Modeling Combustion Processes – A Perspective from past twenty years

ACERC 2005 – Tribute to Dr. L.D. Smoot

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ACERC 1990

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Introduction: CFD based Coal Combustion Modeling

"Development of combustion models is needed to the point where they will find wide application in the management and control of practical systems. This ambitious goal can probably be achieved only with greatly improved understanding of the fluid dynamics and chemical processes occurring in coal combustors, utilization of improved diagnostic techniques in model verification, and evolutionary improvements in the combustion models themselves"

(Penner, S.S., "Assessment of Research Needs for Coal Utilities," DOE Coal Combustion and Applications Working Group (August 1983)

Energy Controls World Economies and our Personal Lives!

- CHEVRONTEXACO CEO CALLS FOR US ENERGY POLICY
  ~David J. O'Reilly, chairman and CEO of ChevronTexaco Corp., called for a new US energy policy in his keynote address at the opening of a weeklong conference of energy executives in Houston, sponsored by Cambridge Energy Research Associates.
  http://ogjo-media.com/lrd1_AAImggAAJ64B
- CHINA LIKELY TO BECOME NET EXPORTER OF HIGH-SULFUR DIESEL
  ~China appears likely to become a net exporter of high-sulfur diesel, or gas oil, starting in February and lasting through March, said a report from Energy Security Analysis Inc. (ESAI), Boston.
  http://ogjo-media.com/lrd2_AAImggAAJ64B
- WORLD OIL PRODUCTION CAPACITY MAY GROW 16 MILLION B/D BY 2010
  ~World oil production capacity could jump by more than 16 million b/d to 101.5 million b/d by 2010, with the addition split "fairly evenly" between members of the Organization of Petroleum Exporting Countries and non-OPEC producers, said an executive of Cambridge Energy Research Associates, a subsidiary of IHS Inc.
  http://ogjo-media.com/lrd3_AAImggAAJ64B

Evolution of PF Coal Combustion & Gasification Models

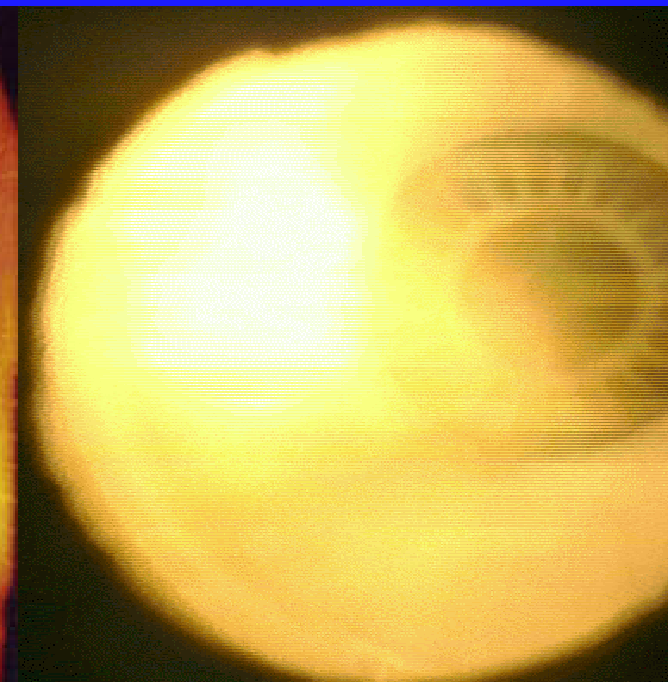
- Government sponsored Coal research
  - Department of Energy, EPA, NSF
- Industry sponsored Coal research
  - UPL, EPRI, Southern Company Services, Dow Chemical, Texaco, Consol
- Combustion Lab formed in mid-70's which evolved to the Combustion Consortium ('85) which led to ACERC ('87)
- Evolution of ACERC Coal models
  - PFFEAM (0-D, empirical, furnace model)
  - 1-DiCOG (1-D, transport, lab reactor)
  - PCGC2 (2-D axi-symmetric, transport, near burner region)
  - PCGC3 (3-D, transport, full furnace model)
  - Banff/Glacier/Fluent/STARCD…

Verification of PF Coal Combustion & Gasification Models

- Initial detailed data taken in 8" pf coal furnace (atmospheric, down fired)
  - Gas Samples via suction/quench probes
  - Gas Temperature via suction pyrometers
  - Coal Burnout via TGA Data
  - Particle size via Coulter Counter
- Detailed validation data taken in CPR (controlled profile reactor) to verify CFD predictions
  - Data book with several well documented cases produced
- Detailed Sensitivity analysis of CFD codes to identify key input data controlling code predictions
- Full-scale data taken in industrial facilities to validate models for full-scale plant operation

Technology Transfer: Application of ACERC technology in Industry

- Incineration
- Coal Conversion
- Chemical Production



CFD Modeling Helps Industry Address Key Issues

- Tighter environmental regulations
  - How can I reduce NOx, CO, PIC's?
- "Best" equipment?
  - Which Burner, flare, nozzle, reactor, etc. is right?
- De-bottleneck/optimize operating plants?
  - How can I increase yield, production rate, safety, etc.?
- Reduce Downtime?
  - How can I shorten time for plant shutdown?

