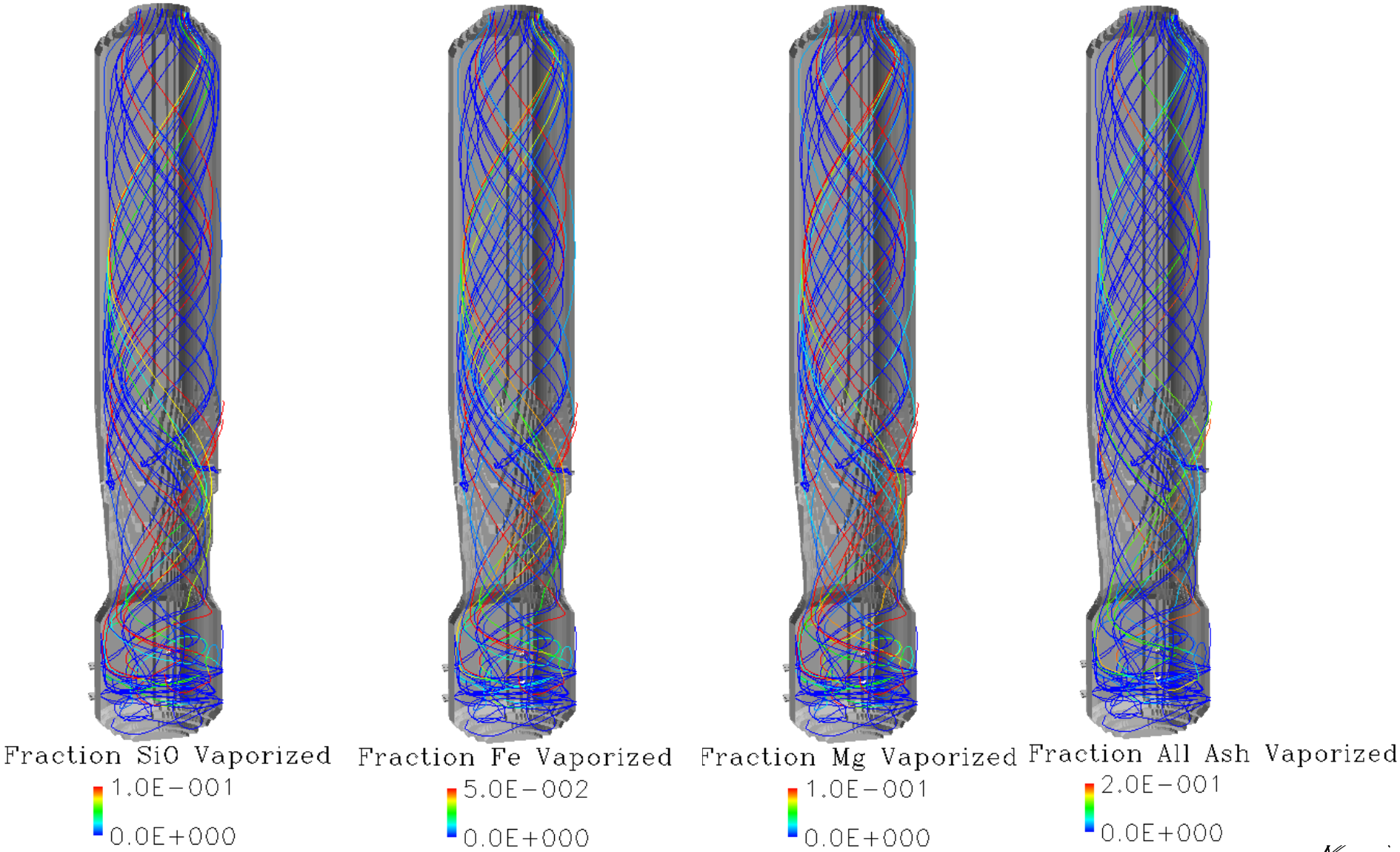
[Lee, 2000]

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)

