APECS Design and Optimization at Alstom Power

NETL 2009 Workshop on Advanced Process Engineering Co-Simulation (APECS)

David Sloan

Pittsburgh, PA, 20-21 Oct 2009

POWER | ALSTOM

Agenda

Topic 1 BSF Emissions Co-Simulation Subtask

Topic 2 Geometric Scaling Co-Simulation Subtask

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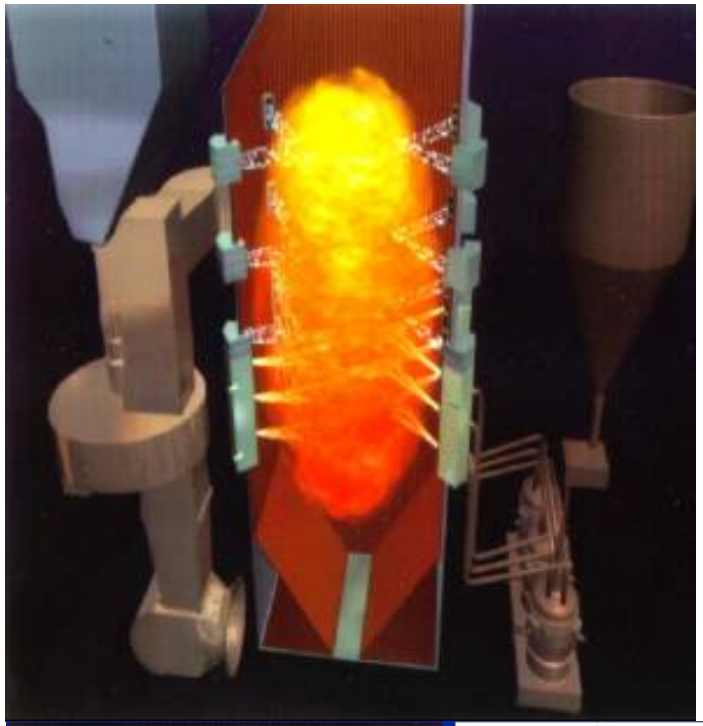
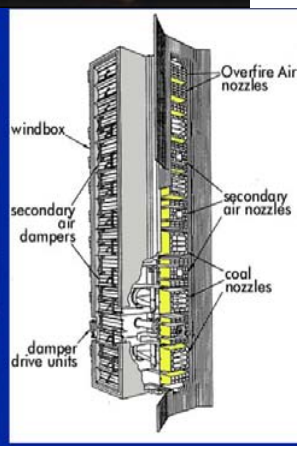
Oxy-Fired Boiler in Co-Simulation
Work Scope

- Conduct an APECS study of the Alstom Boiler Simulation Facility (BSF) island (gas side only) with oxygen firing and flue gas recycling.
- Modify the APECS software to expose the pollutant species to Aspen Plus [ANSYS task] and invoke the special NOx and SOx prediction capabilities in FLUENT.
- Characterize the impact of flue-gas recycle and cleanup on pollutant emissions for a candidate boiler configuration.





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Alstom Boiler Simulation Facility (BSF)
Present Oxy T-Fired Development

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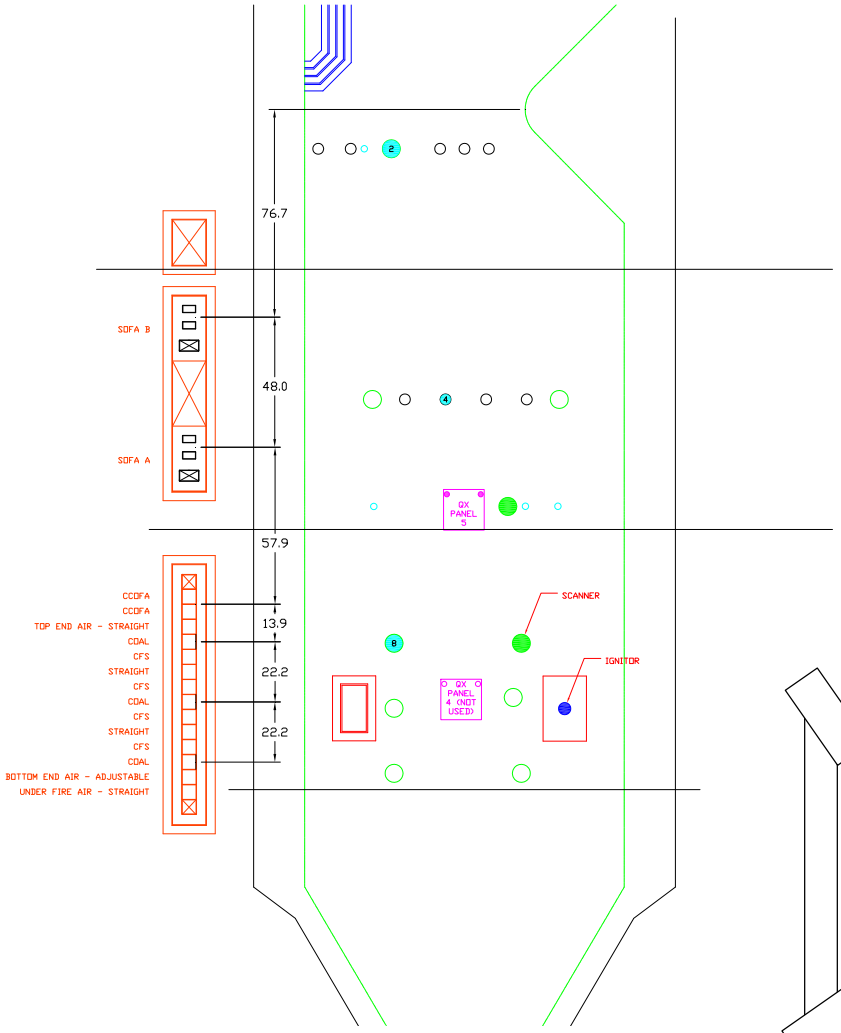
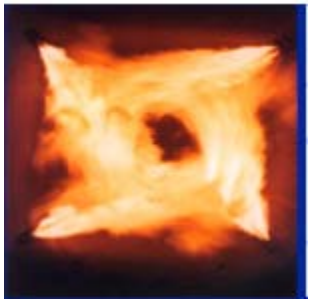
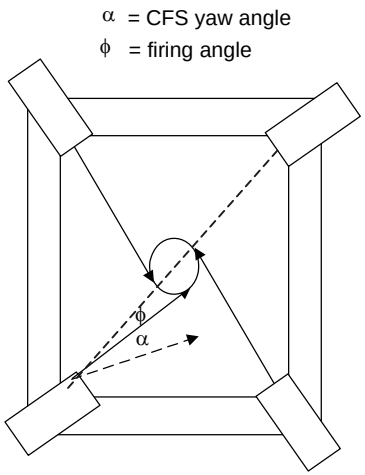
15 MWt BSF Firing System







Windbox

- CCOFA
- CCOFA
- CCOFA
- Top
- Coal
- CFS
- Straight
- CFS
- Coal
- CFS
- Straight
- CFS
- Coal
- Under Firing
- Bottom
- Bottom

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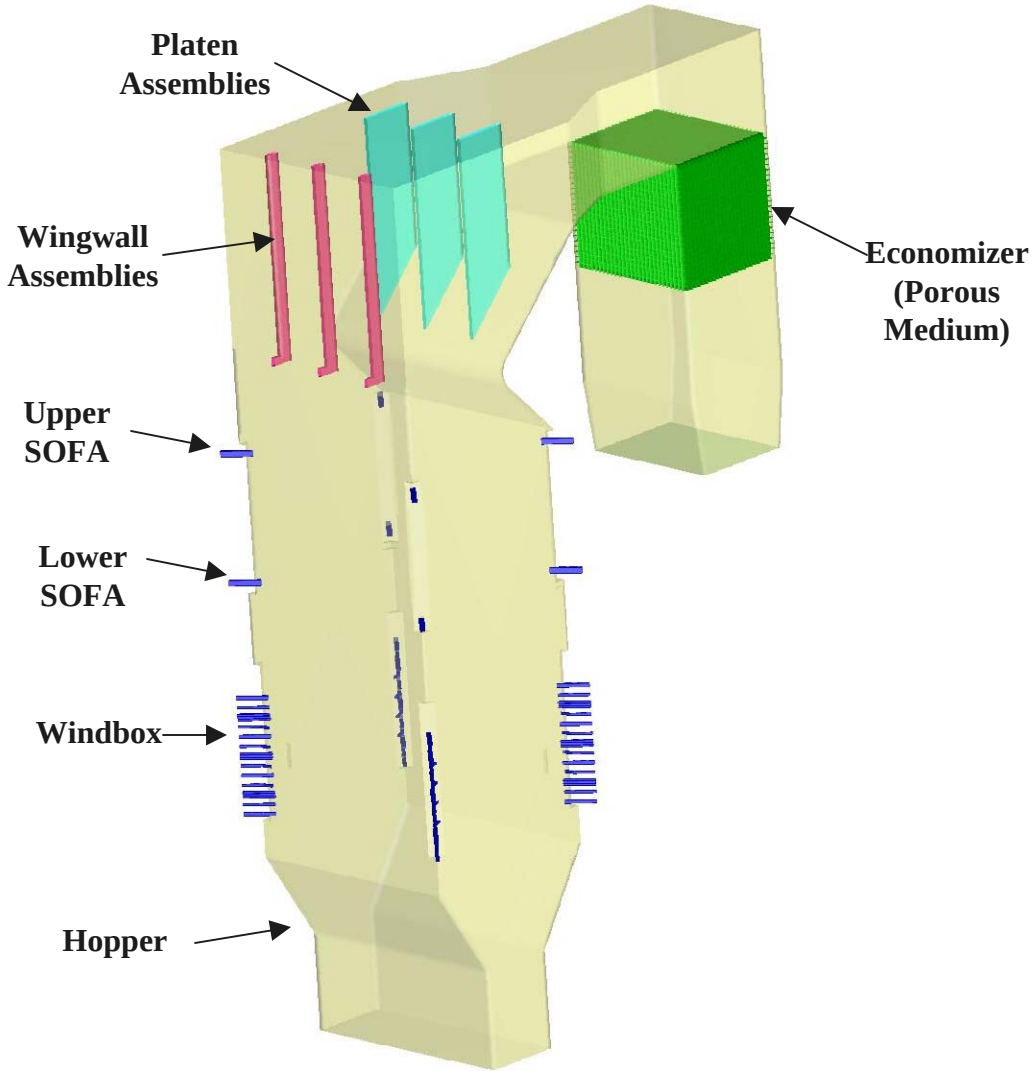
Computational BSF Configuration

- Co-simulation work scope pre-dated latest oxy-fired development
- 1994 BSF configuration
- High-volatile-B (HvB) bituminous coal (Lynnville).
- 3 coal elevations
- A TFS-2000 windbox configuration
  - 2 elevations of SOFA,
  - CFS tips set at 10º from the main firing angle.



