

CFD Analysis of Dynamic TGA Furnace

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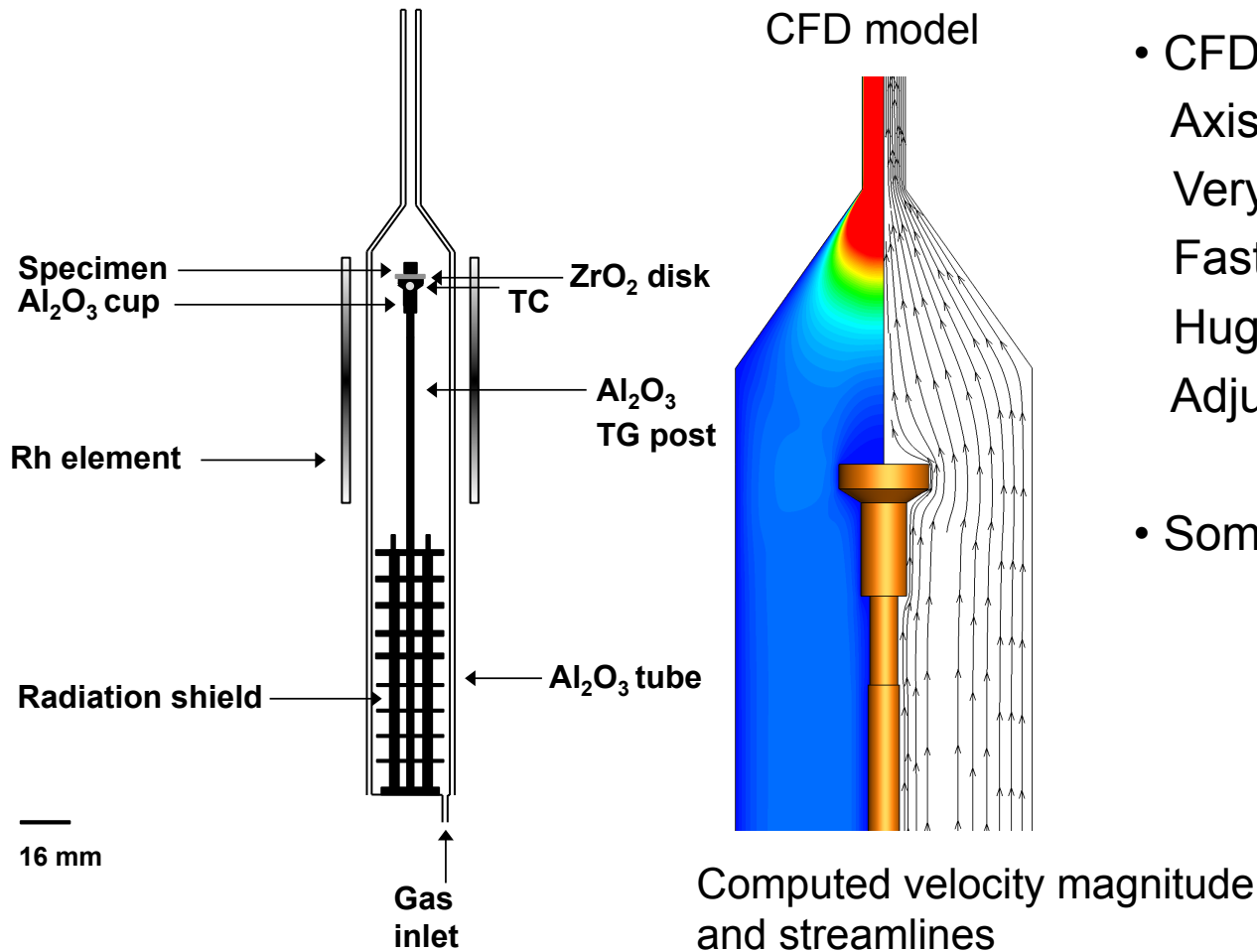
Support from AFOSR

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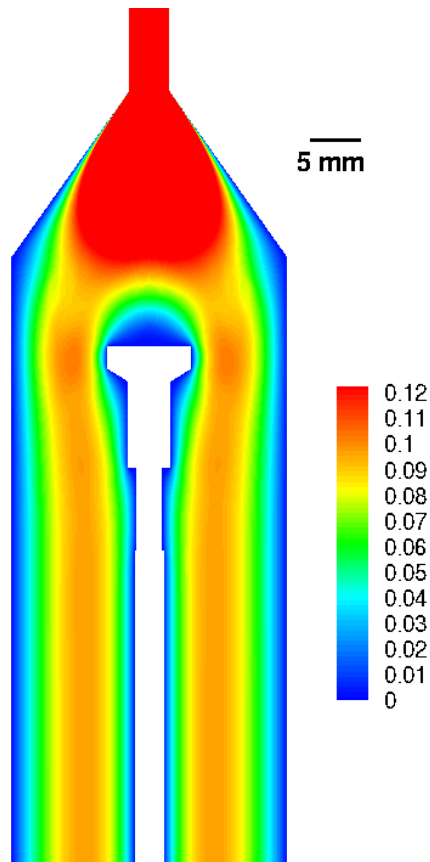
Modeling of U Arizona High Temperature Test Facility