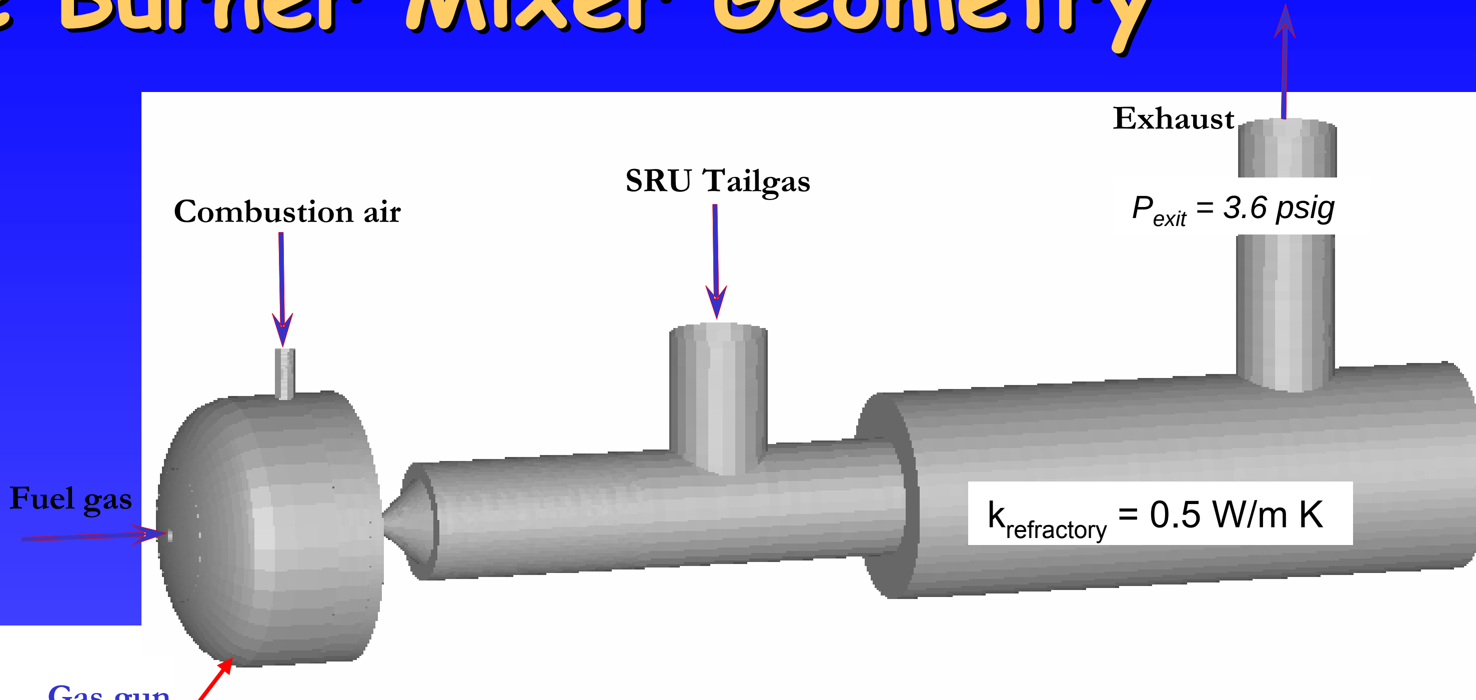
Combustion Models

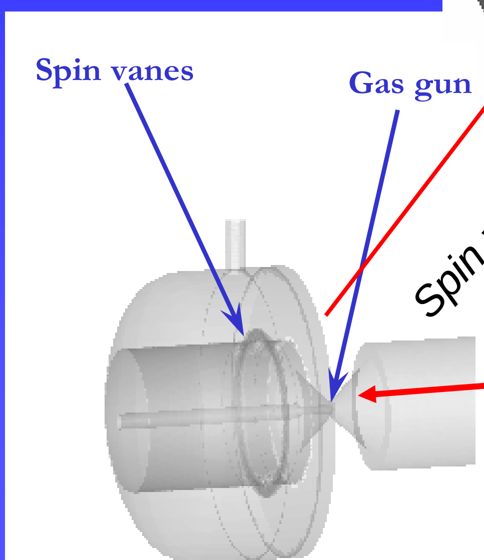
- Kinetically controlled reaction model
  - Fully coupled n-step reactions w/ Arrhenius kinetics
- Gaseous premixed turbulent combustion models
  - Flamelet models for premixed systems
- Extended PPDF non-premixed combustion model
  - Fast reacting non-premixed systems
- NOx formation models
  - Thermal, Fuel and Prompt NOx
- Eddy Break-Up Model (EBU)
  - Rate based on turbulent micromixing
- Hybrid Kinetic/Eddy Break-Up
  - Mixing or kinetics control local rate

SCOT In-line Burner/Mixer System

- Designed to add heat to tailgas from Claus unit
- Tailgas inlet temperature ~260 °F, effluent gas ~530 °F
- Burner provides short-flame w/ rapid-mixing
- Operates sub-stoichiometrically to avoid acid gas oxidization
- STARCD simulation included:
  - Turbulence w/ k-ε
  - Combustion chemistry w/ global reactions
- Combustion species considered H_2, CH_4, CO, CO_2, H_2O, H_2S, O_2, SO_2, N_2
- Combustion reactions included:
  - $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$
  - $CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O$
  - $CO + \frac{1}{2} O_2 \rightarrow CO_2$
  - $H_2S + 3/2\ O_2 \rightarrow SO_2 + H_2O$