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Reaction Calculation Approach

- Main combustion:
  - 3 steps, irreversible, global reactions
  - Magnussen eddy-breakup type model.
  - 9 species (coal volatile, O_2, CO, CO_2, H_2O, H_2S, H_2, SO_2, N_2).
- SOx model:
  - Current FLUENT (post-processing) SOx model is not operational.
  - 10-step (reversible) mechanism (no absorption/catalysis) ← from ANSYS
  - 5 species (H_2S, SO_2, SO, SH, SO_3).
  - Laminar chemistry option with ISAT tables.
  - Radical (H, O, OH) concentrations from main species through UDF.
- NOx model:
  - post-processing mode
  - thermal, prompt, fuel, reburn options
  - 2 species (pollutant NO, pollutant HCN).

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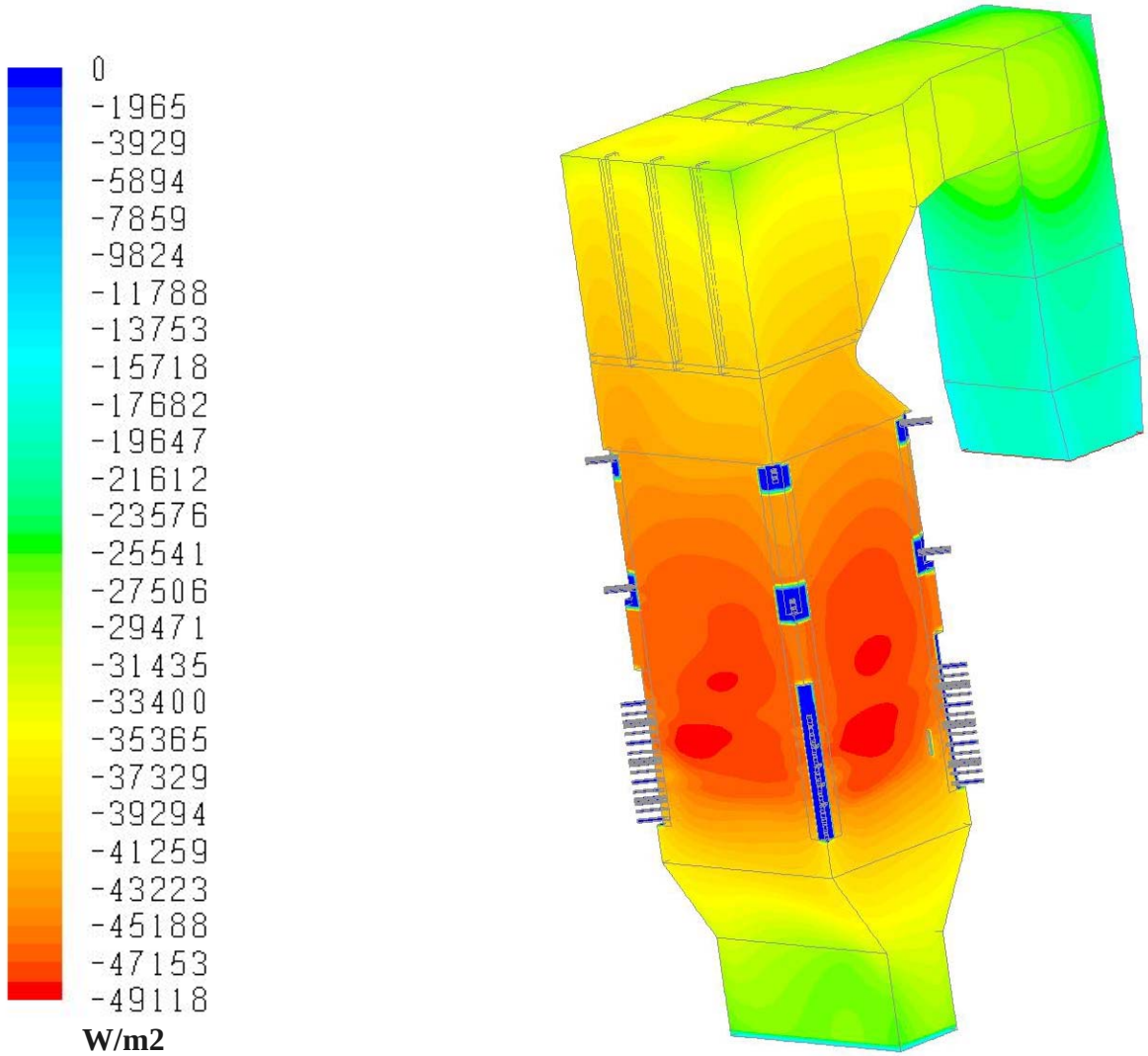
Calculation Example
Total Surface Heat Flux



Total Surface Heat Flux

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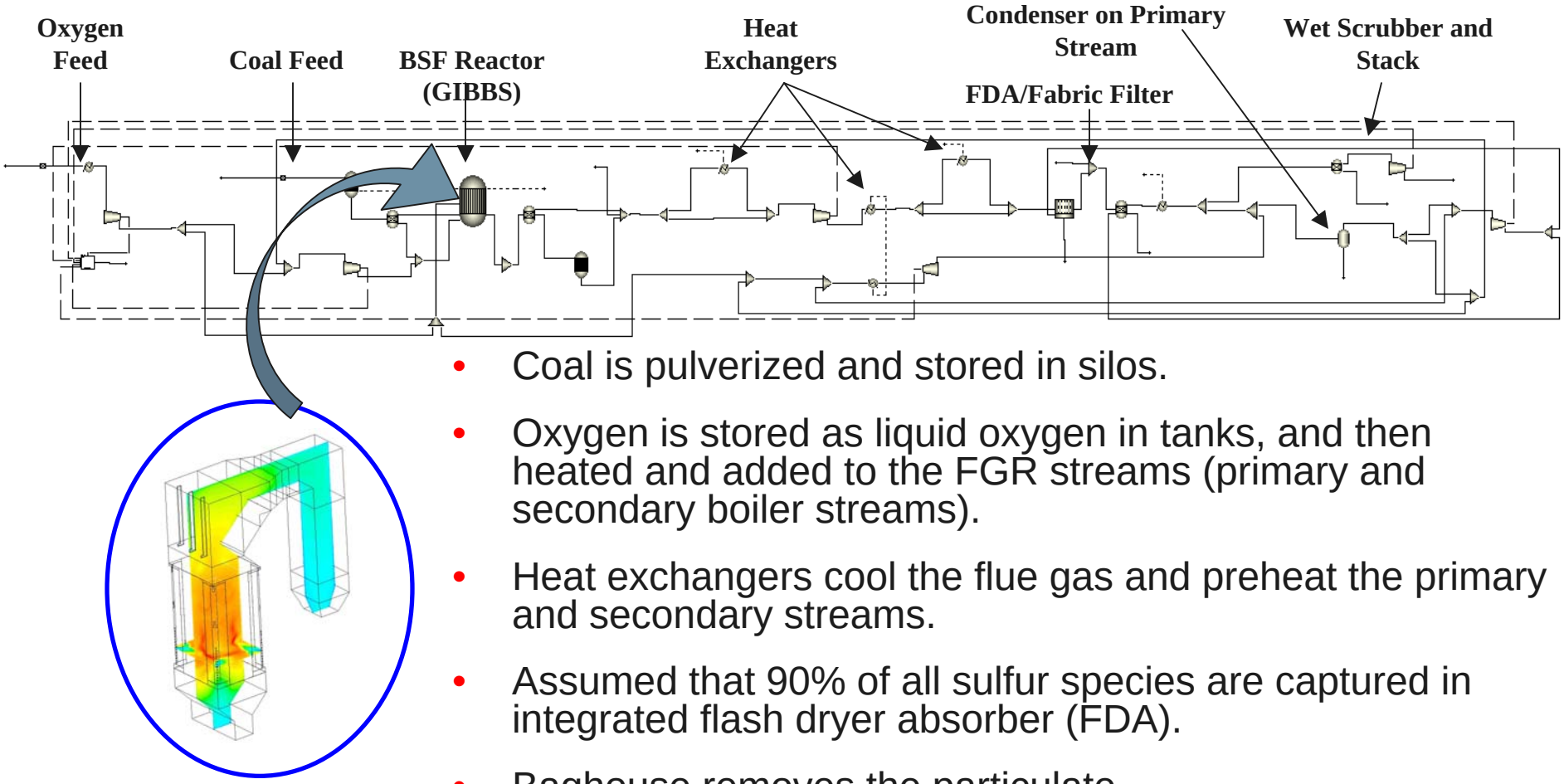
Process Model Description



- Coal is pulverized and stored in silos.
- Oxygen is stored as liquid oxygen in tanks, and then heated and added to the FGR streams (primary and secondary boiler streams).
- Heat exchangers cool the flue gas and preheat the primary and secondary streams.
- Assumed that 90% of all sulfur species are captured in integrated flash dryer absorber (FDA).
- Baghouse removes the particulate.
- A condenser removes much of the moisture from the primary gas feed stream.

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Process Model
Design Specs

Aspen Plus Design Spec	Description
DS-O2PRI	The O2 injected into the primary is varied until the desired O2 mole fraction is achieved.
DS-O2TOT	The total O2 entering the boiler is varied until the desired O2/coal mass ratio is achieved.
DS-RATIO	The volumetric recycle ratio is varied until a target total boiler absorption is achieved.
DS-TPRIM	The flow rate of a primary tempering bypass gas is varied until the desired temperature of the primary stream is achieved (e.g., 140° F).
DS-TRANS	The primary flow rate is varied until the desired transport gas/coal mass ratio is achieved.