- Use CFD to simulate NDE-TGA experimental facility (Corral et al.):



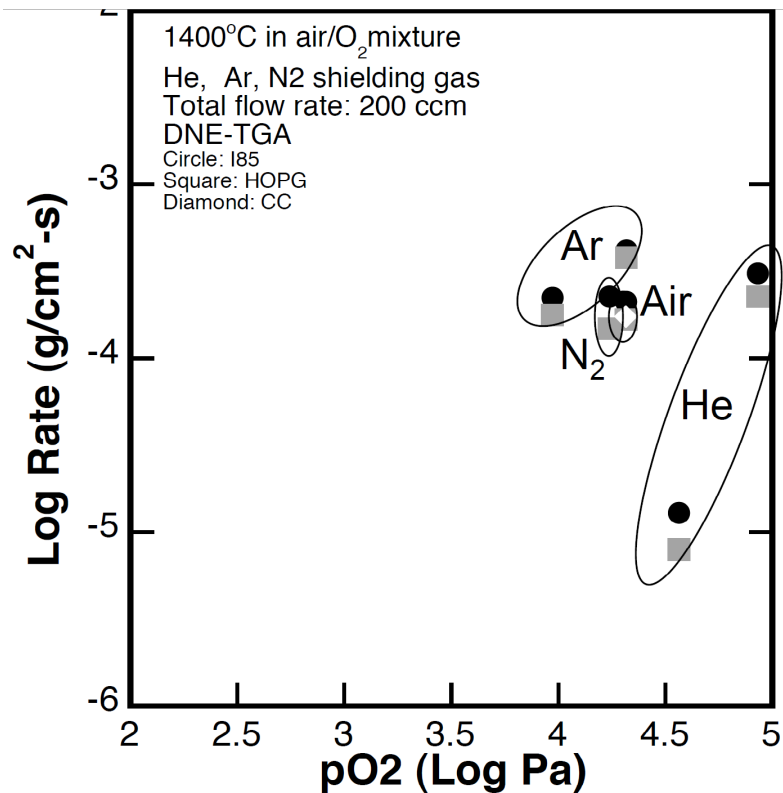
- CFD Simulation:
 - Axisymmetric, non-reacting air
 - Very low flow speeds
 - Fast kinetics
 - Huge range of time scales
 - Adjust Δp to get flow rate
- Somewhat demanding

Modeling of U Arizona High Temperature Test Facility



- Simulation at nominal operating conditions:
 - Flow speeds ~ 0.1 m/s
 - Varying thickness boundary layers
 - Sample sits in low-speed region
 - Simulations are time-consuming
- Represent experiment with a 2D channel:
 - Inert, isothermal surfaces
 - 2 cm section of carbon material
 - Vary flow conditions
 - Vary gas-surface interaction models