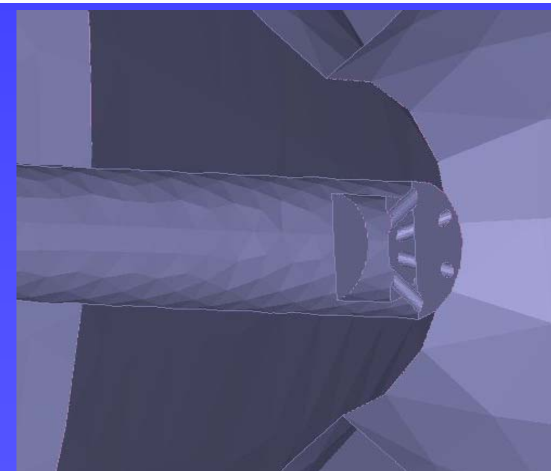
In-line Burner Mixer Geometry





Spin vanes aid mixing

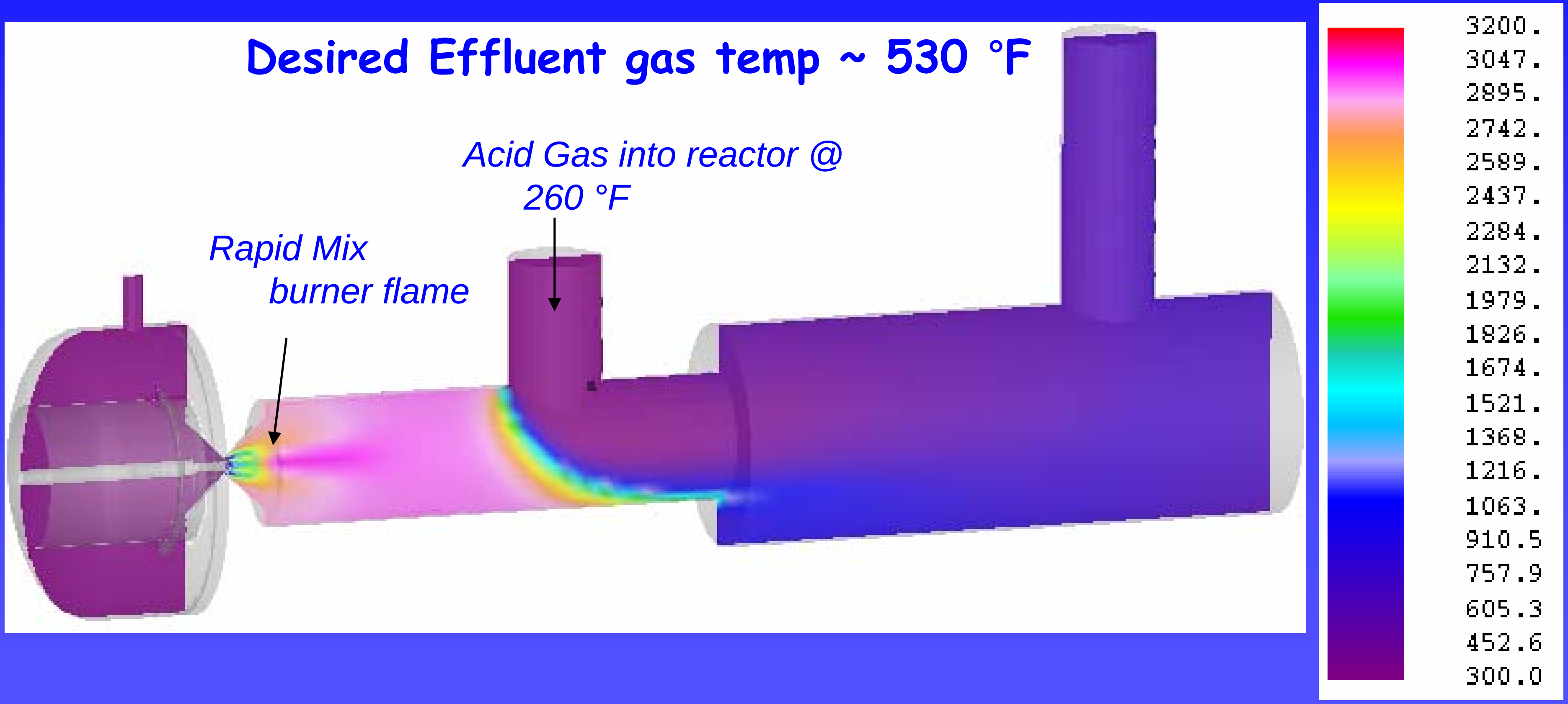
Gas fired through 6 ports



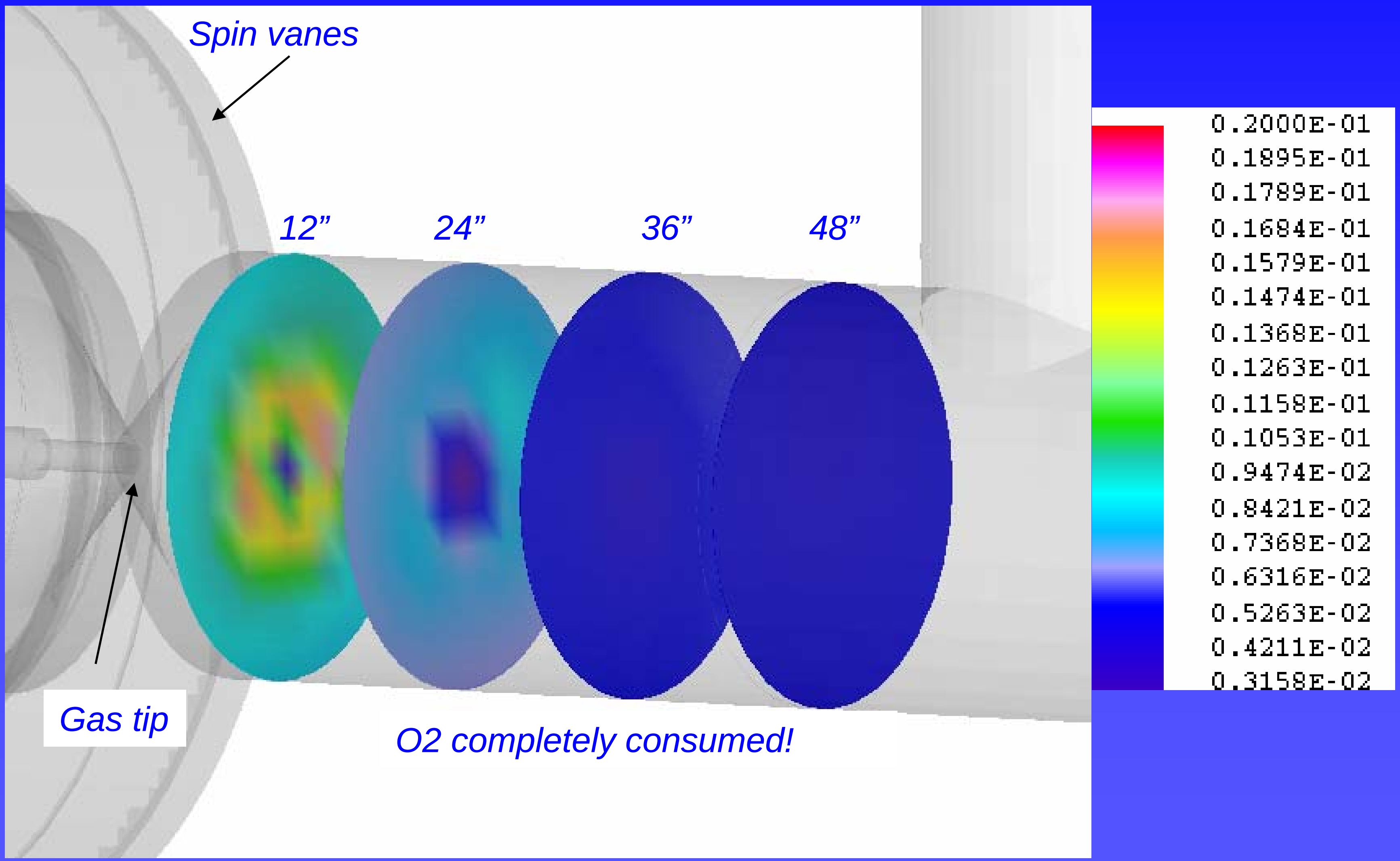
Base Case (nominal operation)

- Concerns:
  - Effluent gas temperature
  - O2 breakthrough
  - Soot Formation
- Firing rate: 2.63MMBtu/hr
- Fuel composition: H_2 = 99 mol% CH_4 = 1 mol%
- Flow rates:
  - 53 lbm/hr Fuel
  - 1736 lbm/hr Combustion air @ 230°F to burner
  - 500 lbm/hr tempering steam @ 350 °F mixed in combustion air
  - 18,105 lbm/hr SRU tail gas @ 260 °F to vessel

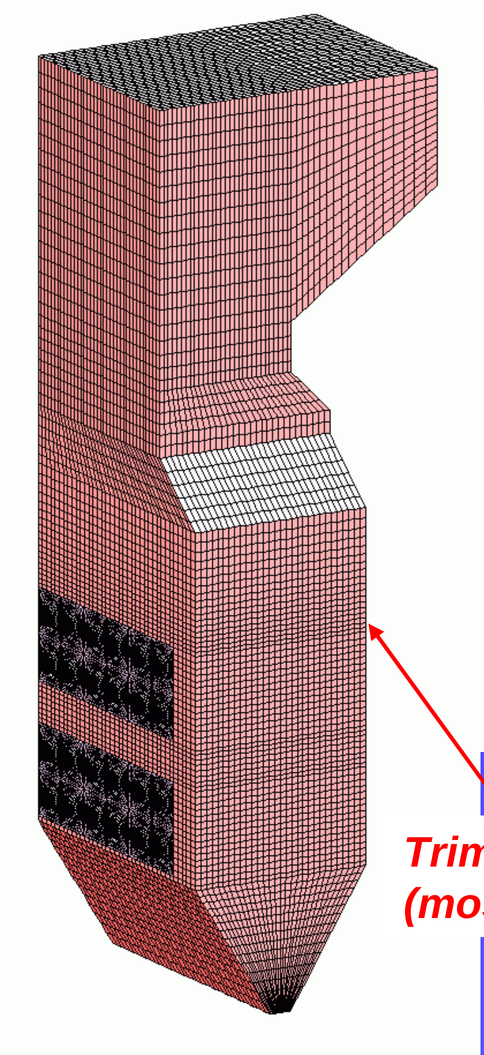
Concern 1: Effluent Temperature (°F)