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

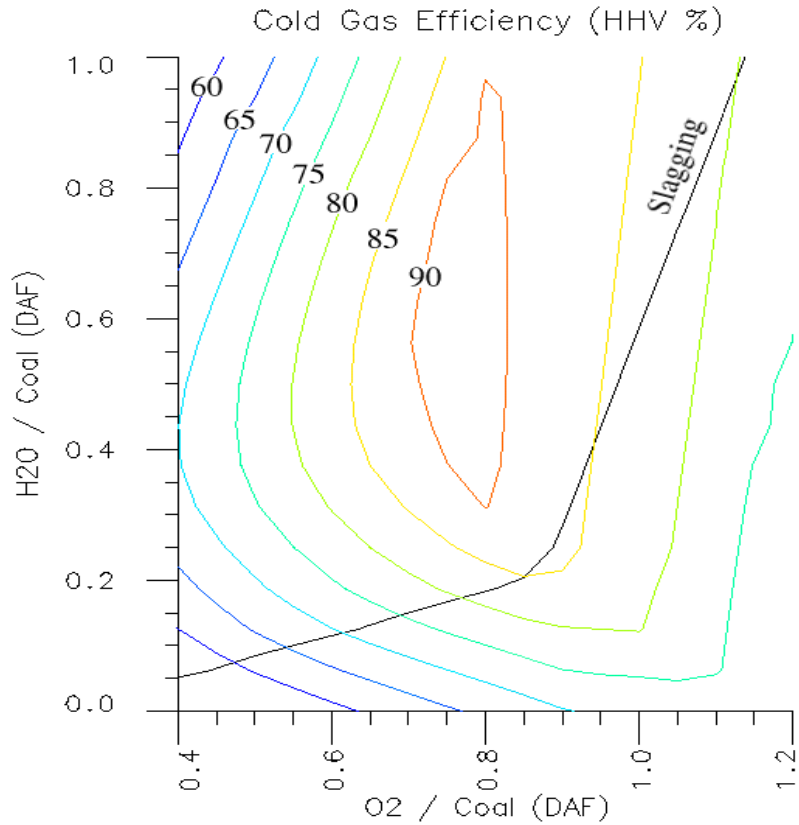
2 Stage Gasifier – Vaporization Along Representative Particle Trajectories