2D Channel Simulations

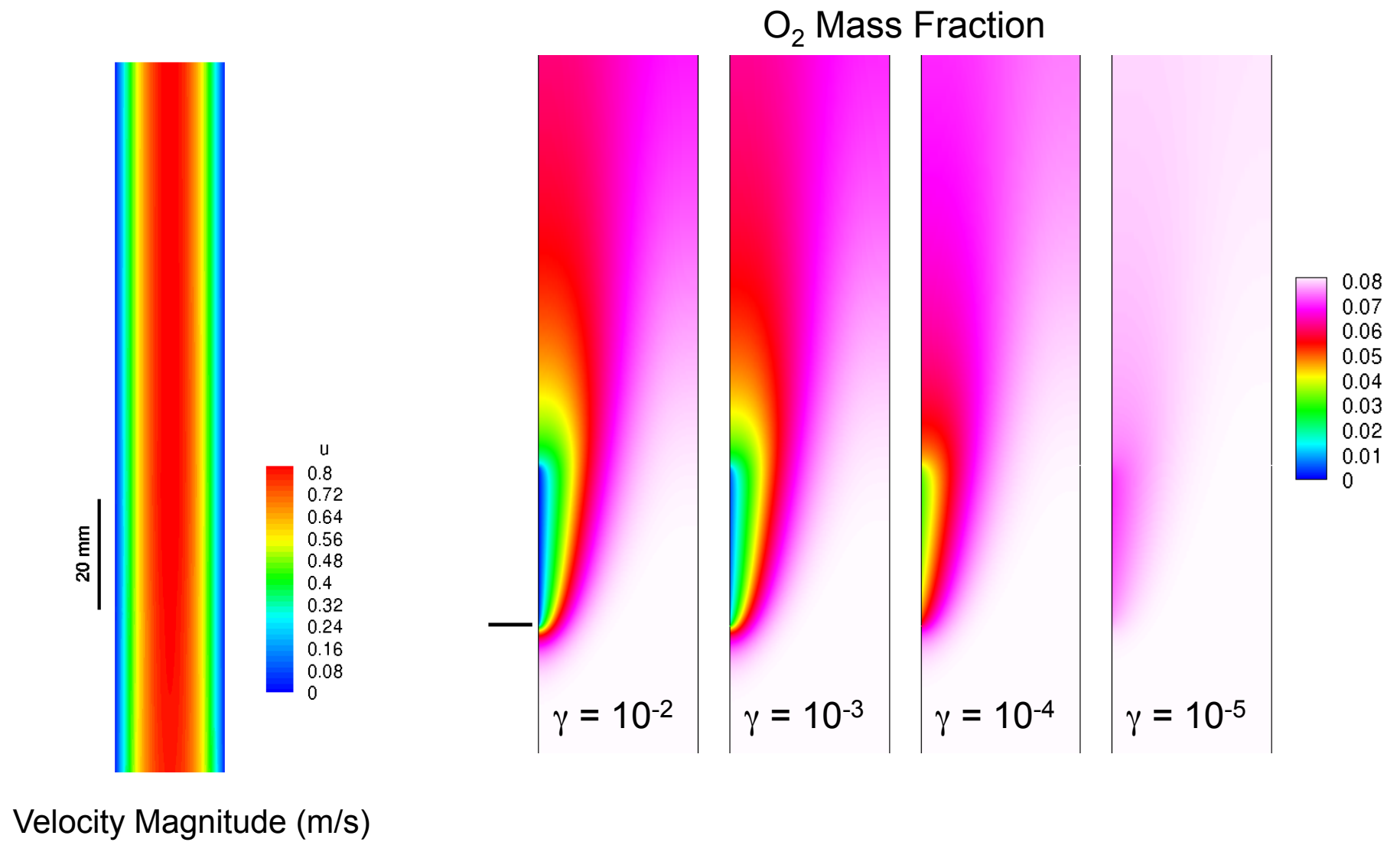


Corral et al. DNE-TGA results at 1400° C

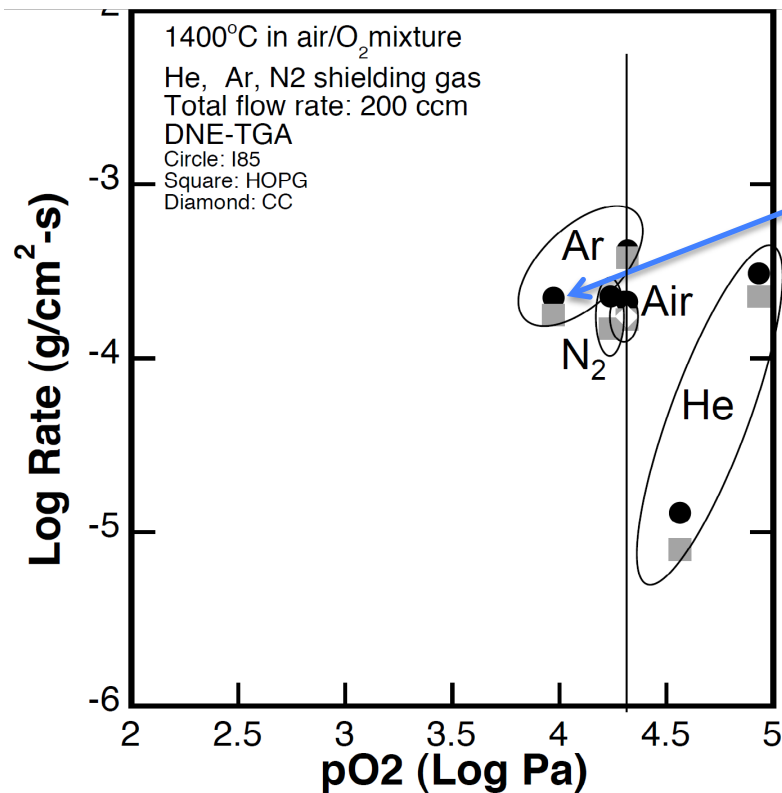
- Focus on DNE-TGA at 1400° C
- Simulations with Zhluktov-Abe model:
 13 species, 12 gas-surface reactions
 Full finite-rate chemical kinetics
 Best available model
- Surface reactions dominated by CO₂:
 CO, C, C₂, C₃ < 10⁻⁷
- Simplify gas-surface interaction model:

$$\text{C(s)} + \text{O}_2 \rightarrow \text{CO}_2$$
 Catalytic efficiency = γ
 Fraction of O₂ that reacts on the surface