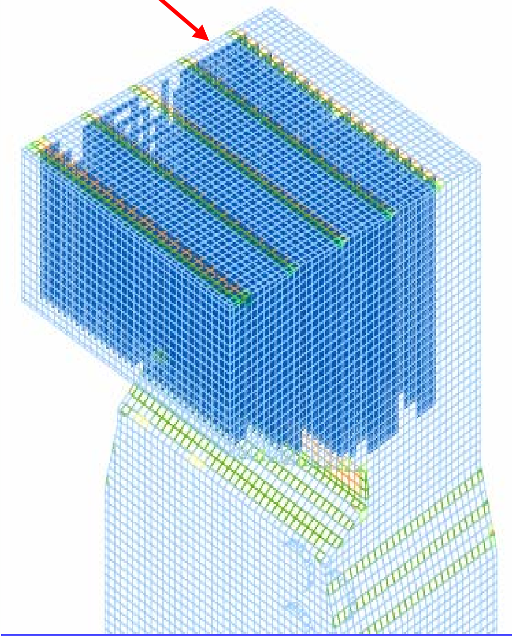


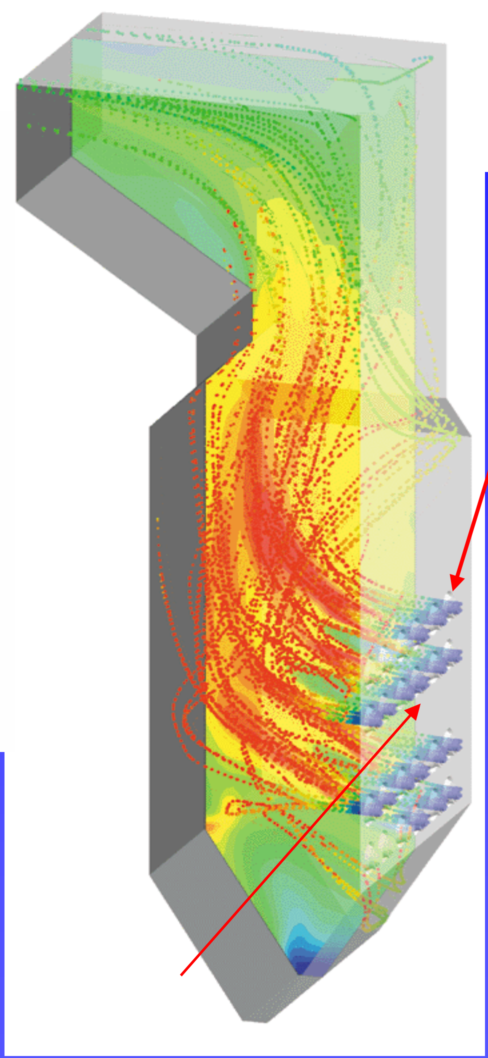
Concern 2: O_2 Breakthrough



DIDCOT COAL FIRED BOILER: Grid





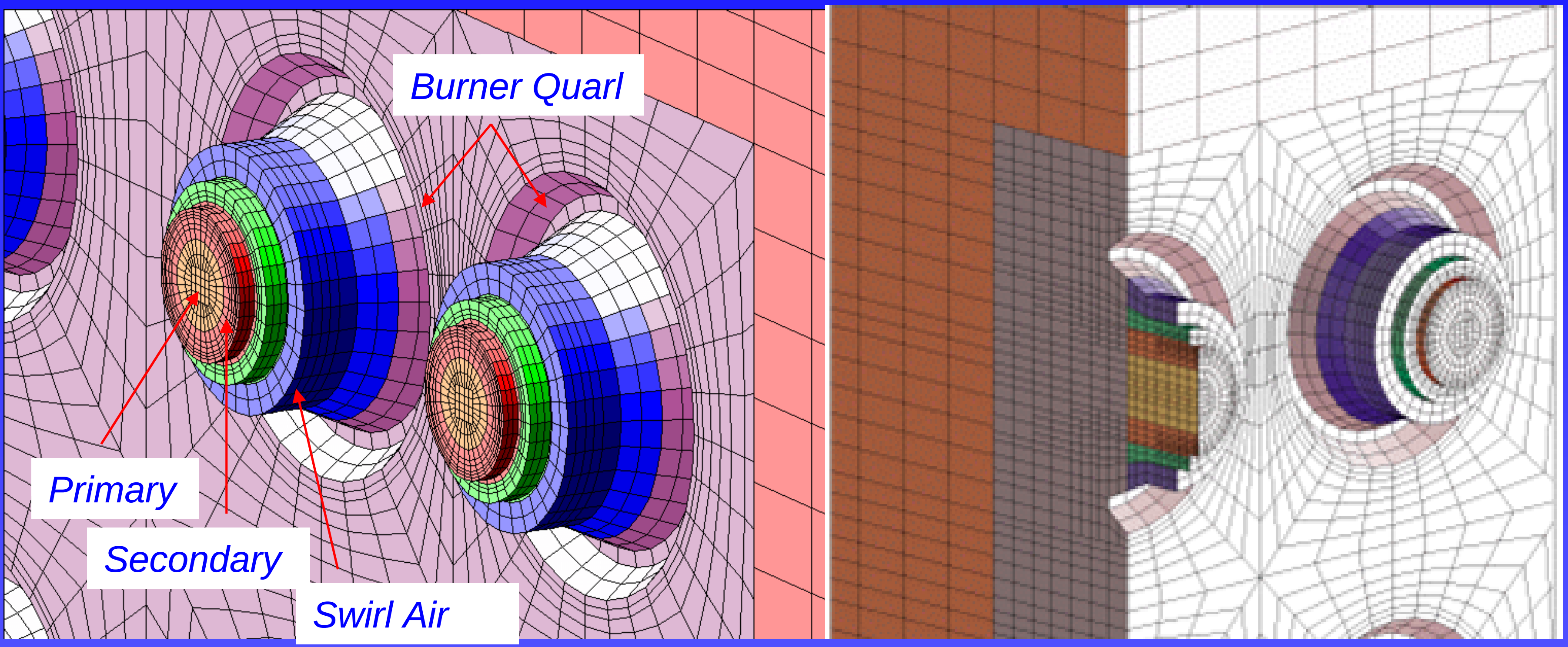


Heat Transfer Surfaces modeled

Individual burner swirl levels modeled

Trimmed mesh (mostly hex)

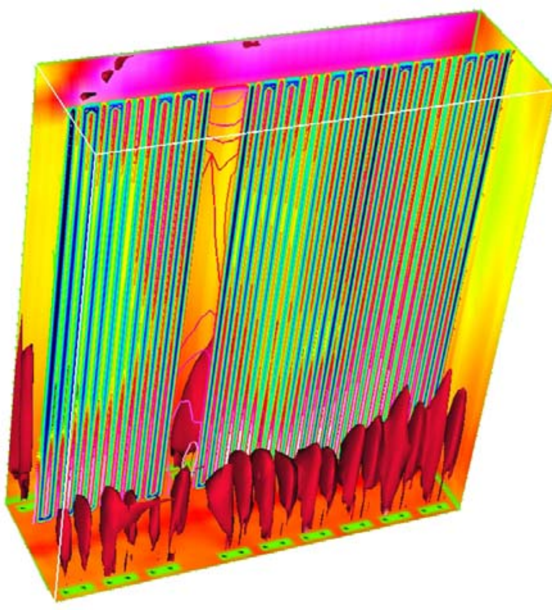
DIDCOT COAL FIRED BOILER
Grid Details - Burners



24 Burners modeled (counter swirl in alternating burners on each row)

"Flame Rollover" in Ethylene Furnace

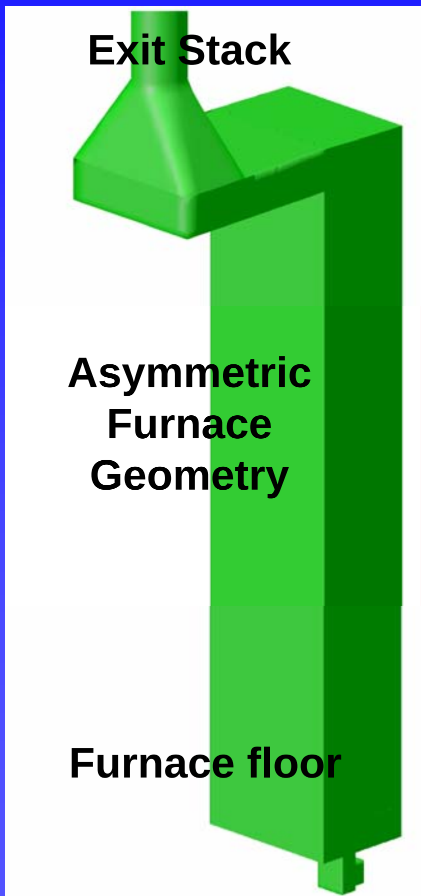
- Ethylene furnace had flame impingement on process tubes
  - De-rated capacity - significant impact on "Bottom-Line"
  - Evaluated 16 different burner/furnace design options
  - Identified most promising solution for implementation
  - Worked First Time – plant operating at full capacity!

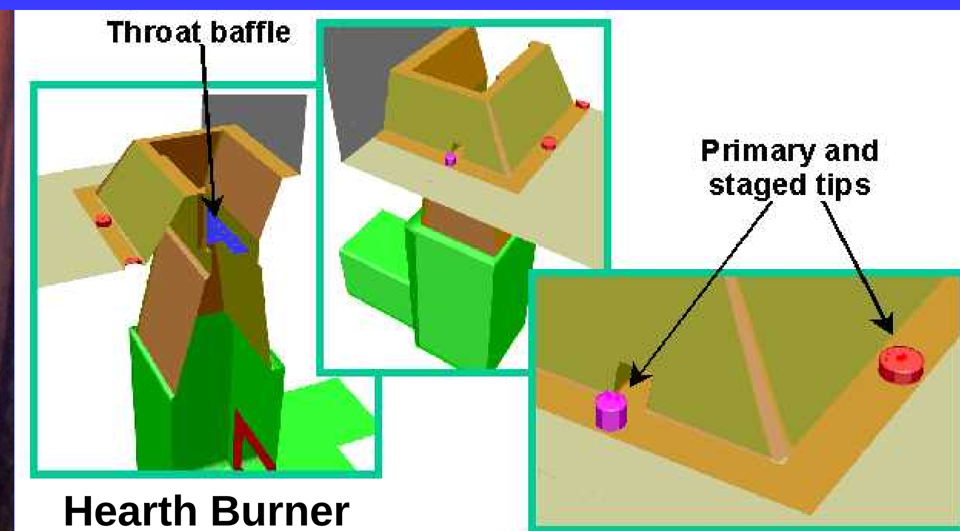


Initial CFD modeling of Ethylene furnaces by Smith, P., et.al, (1993) using BANFF