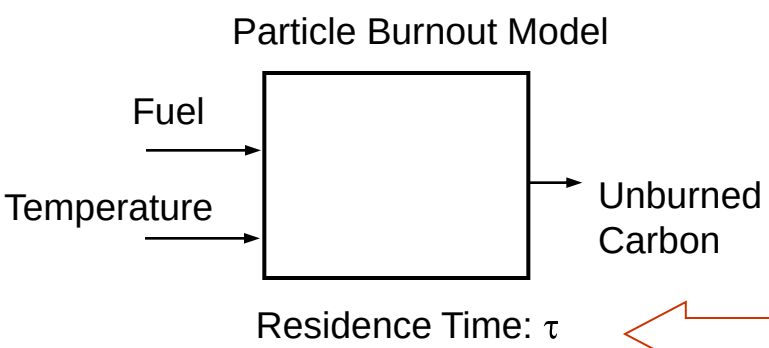
25 to 60 micron

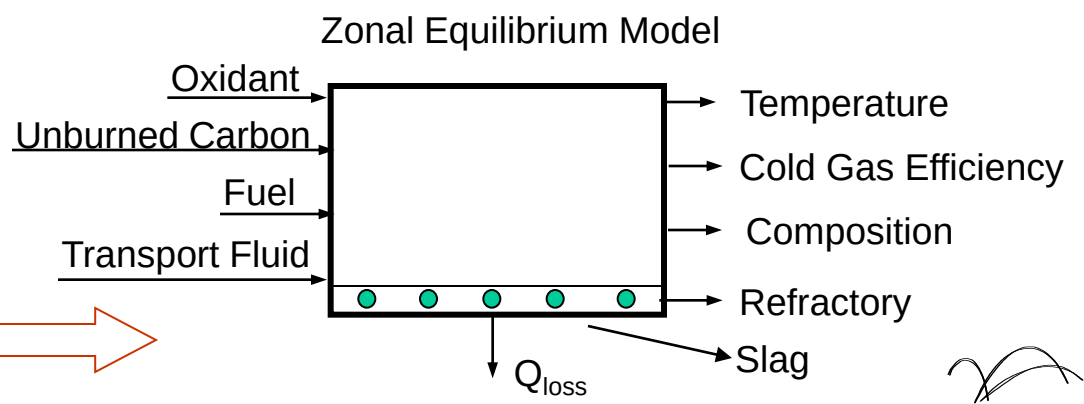


Gasifier – Flow Sheet / Process Model

- 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



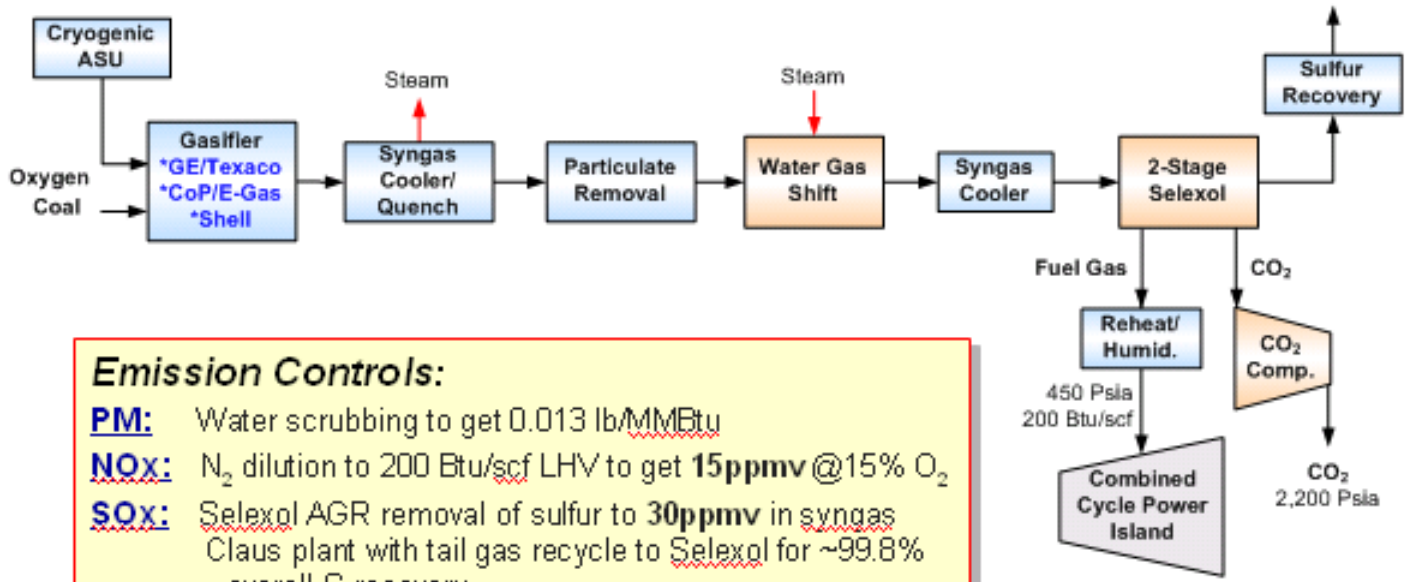




AspenPlus IGCC Flowsheet*

Pre-Combustion Current Technology

IGCC Power Plant with CO_2 Scrubbing



Emission Controls:

PM: Water scrubbing to get 0.013 lb/MMBtu

NOx: N_2 dilution to 200 Btu/scf LHV to get **15ppmv** @15% O_2

SOx: Selexol AGR removal of sulfur to **30ppmv** in syngas
Claus plant with tail gas recycle to Selexol for ~99.8% overall S recovery