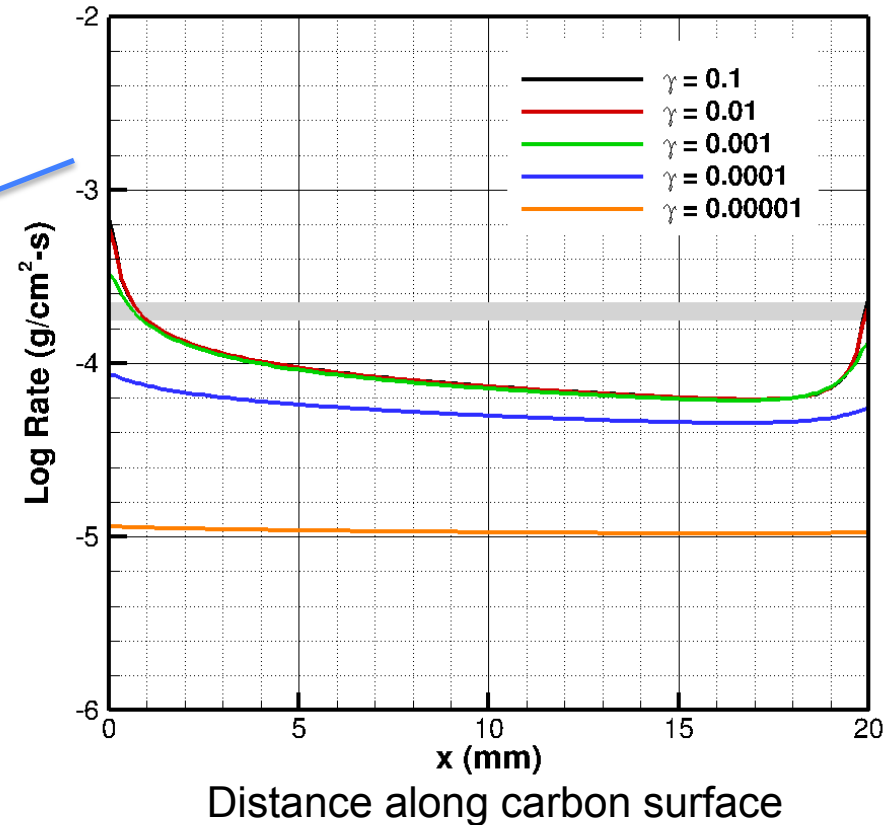
Argon Case 1: $\text{Log PO}_2 = 4.0$



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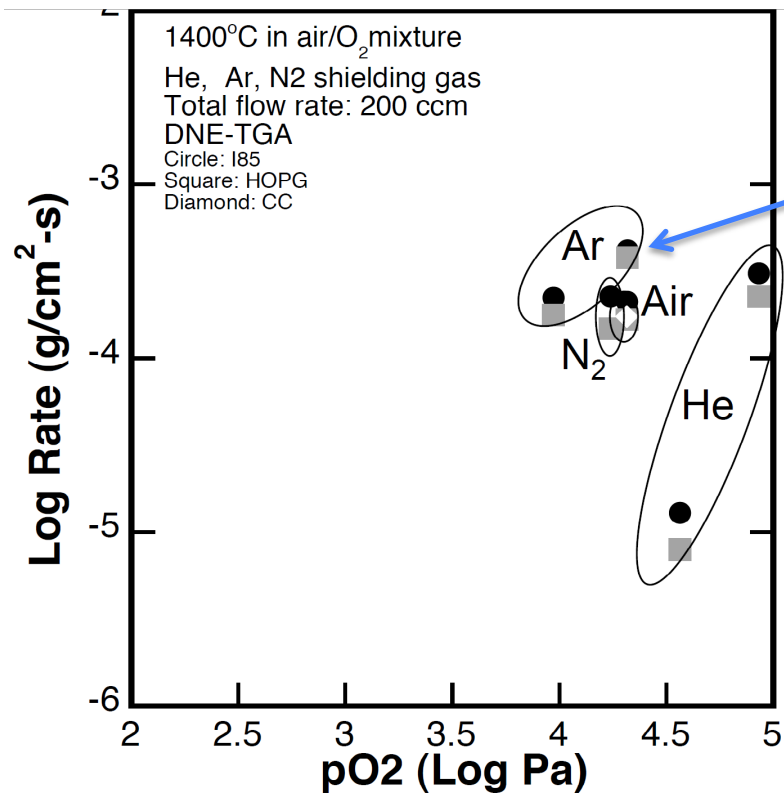