Ethylene Furnace Geometry/Burner Configuration

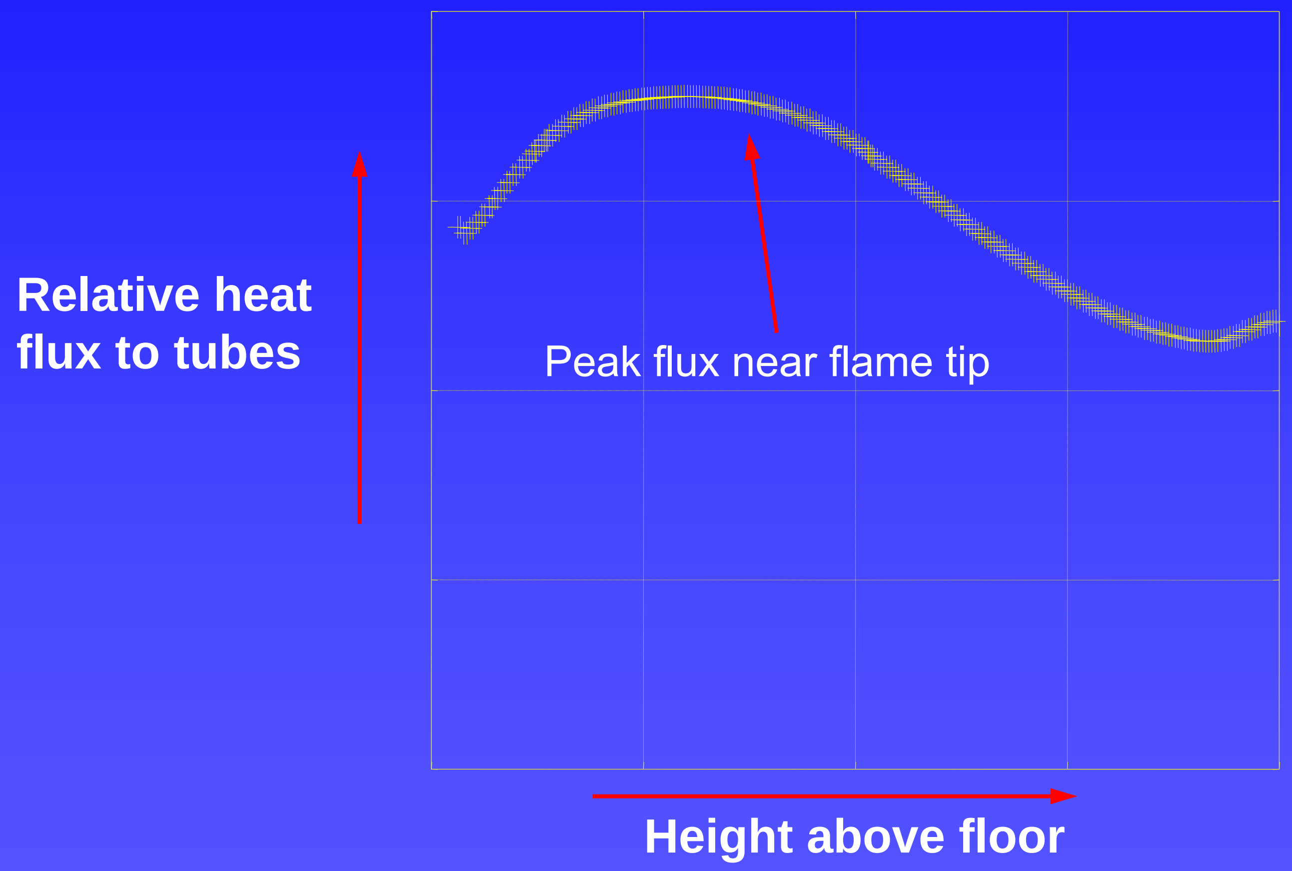
1. Furnace has asymmetric exit creating non-uniform flow inside furnace
2. Low NOx hearth burners fire along refractory wall which radiates to process tubes furnace center

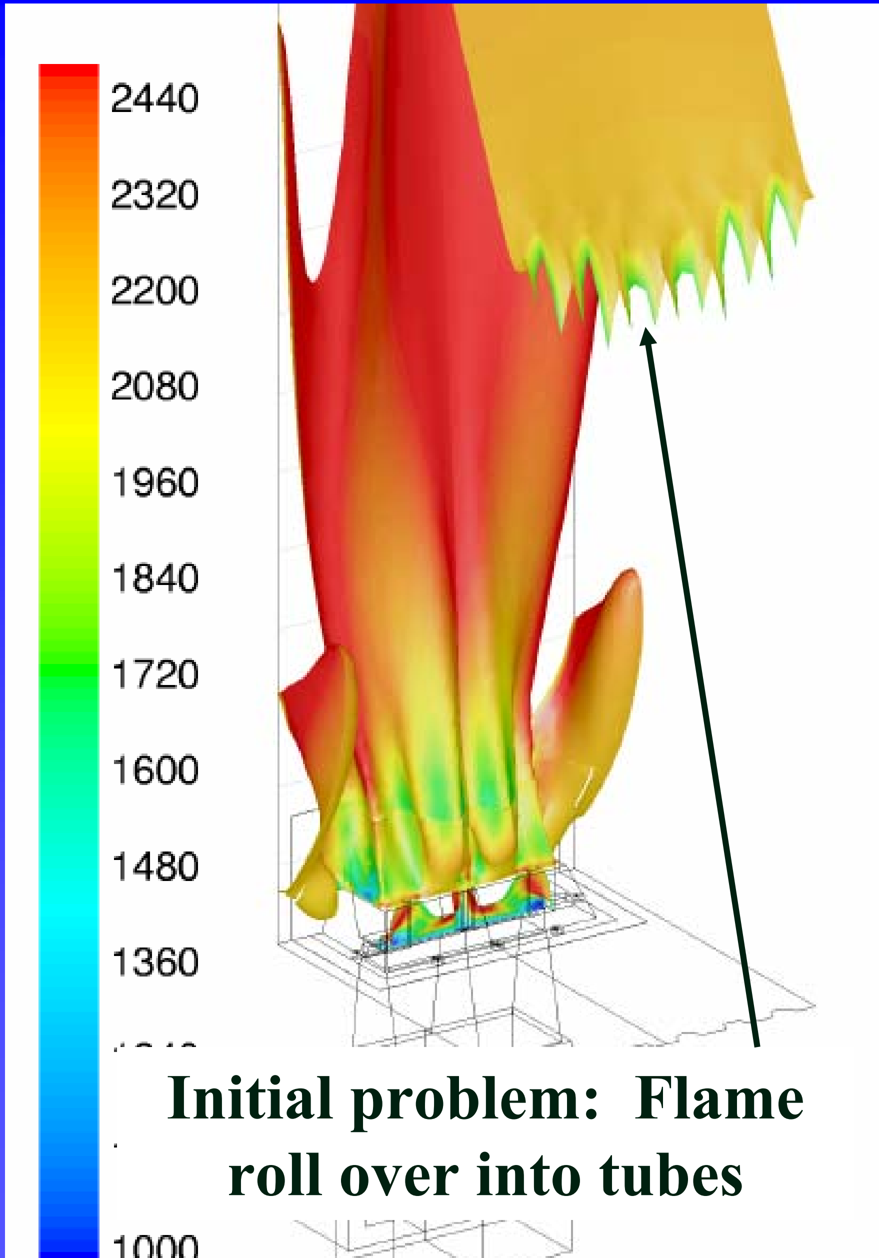




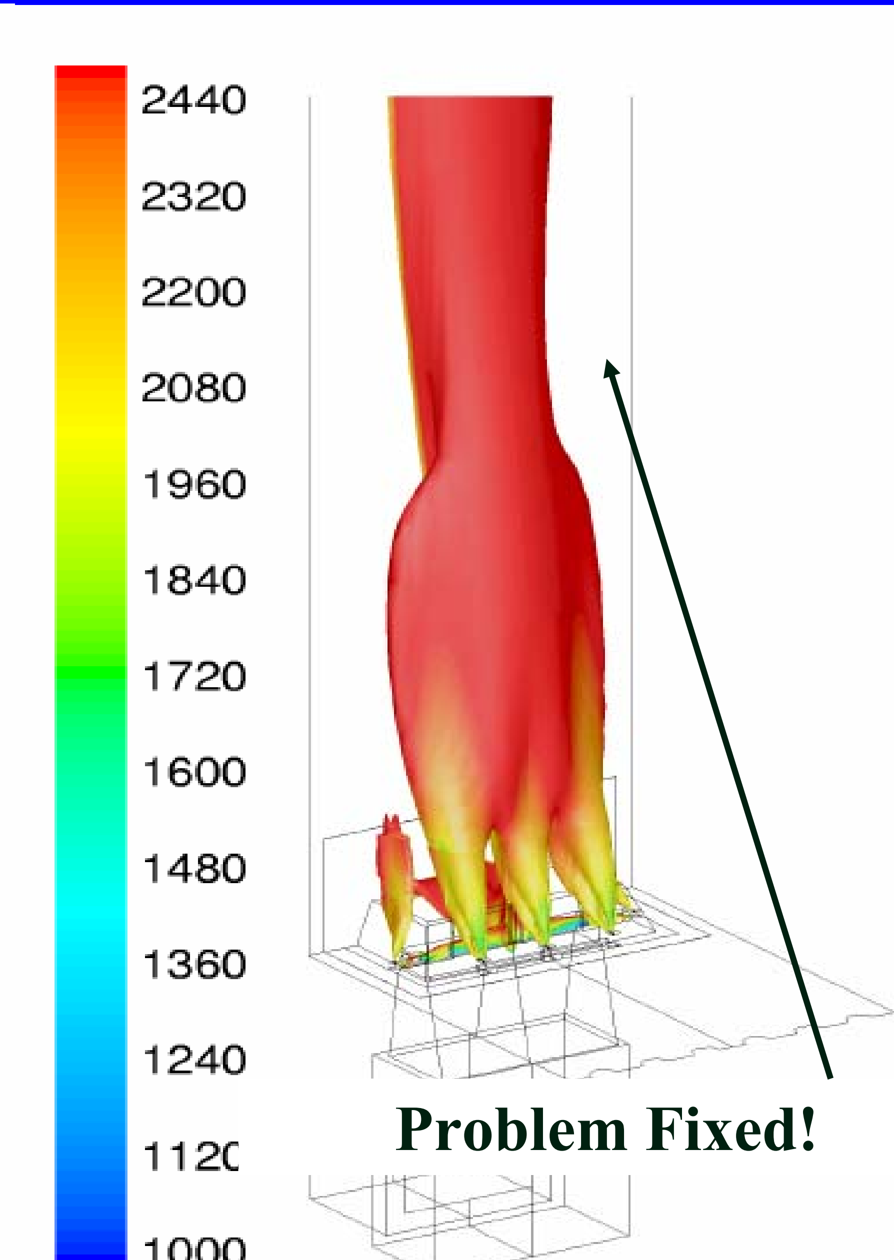
Henneke, et.al., John Zink Handbook, Chapter 9, CRC Press, (2002)