Hg: Activated Carbon beds for ~90% removal

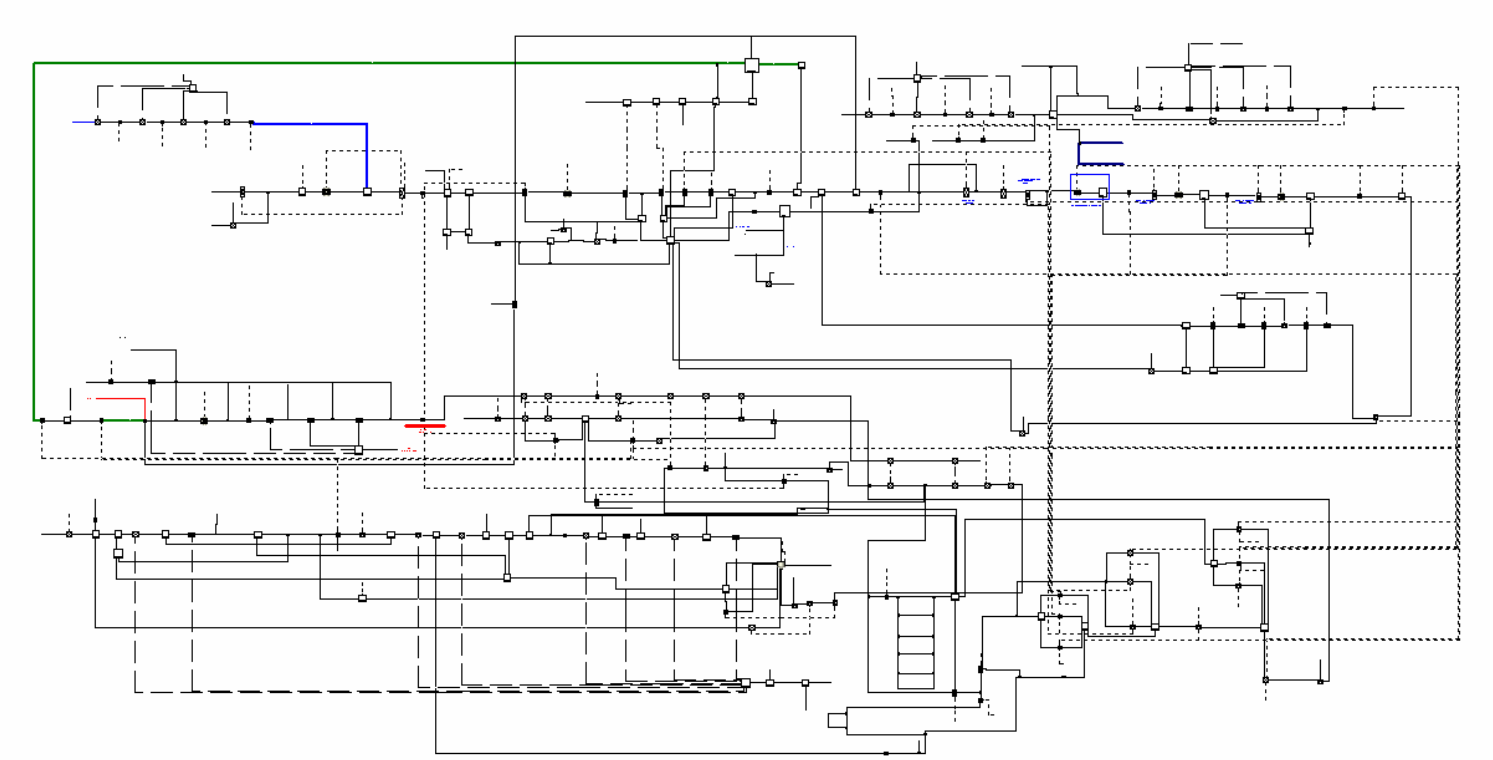
Advanced F-Class Turbine - 232MWe (42% LHV)