RR = volumetric recycle ratio

$$RR = \left[\frac{\textit{total molar flow rate of recycle streams (prior to } O_2 \textit{ addition)}}{\textit{total molar flow rate of } O_2 \textit{ entering boiler}} \right]$$

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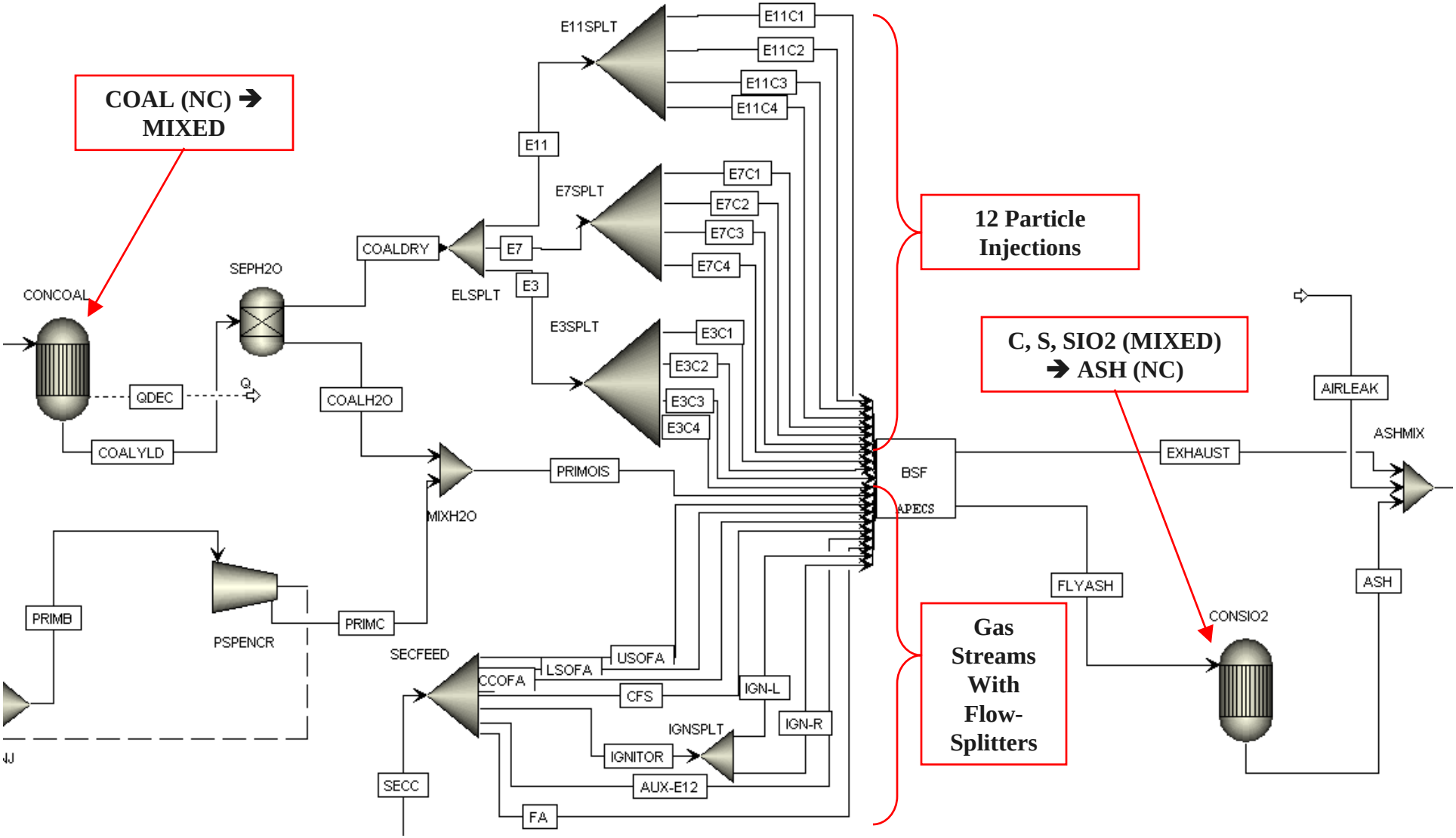
Process Model
Modifications for FLUENT Block



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Process Model
Inlet Flow-Splitter Specifications

- With flow-splitter options, 74 inlet gas streams reduced to 13 material streams.
- 12 DPM injection streams still required. (Can the flow-splitter capability be extended to DPM streams?)

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Reaction Expressions

ALSTOM

Reaction Number	Reaction	Reaction Number	Reaction
(1) - forward	h2s + h → sh + h2	(2) - reverse	sh + h2 → h2s + h
(3) - forward	oh + h2s → h2o + sh	(4) - reverse	h2o + sh → oh + h2s
(5) - forward	so + oh → h + so2	(6) - reverse	h + so2 → so + oh
(7) - forward	sh + o → so + h	(8) - reverse	so + h → sh + o
(9) - forward	o + h2s → sh + oh	(10) - reverse	sh + oh → o + h2s
(11) - forward	so + o2 → so2 + o	(12) - reverse	so2 + o → so + o2
(13) - forward	h + sh + m → h2s + m	(14) - reverse	h2s + m → h + sh + m
(15) - forward	so + o + m → so2 + m	(16) - reverse	so2 + m → so + o + m
(17) - forward	so2 + o + m → so3 + m	(18) - reverse	so3 + m → so2 + o + m
(19) - forward	so3 + o → so2 + o2	[19 - reverse]	[not explicitly prescribed; backward rate option activated]
(20)	vol + (0.974) o2 → (0.253) co + (0.886) h2o + (0.024) h2s + (0.023) n2		
(21)	co + (0.5) o2 + (0) h2o → co2		
(22)	h2 + (0.5) o2 → h2o		
(23)	csolid + (0.5) o2 → co		
(24)	csolid + co2 → (2) co		
(25)	csolid + h2o → h2 + co		
(26)	ssolid + o2 → so2		

Main Combustion Reactions

Particle Reactions

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Species Mapping

	Species in the Materials Listing in FLUENT	FLUENT Species Exposed to the PME	Flow Sheet Species
(1)	vol	vol	CH4
(2)	o2	o2	O2
(3)	co2	co2	CO2
(4)	co	co	CO
(5)	h2o	h2o	H2O
(6)	so2	so2	SO2
(7)	h2	h2	H2
(8)	h2s	h2s	H2S
(9)	cs2	cs2	CARBON
(10)	ss2	ss2	SULFUR
(11)	sio2	sio2	SIO2
(12)	sh	sh	SH
(13)	so	so	SO
(14)	h (private [Note])	so3	SO3
(15)	oh (private [Note])	n2	N2
(16)	o (private [Note])	pollutant-no	NO
(17)	so3	pollutant-hcn	HCN
(18)	n2	Zero Flow Rate Species No. 1	AR
(19)	pollutant-no	Zero Flow Rate Species No. 2	COS
(20)	pollutant-hcn	Zero Flow Rate Species No. 3	NH3
Note:	The private species are not exposed to the PME (Aspen Plus); their flow field values, in the present case, are added to those of the public species "n2".		

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Journal Files
End-User-Journal

- User journal file, called “sxo-apecs-journal.jou,” was used to run the various combustion models in sequence:
  - Default case setup:
    - Activate desired reactions in mechanism listing.
    - Turn on Magnussen eddy-dissipation model
    - Turn on flow, DO, k-ε, main combustion species.
    - Turn off all other species.
    - Set no.-of-cont-phase-iters-per-dpm-iter = 40
  - Set up and solve for NOx:
    - Turn off Adjust UDF (so it doesn’t iterate every iteration).
    - Turn off eddy-breakup model, flow, DO, k-ε, all species.
    - Turn on NOx model species (pollutant-HCN and pollutant-NO).
    - Set no.-of-cont-phase-iters-per-dpm-iter = 0.
    - Do 30 iterations.

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Journal Files
End-User-Journal (cont)

- User journal file “sxo-apecs-journal.jou” (continued):
  - Set up and solve for SOx:
    - Activate stiff chemistry solver.
    - Activate desired reactions in mechanism listing.
    - Activate UDF for calculation of radical (H, O, OH) concentrations.
    - Turn on SOx model species (H2S, SO2, SO, SH, SO3).
    - Do 40 iterations.
  - Return settings to original state for eddy-dissipation model.
    - Turn on Magnussen eddy-dissipation model.
    - Activate desired reactions in mechanism listing.
    - Turn on flow, DO, k-ε, main combustion species.
    - Turn off all other species.
    - Set no.-of-cont-phase-iters-per-dpm-iter = 40
    - Turn on Adjust UDF.

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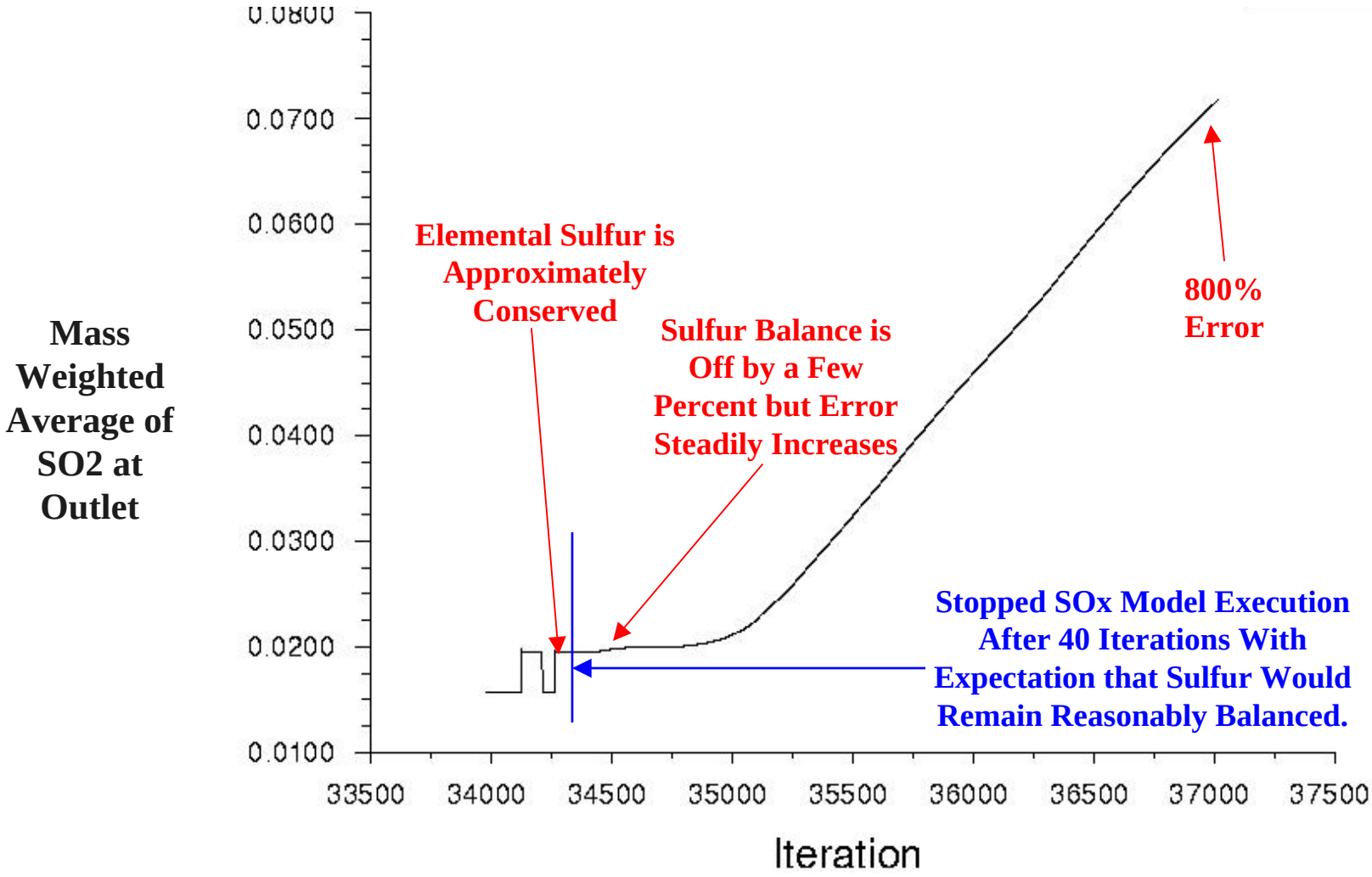
Comment on Sulfur Reaction Model