Predicted Relative Heat Profile in Ethylene Furnace



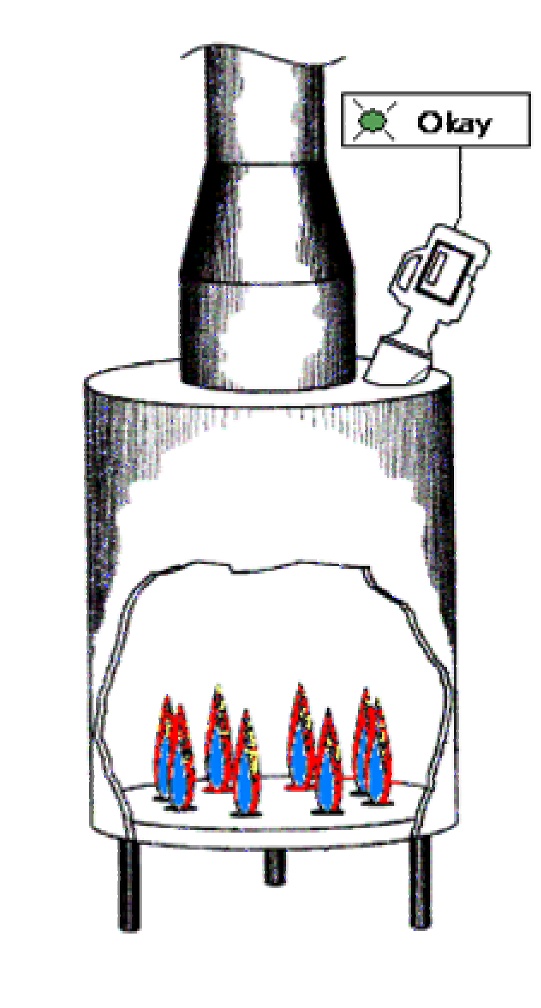


Initial problem: Flame roll over into tubes



Problem Fixed!

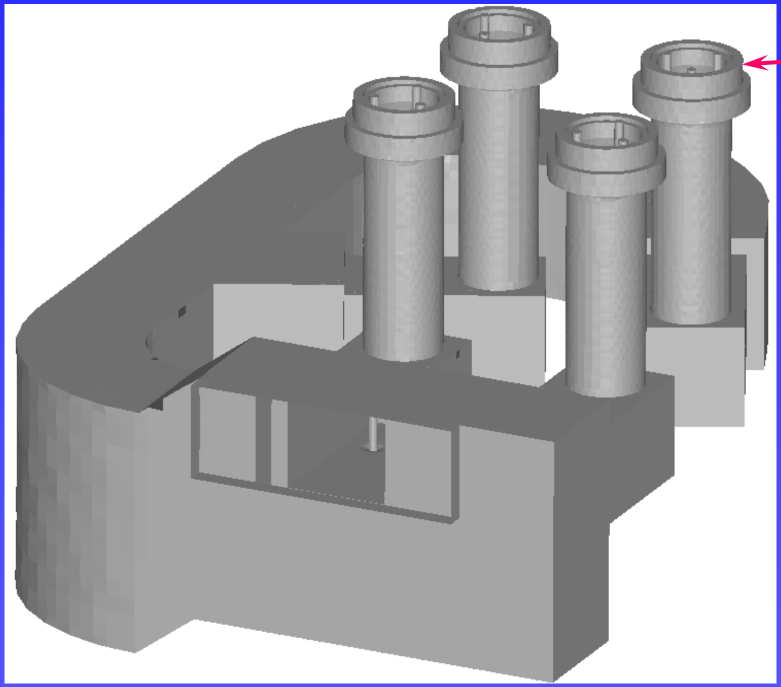
Valero Heater Analysis: Flame Interaction



- Concerned about flame length and shape
- Burner-burner and Burner-furnace interactions can be an issue
- Analyze combustion and furnace flow characteristics to insure furnace operation is "OK!"
- Use "Slice" of overall geometry to approximate full furnace

Operating conditions

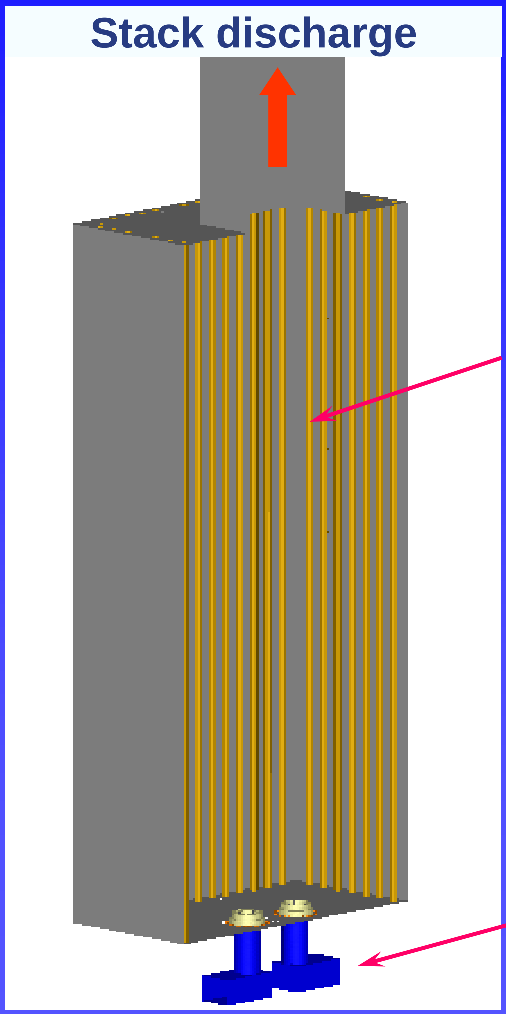
- ~50 acfs per burner (x 8 burners)
- Combustion air temperature 600 °F



Pilots & auxiliaries included

Close-up view of an individual burner cell (group of 4 burners w/ air ductwork

Analysis geometry – Furnace & Burner

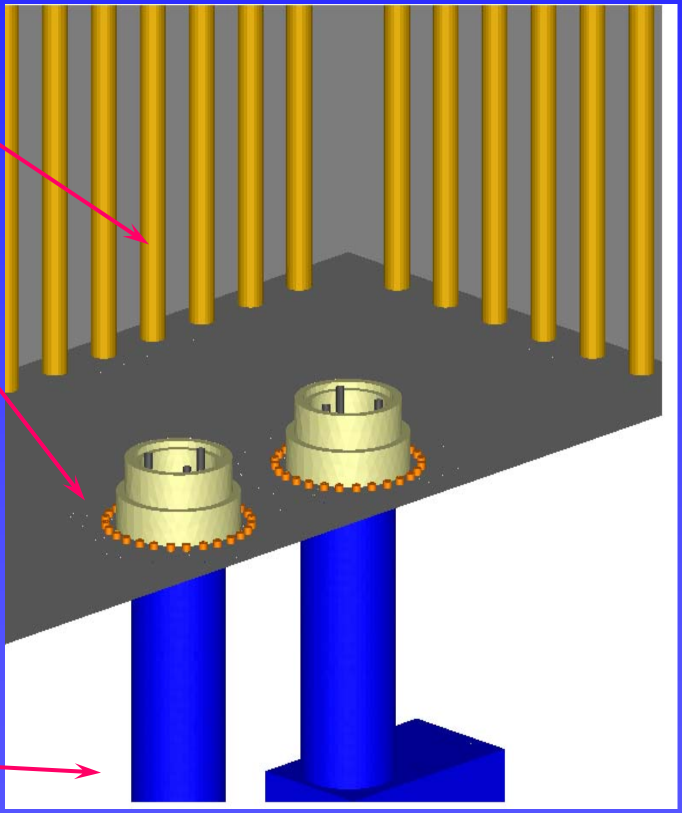


Reflected view – actual model only includes single burner (takes advantage of symmetry planes)