Steam Conditions - 1800psig/1050°F/1050°F

* Ciferno, J. and Klara, J., "2006 Cost & Performance Comparison of Fossil Energy Power Plants," Pittsburgh Coal Conf., 2006b
* Ciferno, J., "2006 Cost & Performance Comparison of Fossil Energy Power Plants," Clearwater Conf. 2006a

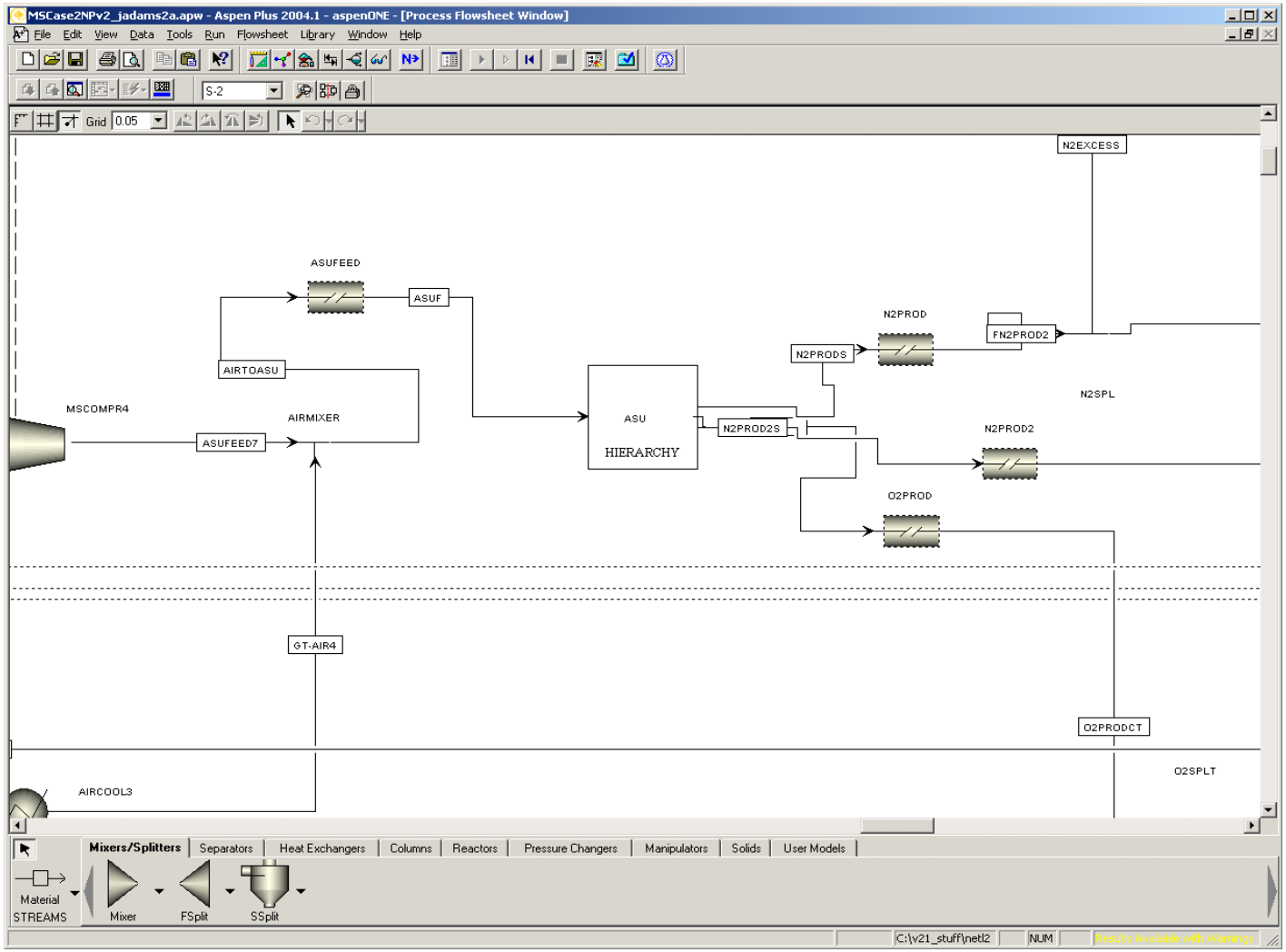
AspenPlus IGCC Flowsheet*

- Using NETL AspenPlus IGCC flowsheets [Ciferno et al., 2006]* (NP)
  - Cost and Performance evaluations with AspenPlus flowsheets for plant configurations with different gasifiers with and w/o CO2 capture
  - Extensive AspenPlus process simulations
    - Flowsheets use ~200 blocks and 500 streams
    - NP = non-proprietary information version of flowsheets