➔Issue Elevated to FLUENT Developers

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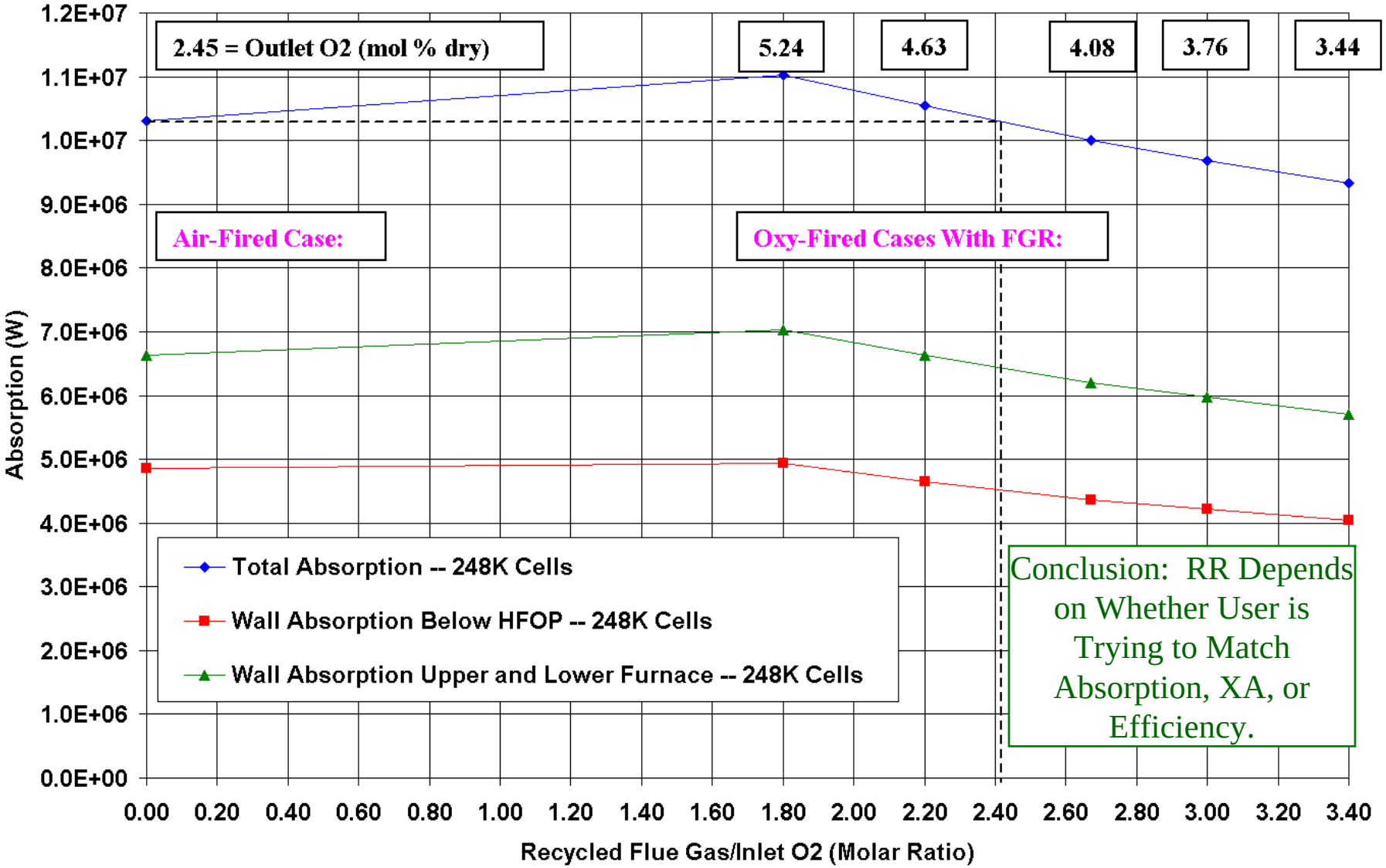
Total Absorption
Air-Fired vs Oxy-Fired



Conclusion: RR Depends on Whether User is Trying to Match Absorption, XA, or Efficiency.

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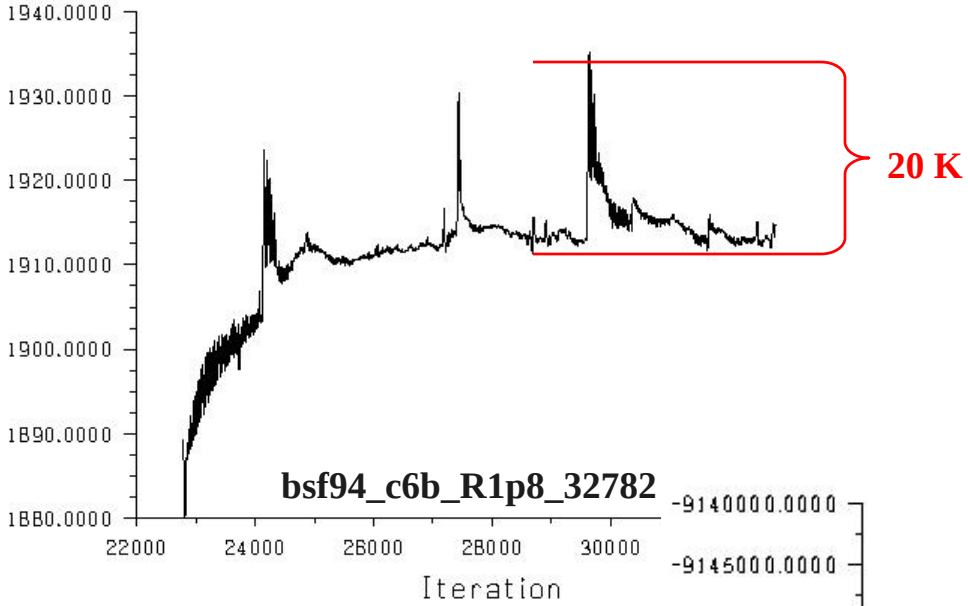
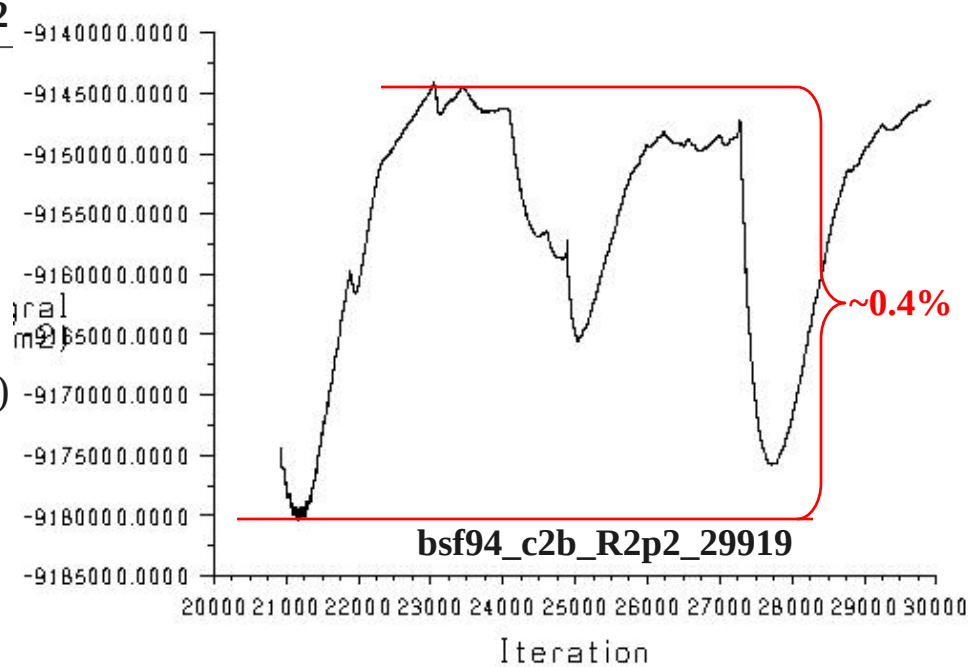
Convergence Behavior

Mass-Weighted Temperature at HFOP (K)



Total Surface Heat Flux (W)



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Results from Co-Simulations

- Each FLUENT block execution requires 8 hrs elapsed time on 8-processors of a Linux workstation.
- 2 runs at different target absorptions (cases stopped manually after sufficient iterations)

Parameter	Results from Oxy-Fired Flow Sheet	
	Run 1	Run 2
Target Absorption	10.314 MW (35.216 MBtu/hr)	9.7 MW (33.12 MBtu/hr)
% Recycle	69.6	74.1
Volumetric Recycle Ratio	2.48	3.13
Outlet O2 (%, Dry, by Volume)	4.65	3.99
NOx (oxy-fired) / NOx (air-fired) [Note 1]	0.18	0.25
SOx (oxy-fired) / SOx (air-fired) [Note 2]	1.13	1.1
Exit SO3 Mole Fraction	negligible	negligible
Number of FLUENT® Executions	10	51
CPU Days	3.3	16.7
Note 1:	At location downstream of recycle take-off	
Note 2:	At exit of boiler. FDA removes 90% of sulfur species from boiler exhaust before the recycle is split off.	

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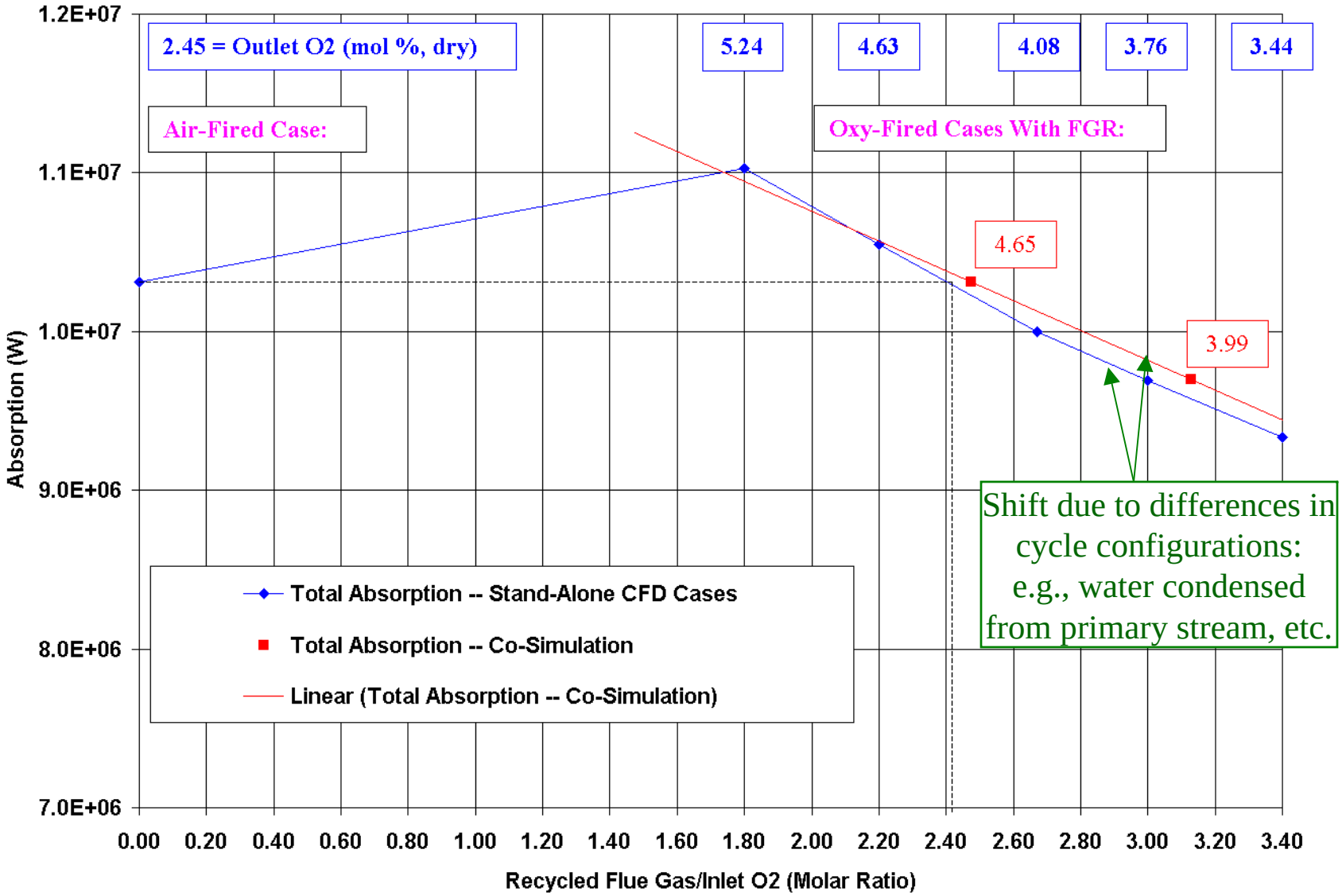