Simulation results for C loss rate

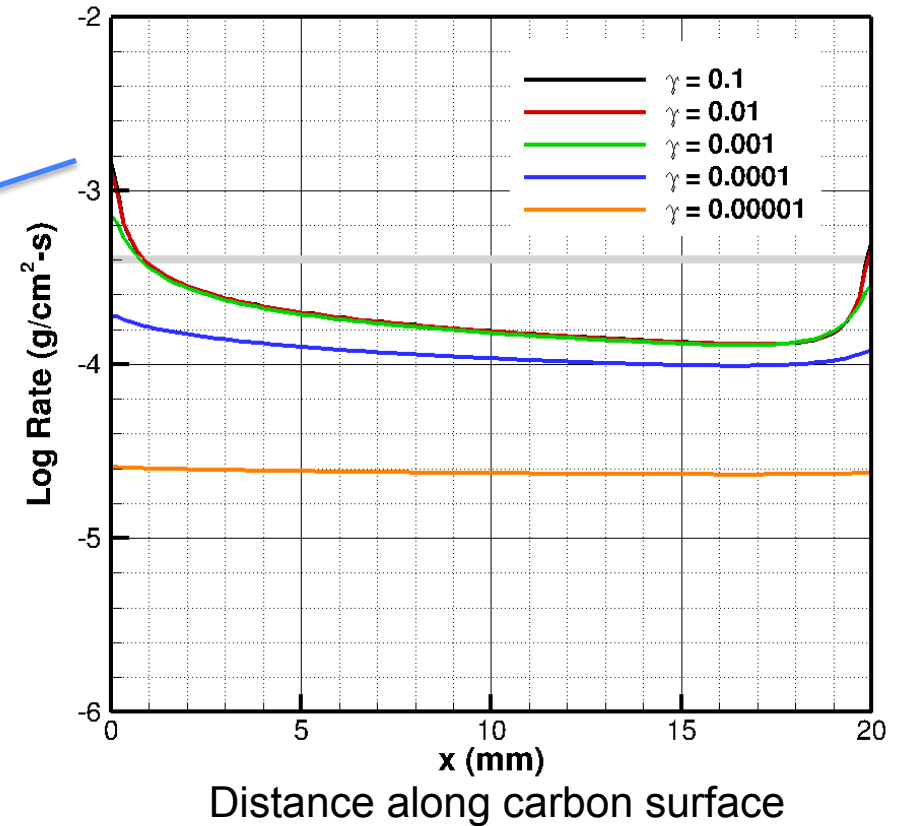


- Large variation in reaction rate along plate
- Diffusion limited for $\gamma > 10^{-3}$, approximately brackets data