* Ciferno, J. and Klara, J., “2006 Cost & Performance Comparison of Fossil Energy Power Plants,” Pittsburgh Coal Conf., 2006b
* Ciferno, J., “2006 Cost & Performance Comparison of Fossil Energy Power Plants,” Clearwater Conf. 2006a

NETL IGCC Flowsheet with ASU



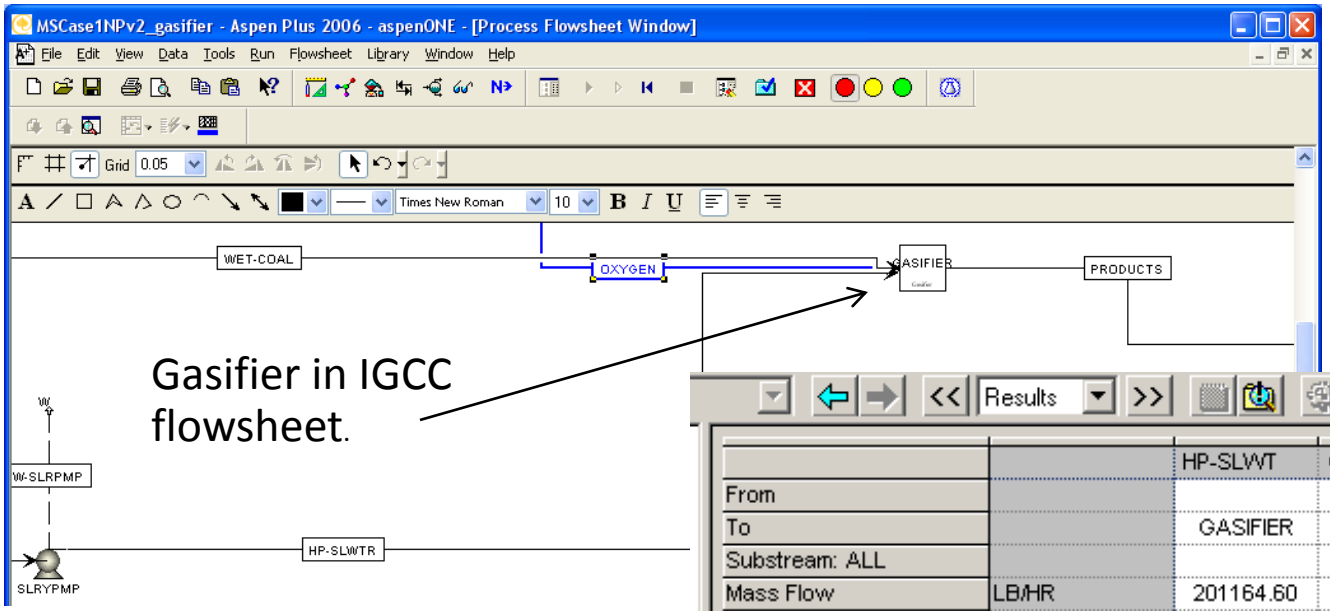
- Import as hierarchal library to replace single unit op ASU
- Must alter flowsheet convergence parameters / sequence