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Conclusions and Recommendations

- Important advancement in integrated simulations – demonstration of the use of SOx and NOx emissions calculations in a co-simulation.
- BSF case successfully run in Aspen Plus flowsheet with separate emissions models.
- Recommendations:
  - Cape-Open Booleans and variables for pollutants are currently limited in capability and could be made more versatile.
  - The FLUENT SOx model requires additional work in order to conserve elemental sulfur; mechanism needs to be validated.
  - When FLUENT block execution is spawned to Linux (or PC) platform, it is desirable for the user to be able to halt execution and interact with the case.
  - User should have the option of mandating that the FLUENT case be automatically saved to the “temp” directory after every successful FLUENT block execution.
  - Use “flow-splitters” for particle injections (in a similar manner to that done for the gas inlets).
  - Methodology for particle tracking at the outlet plane needs to be changed so that the UDF can be parallelized (and the “message passing” option can be used).

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Topic 1 BSF Emissions Co-Simulation Subtask

Topic 2 Geometric Scaling Co-Simulation Subtask

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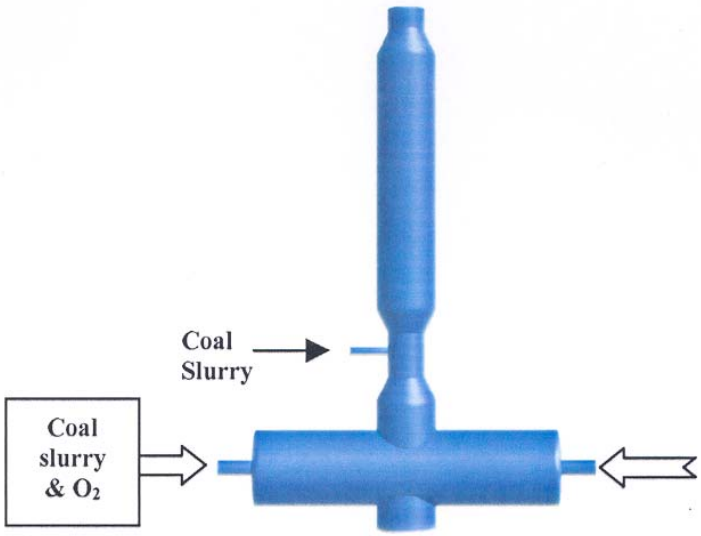
Geometric Scaling Module
Gasifier

- Entrained flow gasifier selected by NETL

- Gasifier Description
  - Two stage
  - Oxygen blown
  - Entrained flow
  - Coal slurry



Shi, et al., 4th ICCHMT (2005)

- Gasifier Model
  - Dilute flow regime ➔ DPM applied
  - Water droplets and coal particles treated separately
  - 8 species
  - 25,000 cells (requires 4-5 CPU hours from scratch)

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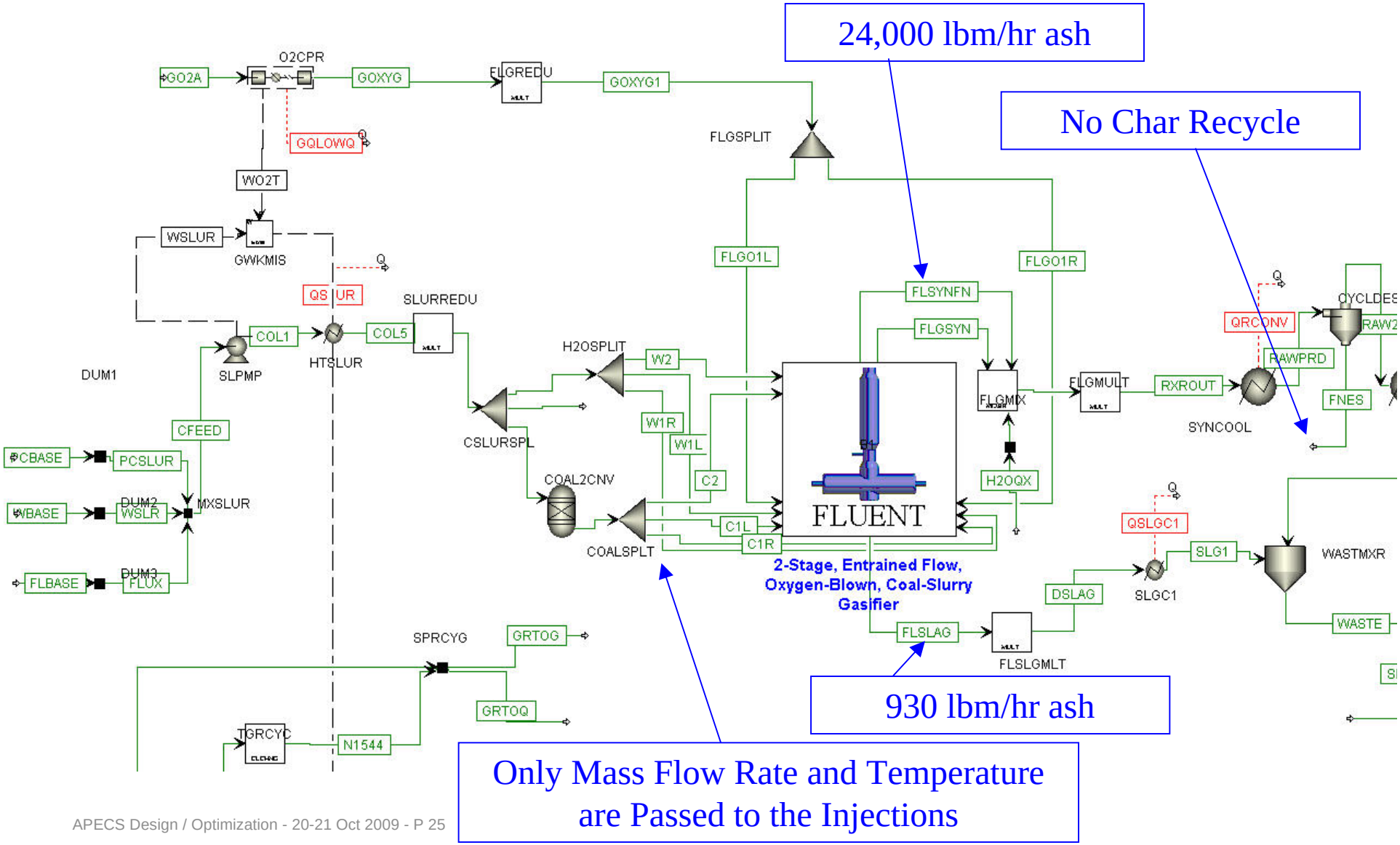
Geometric Scaling
Gasifier Module [from Demo]



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Geometric Scaling
Fixed Parameters and Constraints

- The H2O/coal ratio is set.
- The splits in the flow rates of the constituent H2O, coal, and oxygen streams feeding the first and second stages are set.
- The relative lengths of the geometrical sections and the height of the riser are set.
- The walls will remain adiabatic.
- No char or ash recycle.

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Geometric Scaling
Primary Factors Allowed to Vary

- The “throughput,” defined as the overall coal flow rate to the gasifier, is varied in order to achieve a process model “design spec” target.

- The overall oxygen flow rate is varied, through an optimization methodology, in order to achieve the maximum CGE for a given coal throughput.

$$CGE = \frac{(\dot{m}_{syngas})(HHV_{syngas})}{(\dot{m}_{fuel})(HHV_{fuel})}$$

- The geometry and inlet cross-sections scale with the coal throughput in order to preserve the cross-sectional velocities and residence times.

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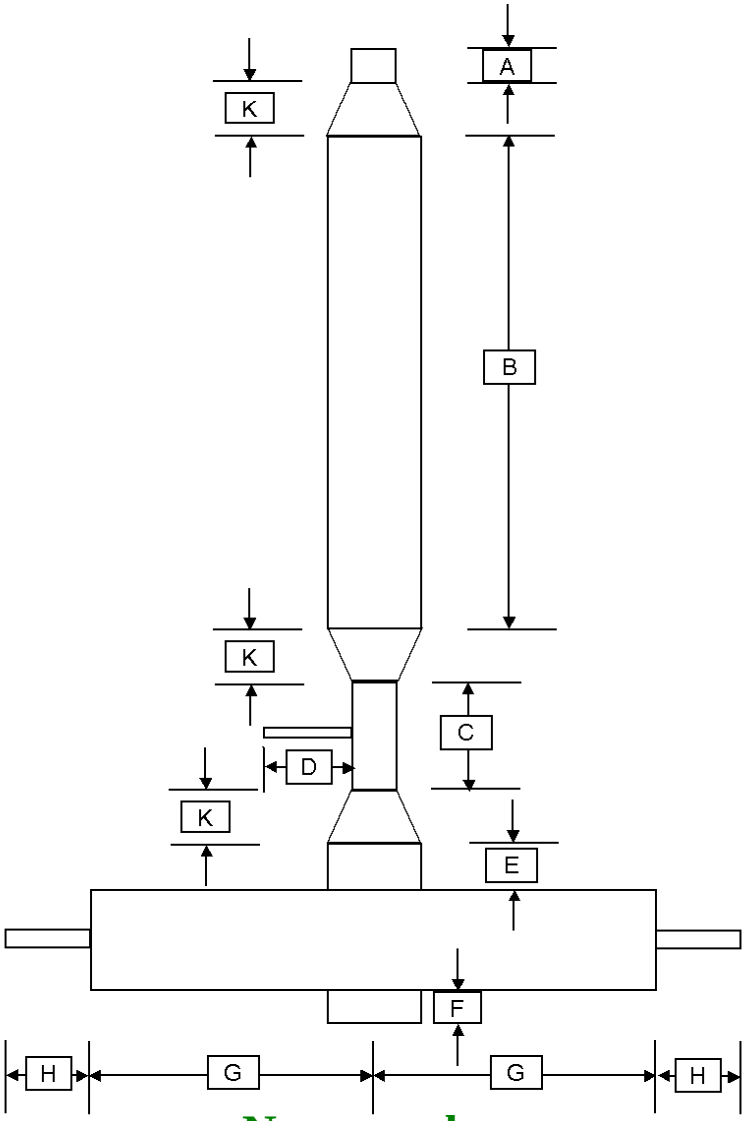
Geometric Scaling
Potential (Exposed) Scaling Parameters