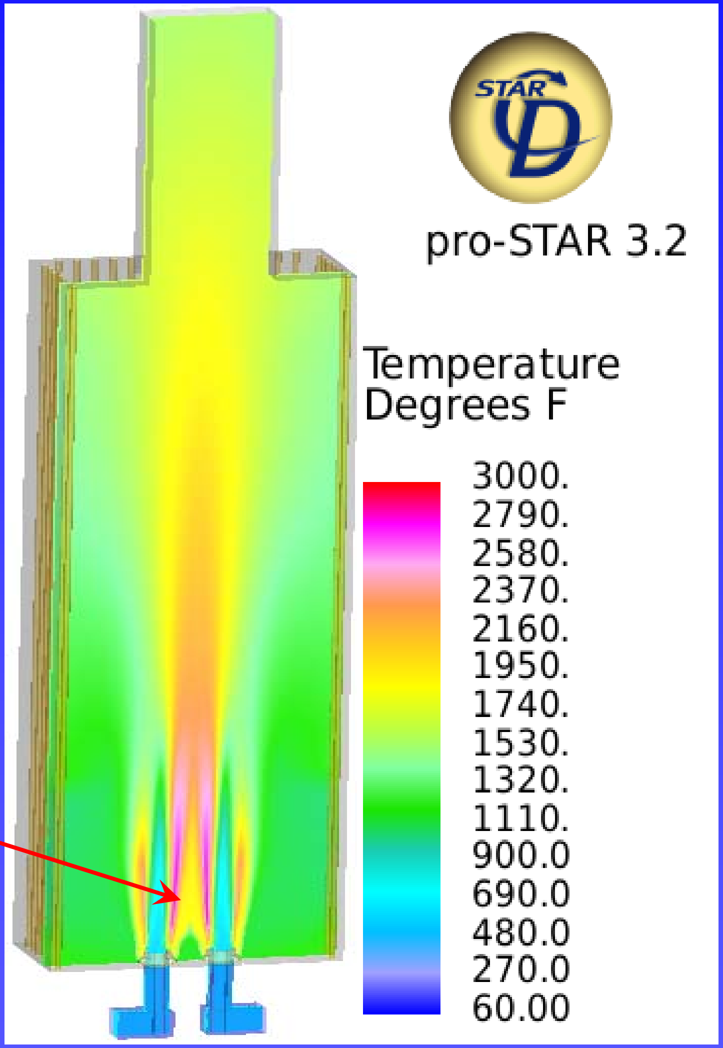
Process Tubes shown in brown

Free Jet Burner w/ gas tips

Air inlets



Predicted Firebox Temperature (°F)



Gas tips near center appear to interact because flames are too close

Natural Gas Gasification

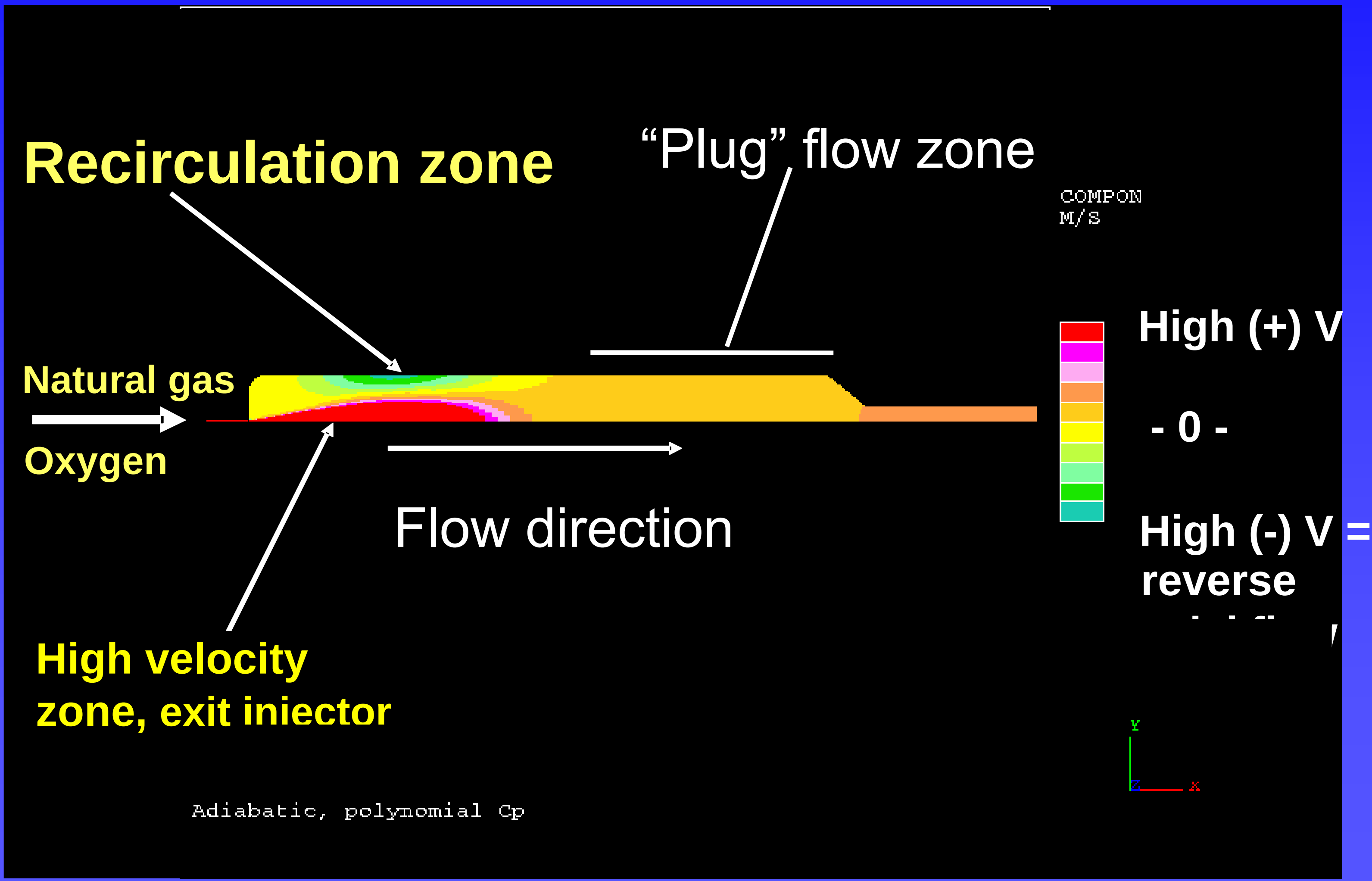
- Is applied industrially for H_2 and CO production.

- Provides the simplest chemical system as departure point for modeling:

$$CH_4 + O_2 \rightarrow CO + H_2 + (H_2O + CO_2 + CH_4)$$

- Provides opening opportunity to implement full reaction kinetics vs. equilibrium only CFD calcs.