Simple vs. Detailed ASU

	Case 1		Case 2	
Gross Plant Power Output	**NETL**	**REI**	**NETL**	**REI**
Gas Turbine Gross Power	463,940	463,940	464020	464,020
Sweet Gas Expander Gross Power	8,340	8,340	8010	8,010
Steam Turbine Gross Power	300,470	300,510	266860	266,850
Total	**772,750**	**772,790**	**738890**	**738,880**
Auxiliary Load				
Coal Handling	630	630	650	650
Coal Milling	1,280	1,280	1320	1,320
Coal Slurry Pumps	420	420	440	440
Slag Handling and Dewatering	280	280	290	290
Air Separation Unit Auxiliaries	2,000	2,000	2000	2,000
ASU Main Air Compressor	59,610	59,080	72760	72,140
Oxygen Compressor	11,530	11,530	11030	11,030
Nitrogen Compressor	22,803	22,258	28373	28,373
Sulfur Removal	2,962	2,962	3057	3,057
Tail Gas Recycle Compressor	1,070	1,070	1030	1,030
Boiler Feedwater Pumps	4,880	4,890	4880	4,880
Condensate Pumps	250	250	260	260
Flash Bottoms Pump	200	200	200	200
Circulating Water Pump	3,290	3,290	2850	2,850
Cooling Tower Fans	1,650	1,650	1420	1,420
Gas Turbine Auxiliaries	2,105	2,106	2013	2,013
Steam Turbine Auxiliaries	1,053	1,053	1007	1,007
Claus Plant Auxiliaries	211	211	201	201
Miscellaneous Balance-of-Plant	3,158	3,158	3020	3,020
Transformer Losses	2,250	2,250	2160	2,160
Total	121,632	120,567	138960	138,341
Net Plant Performance				
Auxiliary Load	121,632	120,567	138960	138,341
Net Plant Power	651,118	652,223	599930	600,539
Net Plant Efficiency (HHV)	38.89%	38.96%	34.72	34.76
Net Plant Heat Rate (HHV)	8,774	8,759	9827	9,817
Coal Feed Flowrate	489,685	489,685	505381	505,381
Thermal Input[1]	1,674,216	1,674,216	1727883	1,727,882
Oxygen Flowrate	416,677	416,180	429948	429,948
Condenser Duty	1,480	1,480	1280	1,280

- Detailed ASU
  - not as robust as simple model
  - provides much more information about localized processes important for ASU operation
- But only minor differences in predicted overall plant performance

NETL IGCC Flowsheet with Gasifier Process Model



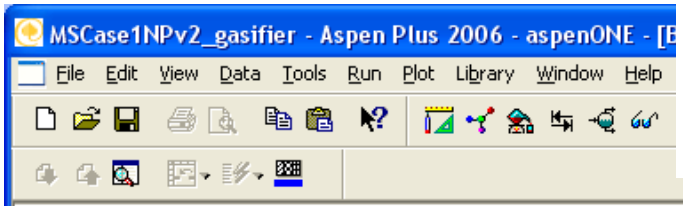
Gasifier in IGCC flowsheet.

Gasifier Oututs

Results

		HP-SLWT	OXYGEN	PRODUCT	WET-COA
From				GASIFIER	
To		GASIFIER	GASIFIER		GASIFIER
Substream: ALL					
Mass Flow	LB/HR	201164.60	409899.70	1131147.00	520107.00
Mass Enthalpy	BTU/HR	-1373701000.	11619940.00	-1865675000.	-524727700.0
Substream: MIXED					
Phase:		Liquid	Vapor	Vapor	Missing
Component Mole Flow					
H2O	LBMOL/HR	11166.33	0.00	8412.37	0.00
AR	LBMOL/HR	0.00	407.59	407.58	0.00
CO2	LBMOL/HR	0.00	0.00	5086.27	0.00
O2	LBMOL/HR	0.00	12100.29	0.00	0.00
N2	LBMOL/HR	0.00	229.27	513.61	0.00
O2S	LBMOL/HR	0.00	0.00	0.00	0.00