Not to scale

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Geometric Scaling
Gambit Journal File (“gasifier.jou”)

```
/     assign cape-open parameters to physical parameters

$section_A_diameter = $geometry_parameter_1
$section_A_length = $geometry_parameter_2
$section_B_diameter = $geometry_parameter_3
$section_B_length = $geometry_parameter_4
$section_C_diameter = $geometry_parameter_5
$section_C_length = $geometry_parameter_6
$section_D_diameter = $geometry_parameter_7
$section_D_length = $geometry_parameter_8
$section_E_diameter = $geometry_parameter_9
$section_E_length = $geometry_parameter_10
$section_F_diameter = $geometry_parameter_11
$section_F_length = $geometry_parameter_12
$section_G_diameter = $geometry_parameter_13
$section_G_length = $geometry_parameter_14
$section_H_diameter = $geometry_parameter_15
$section_H_length = $geometry_parameter_16
$section_K_length = $geometry_parameter_17
/
```

Gambit Physical Parameter

CAPE-OPEN Geometry Parameter

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Geometric Scaling
Sequence for CO Parameter Utilization

- The CAPE-OPEN parameter “geometry-parameterization” is set equal to unity (in calculator block SWITCH), which will then notify the APECS controller, when Aspen Plus executes the FLUENT block, to regrid the FLUENT mesh.
- Whenever the parameter “geometry-parameterization” is activated (i.e., set equal to unity), then in a subsequent calculator block (C-PREUSR), the values for each CAPE-OPEN “geometry_parameter_#” are overwritten based on the ratio of the current coal throughput to the baseline throughput.
- When the FLUENT block is executed, APECS generates a boundary condition file, as well as an interpolation file from the current FLUENT .cas and .dat files.
- The Gambit journal file (i.e., gasifier.jou) then uses the newly scaled diameter and length values to construct a new mesh. The CAPE-OPEN parameter “geometry_model_name” is used for the file name for the Gambit journal file, and the “geometry_parameter_#” variables provide the baseline or default geometric values.

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Geometric Scaling
Sequence for CO Parameter Utilization (cont)

- The APECS controller reads the boundary condition file and the interpolation file into the newly created mesh file.
- A second journal file is used to complete post-interpolation operations (e.g., changing URFs or executing DPM to re-establish particle source terms).
  - The name of this second journal file is provided through the CAPE-OPEN variable “geometry_user_journal_name”
  - The journal file is read by the APECS controller whenever the integer switch “geometry_user_journal_activate” is set to unity.
- All of the above APECS operations are performed without ever exiting FLUENT (➔helps to preserve plotting planes, etc.)

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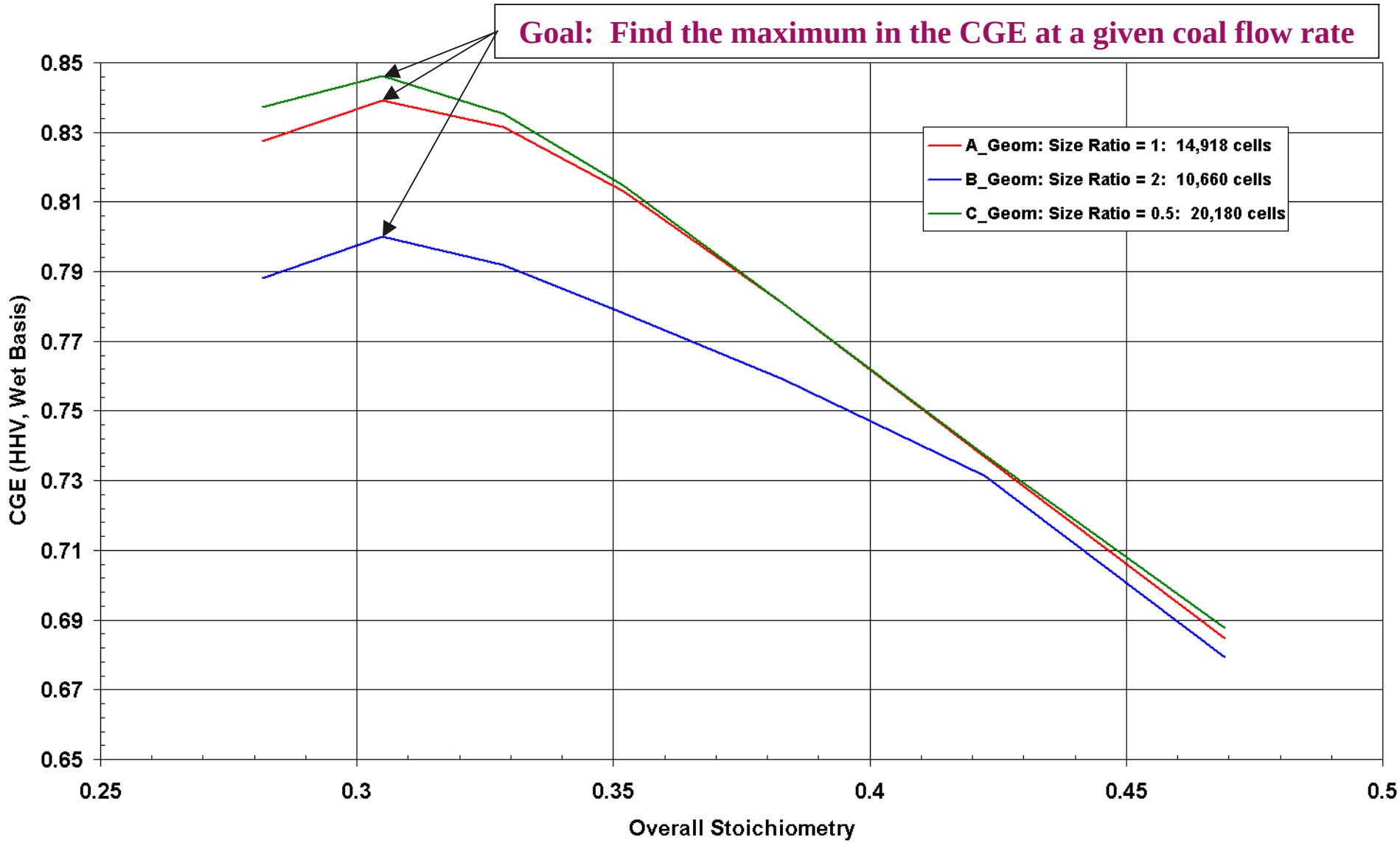
Geometric Scaling
Preliminary Sensitivity Assessment



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Geometric Scaling
Solution Issues

- Complex method – feasible path “black-box” pattern search.
  - Handles inequality constraints and bounds on decision variables
  - Does not require numerical derivatives
  - Takes many iterations to converge
- SQP method – state-of-the-art, quasi-Newton nonlinear programming algorithm
  - Can converge tear streams, equality constraints, and inequality constraints simultaneously with the optimization problem.
  - Converges in fewer iterations
  - Requires numerical derivatives for all decision and tear variables at each iteration
- Problem: Both methods bogged down and ultimately failed
- Reason: CFD solutions must be reliable and repeatable
  - Lack of convergence
  - Solution noise

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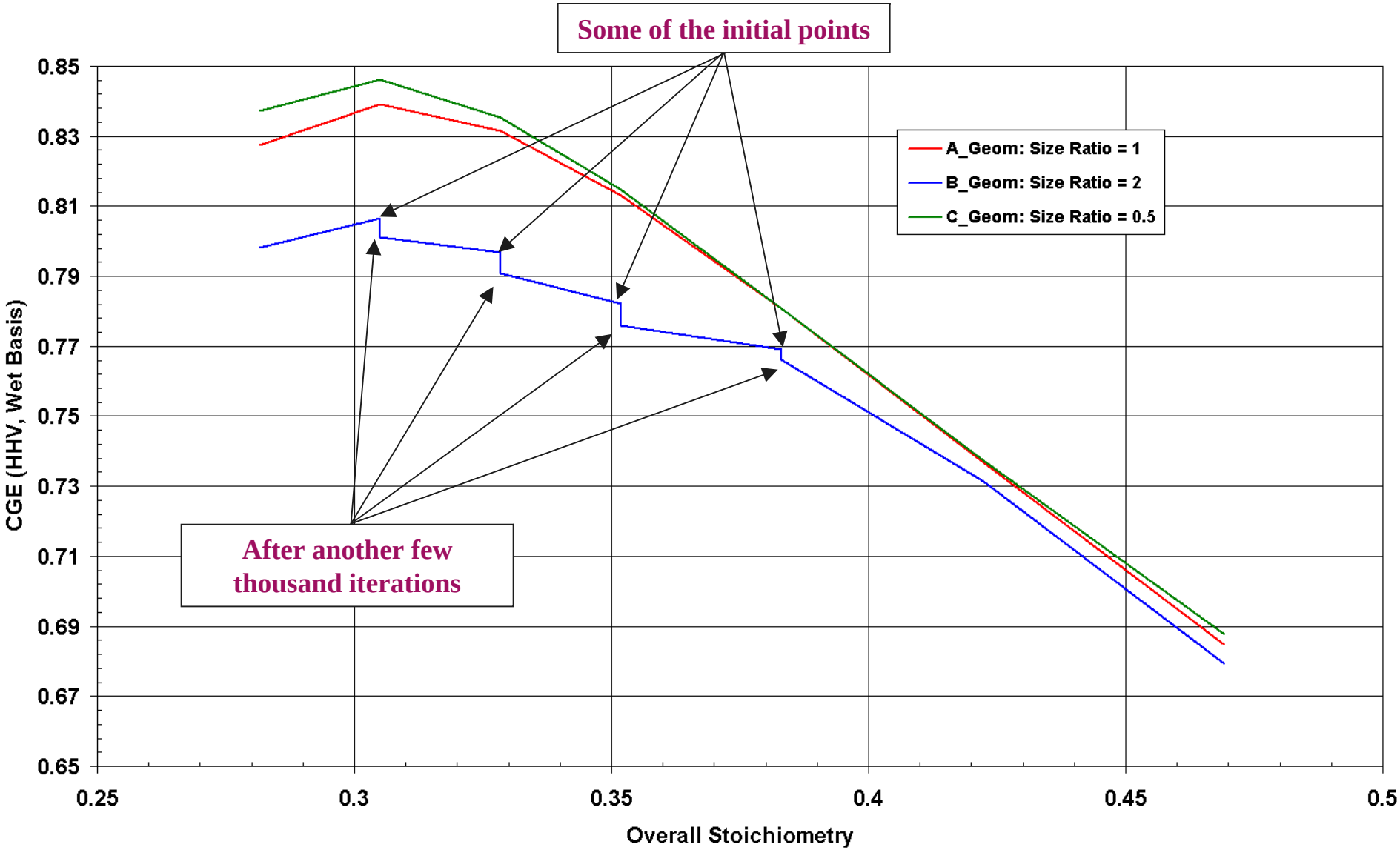
Geometric Scaling
Preliminary Sensitivity Assessment