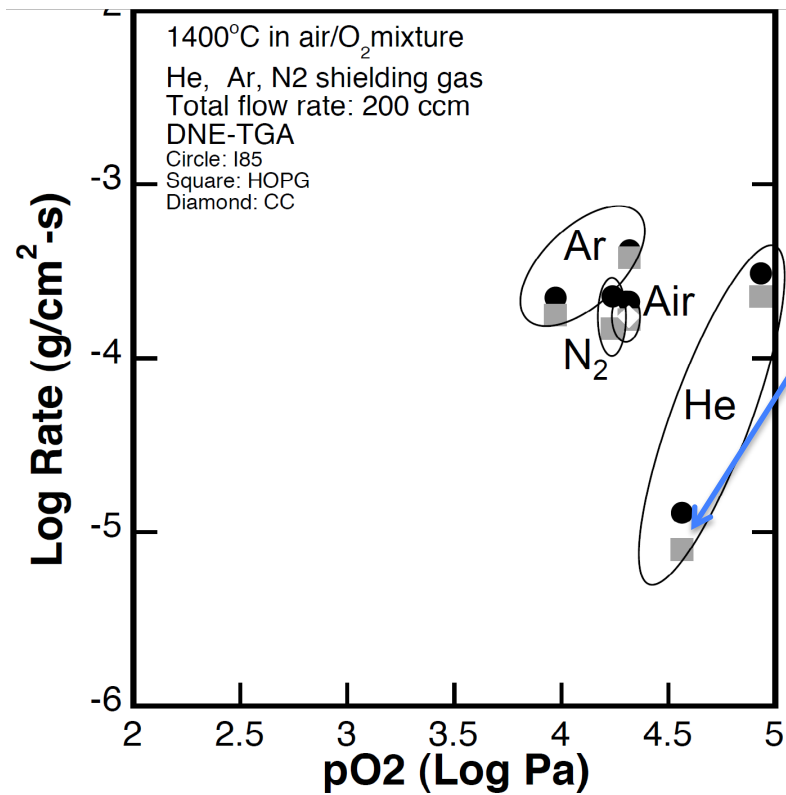
Argon Case 2: $\text{Log PO}_2 = 4.3$



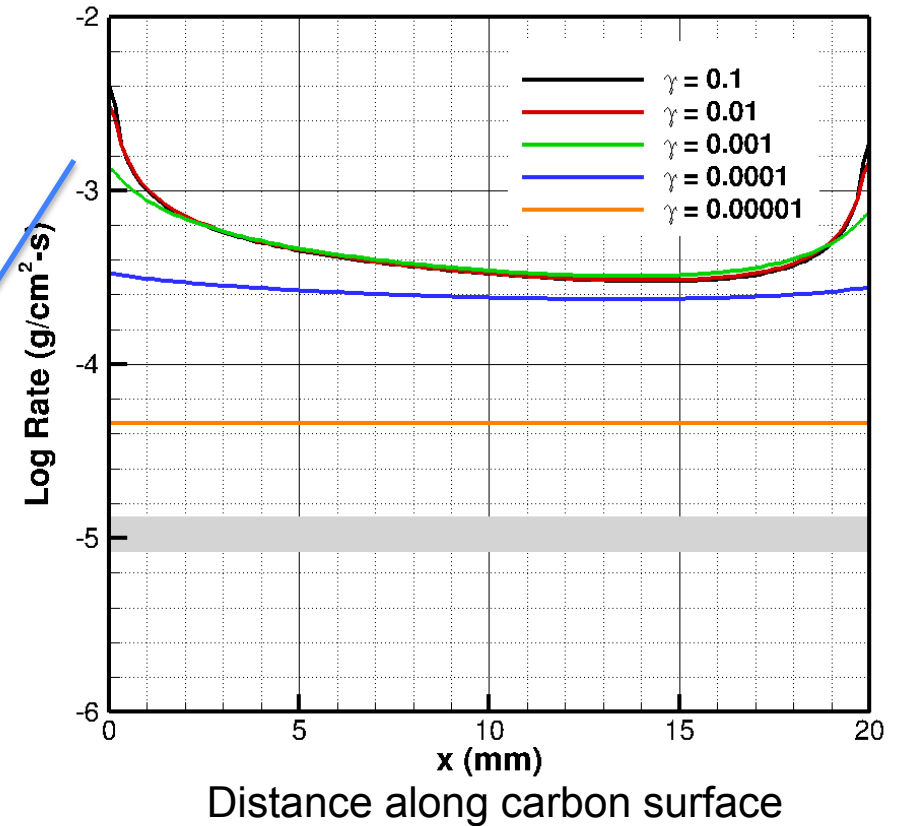
Simulation results for C loss rate



Helium Case 1: $\text{Log PO}_2 = 4.6$

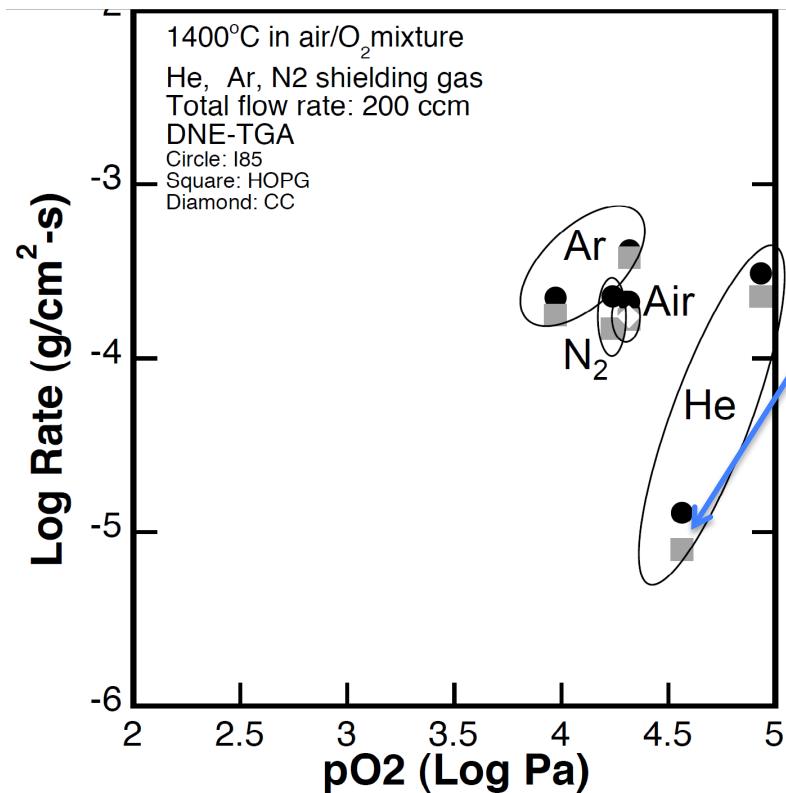


Simulation results for C loss rate