Gasifier Inputs



GASIFIER

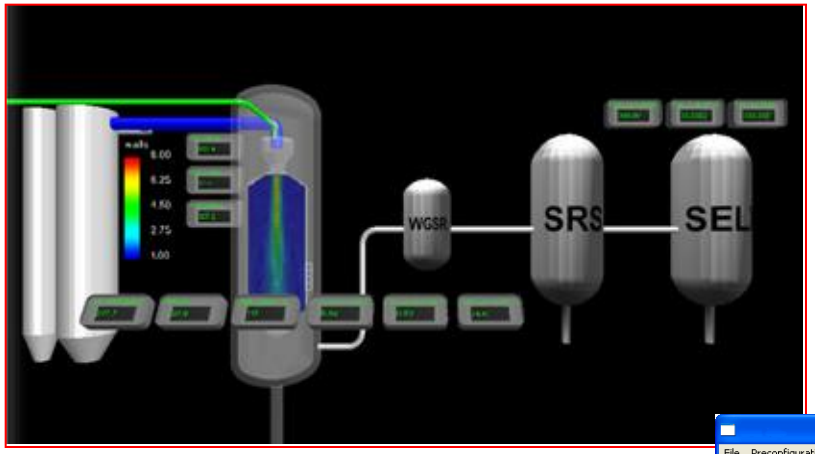
- GASHEAT2
- GASIFIER
  - Ports
  - Parameters
  - Block Options
  - Stream Results

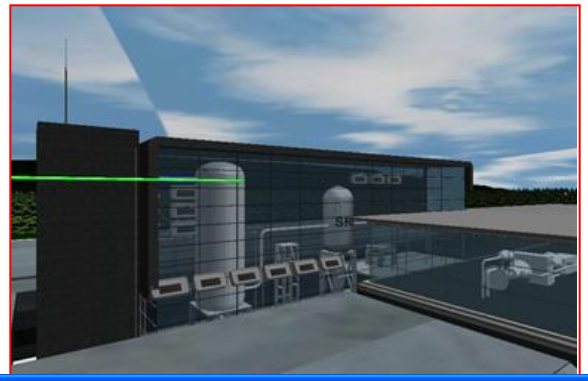
All

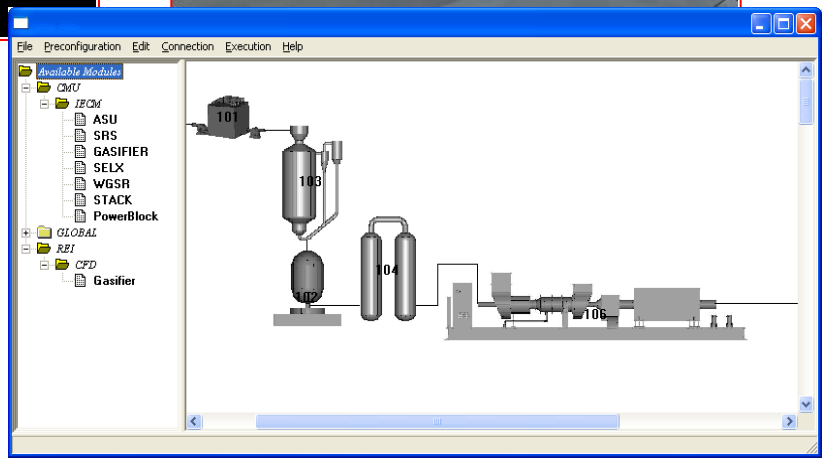
Name	Value	Units	Read Only	Description	Base Type
PresDrop	0		READ-WRITE	Pressure Drop, Pa	DOUBLE
SizeThru50	90		READ-WRITE	Size Thru 50, %	DOUBLE
SizeThru200	80		READ-WRITE	Size Thru 200, %	DOUBLE

A Framework for Virtual Simulation of Advanced Power Systems

A CMU, ISU, REI coordinated effort







Key Features

- Virtual engineering based
- Hierarchy of Models
- View and Interrogate at Multiple Levels
- Platform Independent
- Open Source, Extensible, Flexible
- Supports CO_2 capture and FutureGen

Carnegie Mellon

Iowa State University

REACTION ENGINEERING INTERNATIONAL

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