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Geometric Scaling
Investigation of Lack of Convergence

CFLOW = 502331.3

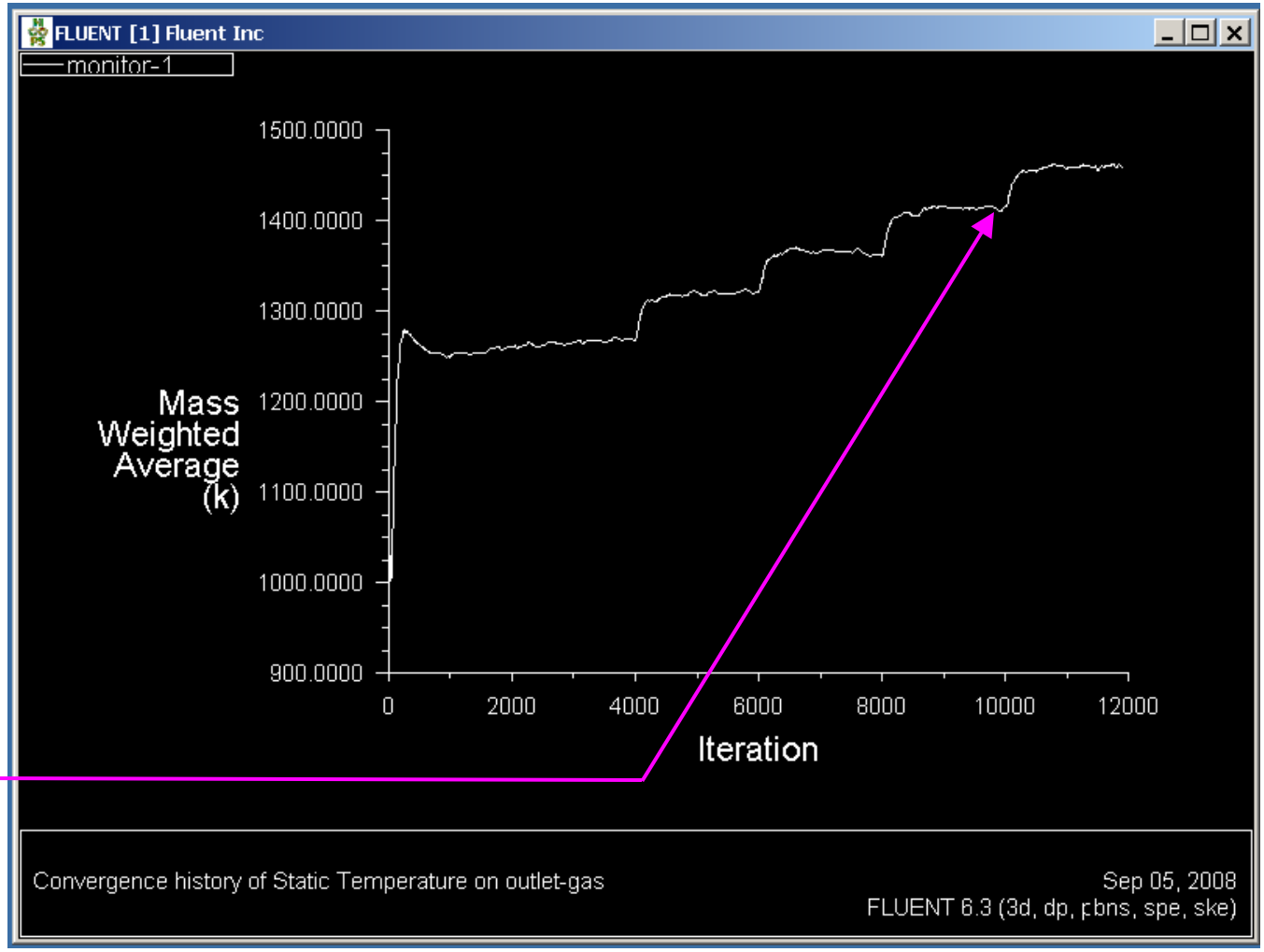
XFLUX = 10251.66

CGE = 0.8094

STOICH = 0.3175

XO2FLO = 346824.7 lbm/hr

- Took restart formed at 10,000 iteration point (which had run for 2,000 iterations)
- Subsequently ran in stand-alone mode



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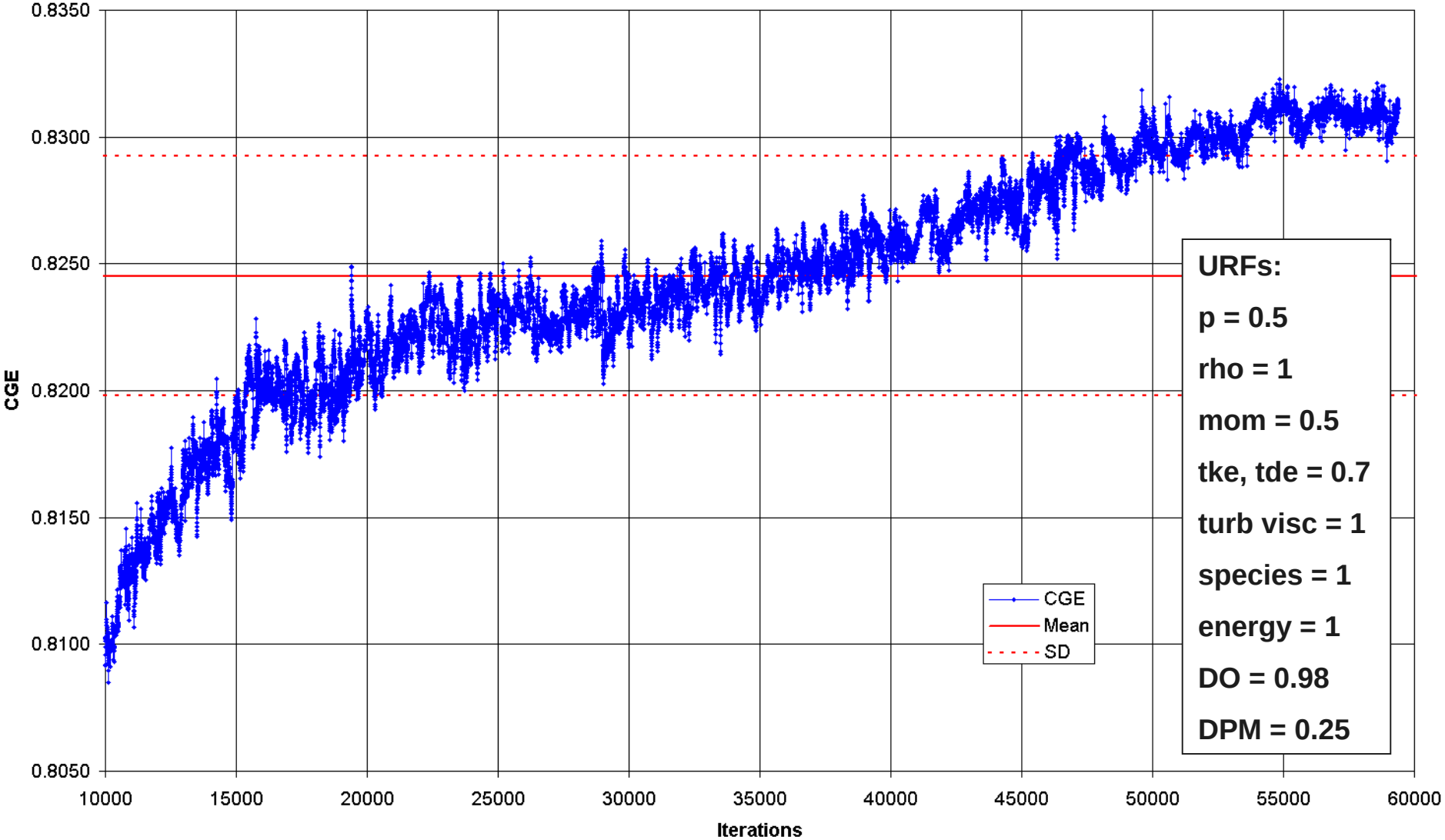
Geometric Scaling
Lack of Convergence in CGE



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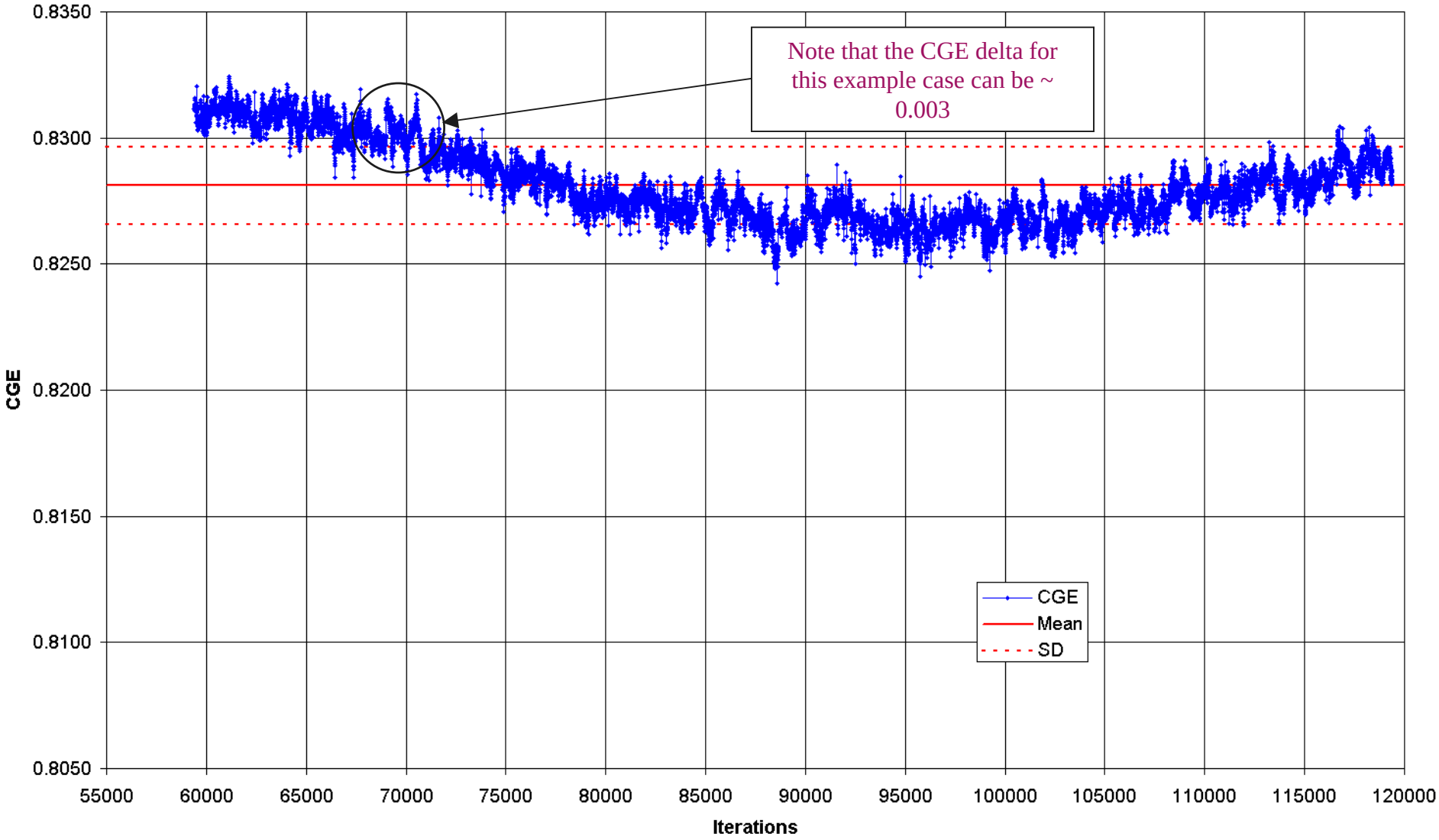
Geometric Scaling
Lack of Convergence in CGE (cont)