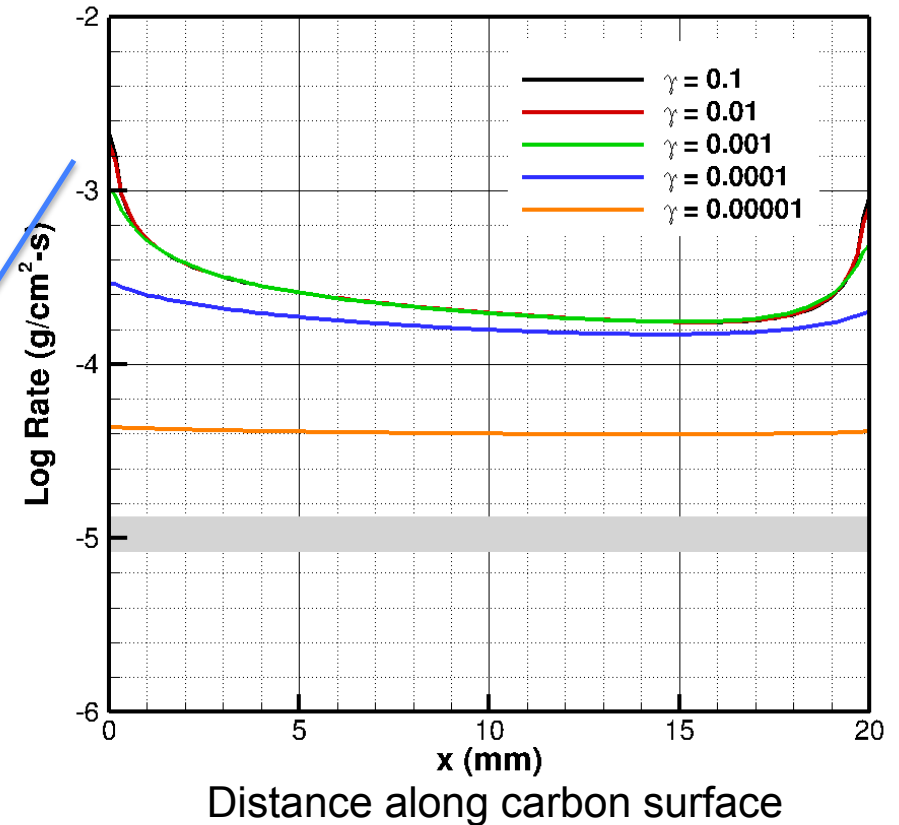


- Fickian diffusion with $Le = 1.4$
- Simulations are 2 orders of magnitude high

Helium Case 1: $\text{Log PO}_2 = 4.6$



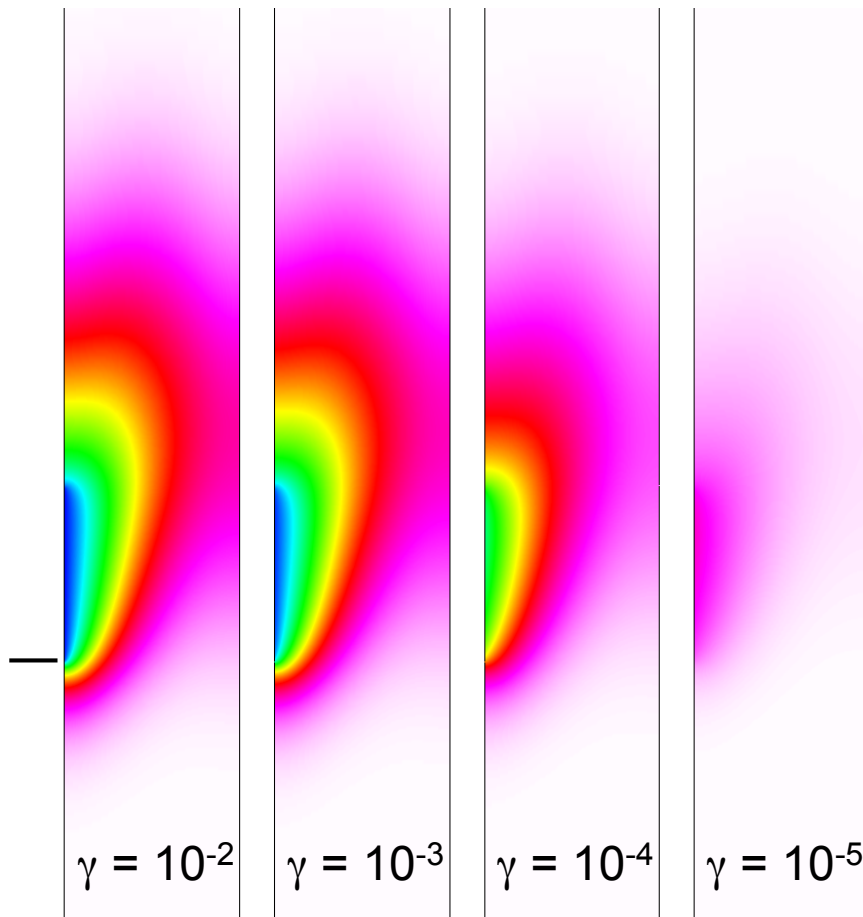
Simulation results for C loss rate