Equilibrium Model: Contours of Axial Velocity in Pilot Gasifier, Steady state simulation



Kinetics Model: Transient Velocity Profile

t = 0 to t = 5.9 sec (~ 1.5 res. time)

High Velocity

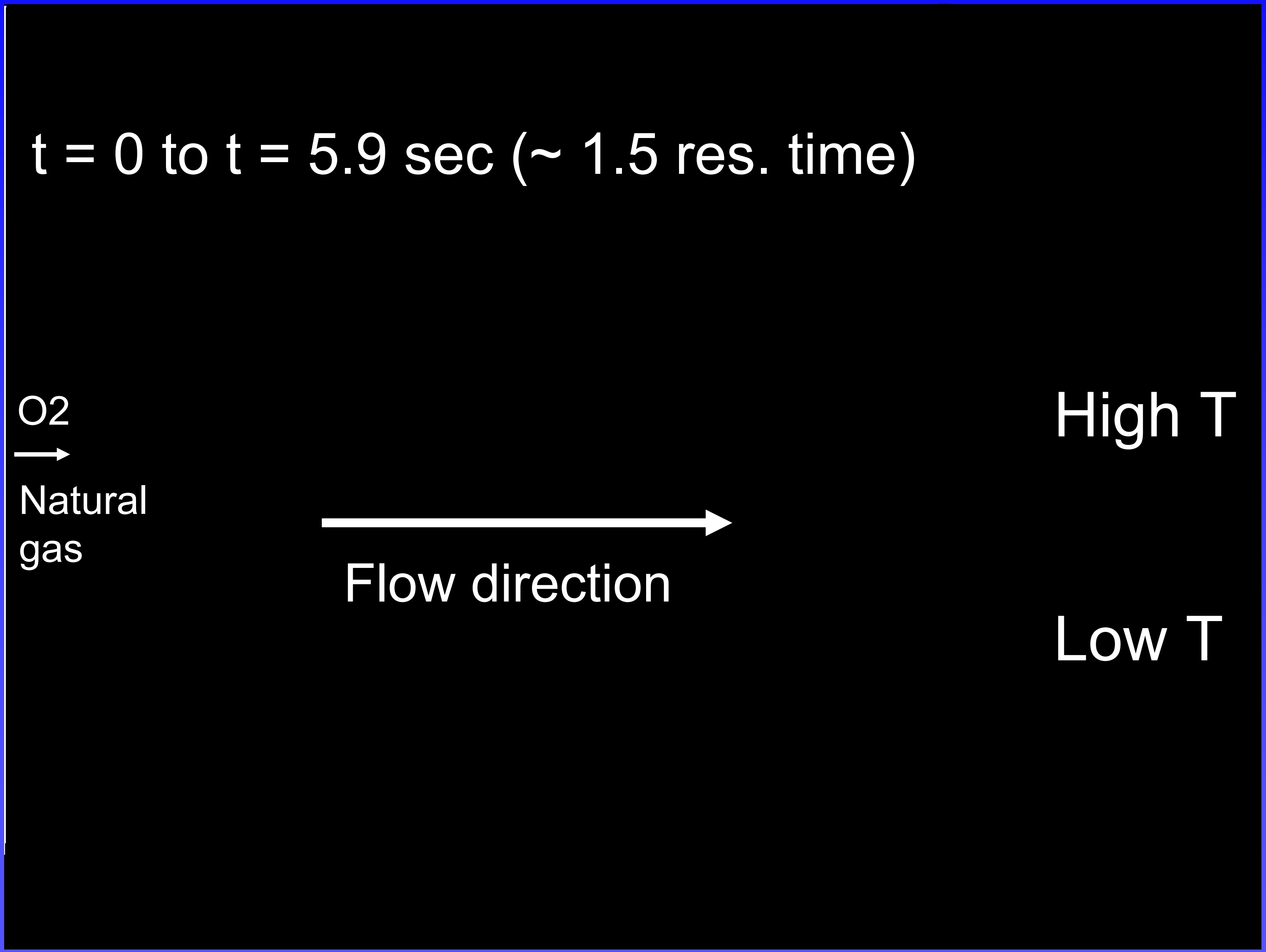
O2

Natural gas

Flow direction

Low Velocity

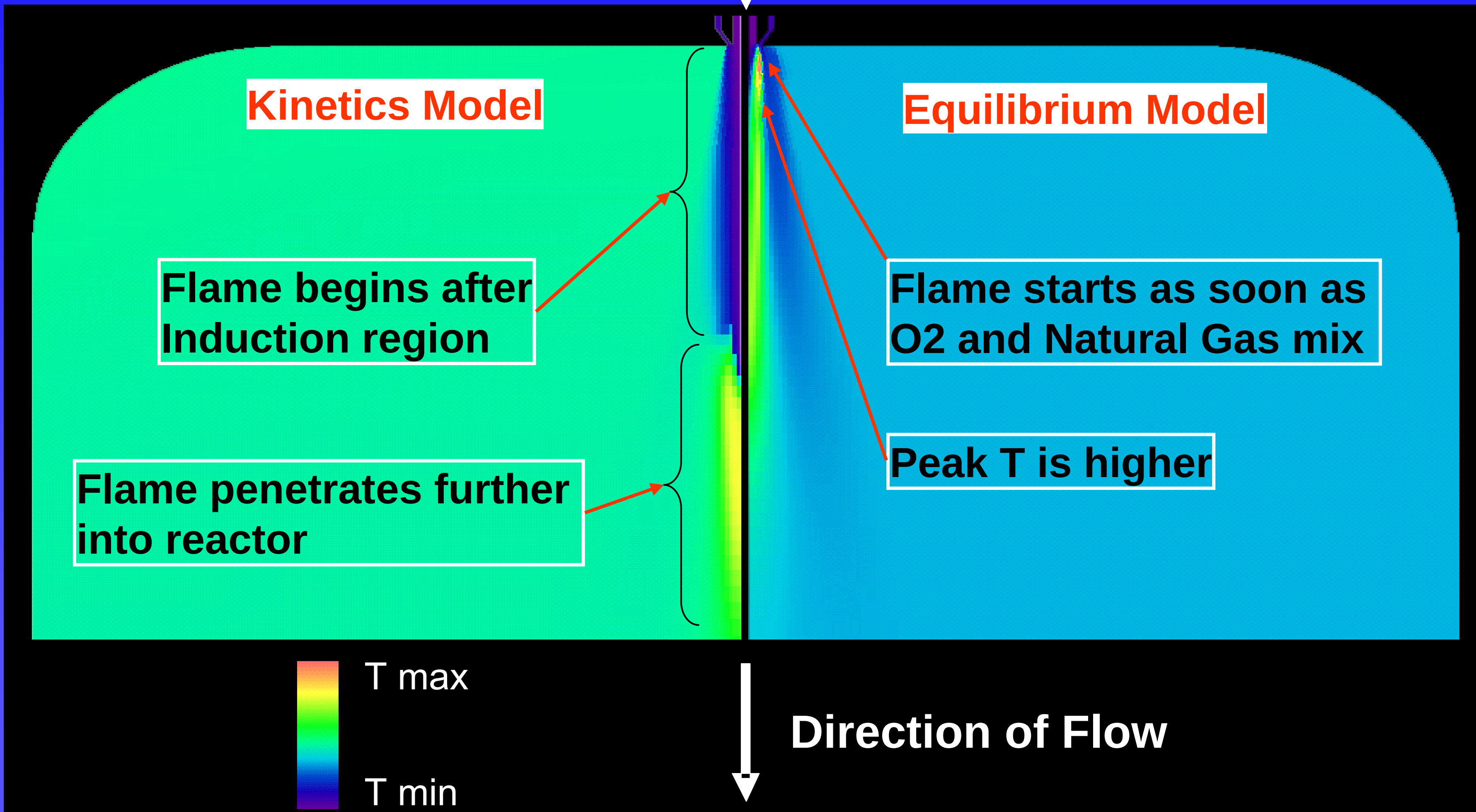
Kinetics Model: Transient Gasifier Temperature



The Models Predict Different Flame Shapes....

Top of gasifier

Injector: O2 + Natural Gas



Conclusions and Summary

- Combustion CFD started in early 70's at National Labs (i.e., Harwell, Los Alamos, etc.) and Universities (Imperial College, Sheffield, BYU, etc.) and evolved through 80's (limited funding in 90's)
- Initial technology ported to commercial CFD codes to support technology transfer to industry
- Parameterization of CFD geometry/operating data allows coupling to optimization software (i.e., mod-frontier) to quickly investigate engineering designs
- Advanced Physics (fluid/solid interaction, combustion acoustics, detailed reaction kinetics, etc.) possible with better/cheaper computers
- CFD linked to Design software (i.e., ProE, Solidworks)
- Challenges remain slagging/fouling, detailed chemistry, conjugant heat transfer, full plant models

Acknowledgements

- Jan Garvey/Kerry Irons and Dow Chemical for support of work on RCl Incineration
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