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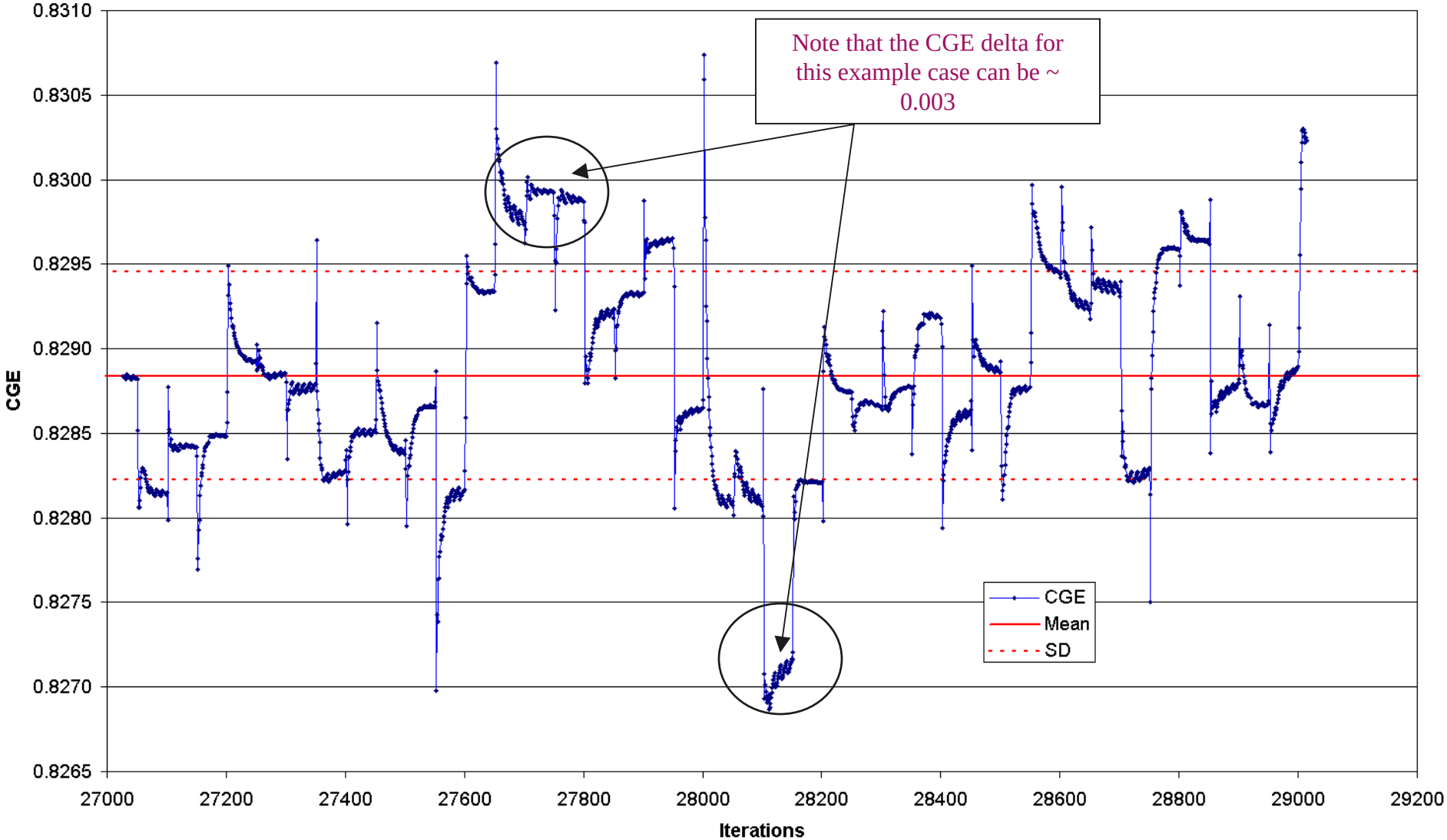
Geometric Scaling
CGE Calculation Variability -- Noise

Average = 0.82884, Standard Deviation = 0.0006164



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Geometric Scaling
Hard-wired Optimization

- Substantial lack of convergence (sometimes requiring 40,000 to > 60,000 iterations)
- Significant computational noise:
  - For a change in the STOICH of 0.01, the change in the CGE may be about 0.003 - 0.005 (depending upon proximity to maximum).
  - This is approx. equal to the size of the FLUENT-computed noise.
- The A+ optimization routines require repeatable solutions (problematic for finite-difference derivatives and line searches)
- Hard-wired optimization attempt:
  - Assumed 2000 to 4000 iterations per run
  - The tolerance on STOICH has to accommodate a change in STOICH of ~0.01 (or larger) to produce a consistently perceptible and reliable change in CGE
  - Aspen Plus computes the optimum by calculating the CGE at 5 discrete STOICH values 0.0125 apart
  - Selects the largest value as the optimum and repeats the calculation at that STOICH before exiting loop

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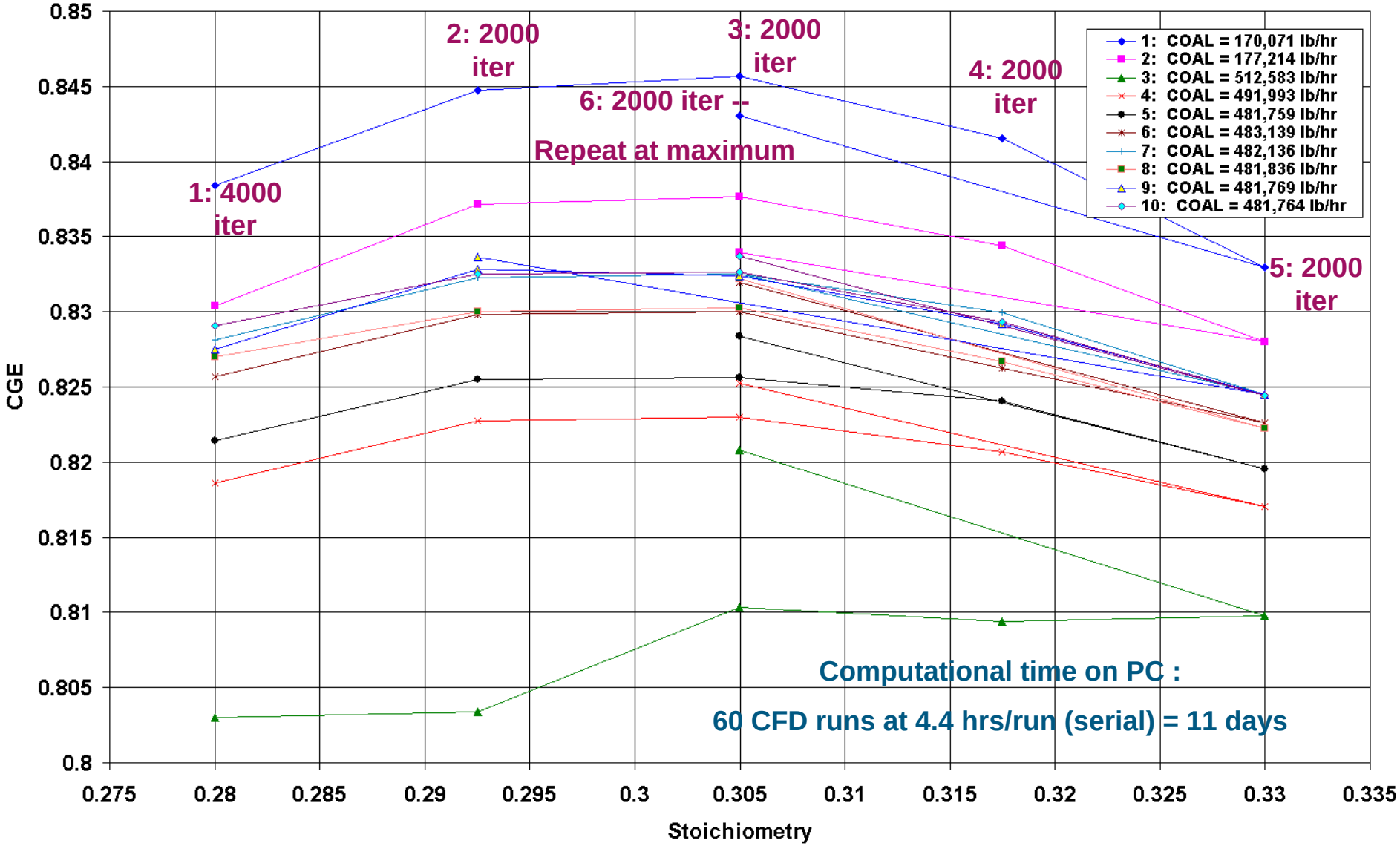
Geometric Scaling
Results for Hard-wired Optimization



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Geometric Scaling
Discussion

- CFD case issues:
  - extreme convergence times (stiffness?)
  - fluctuating noise superimposed on changing or rolling mean
  - robustness of the chemistry solver
- The A+ optimization routines require repeatable solutions. Convergence issue must be solved and times shortened.
  - Unlikely that Complex method is practical (i.e., too many solutions required)
  - SQP should be given another opportunity to be tested:
    - What is the detailed methodology and how can it be adjusted to accommodate stochastic or oscillatory behavior?
    - Will finite difference derivatives always be an issue?
  - Perhaps other optimization approaches more amenable with CFD: e.g., cover sensitivity range with discrete calculation points and then apply curve fit to find max/min (?), then repeat with reduced range (?).

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