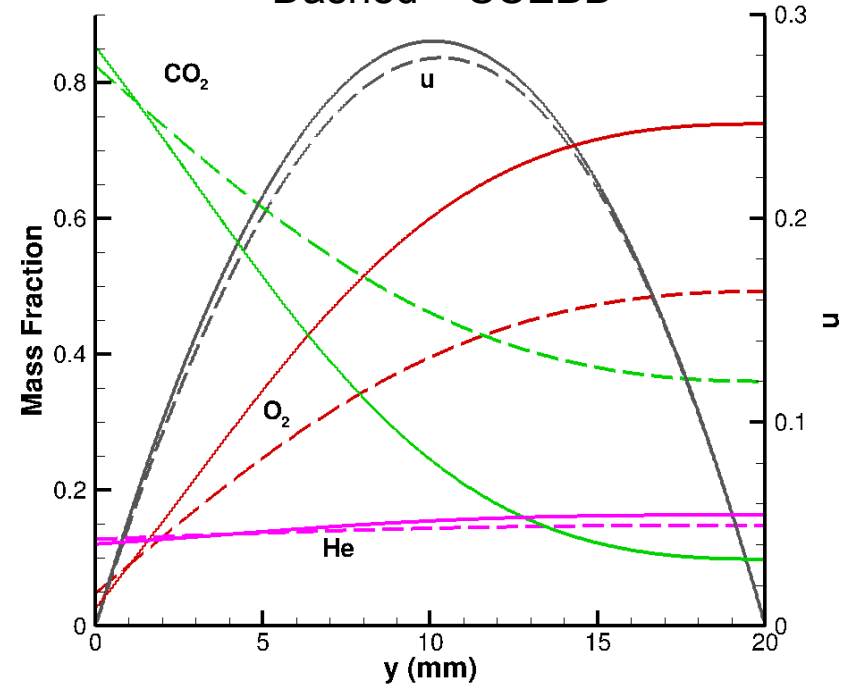
- Self-consistent effective binary diffusion
- Closer, but still over-predicts data

Helium Case 1: $\text{Log PO}_2 = 4.6$

O_2 Mass Fraction: SCEBD

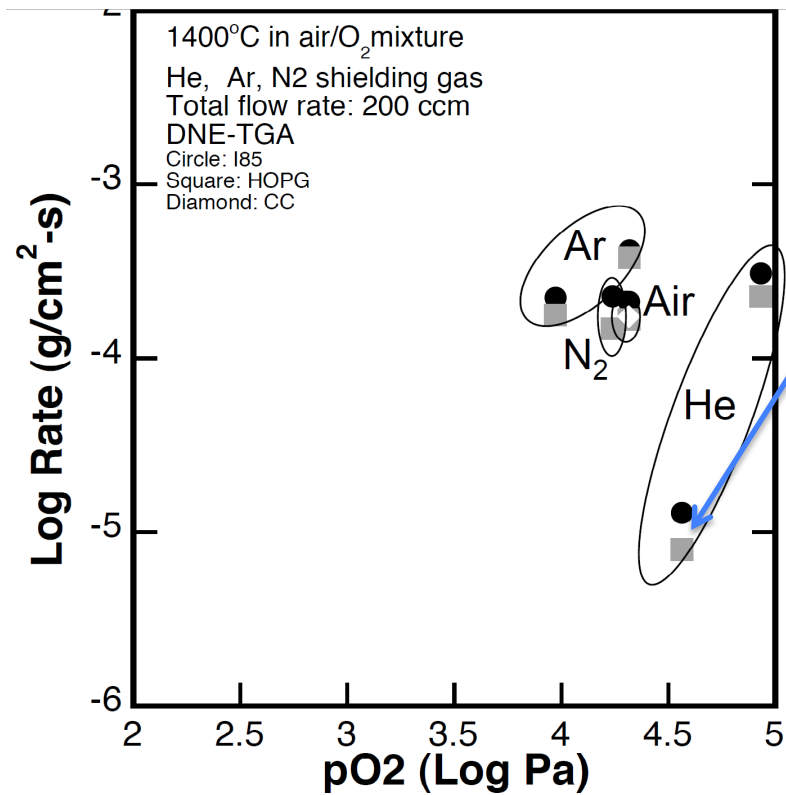


Solid = Fickian
Dashed = SCEBD

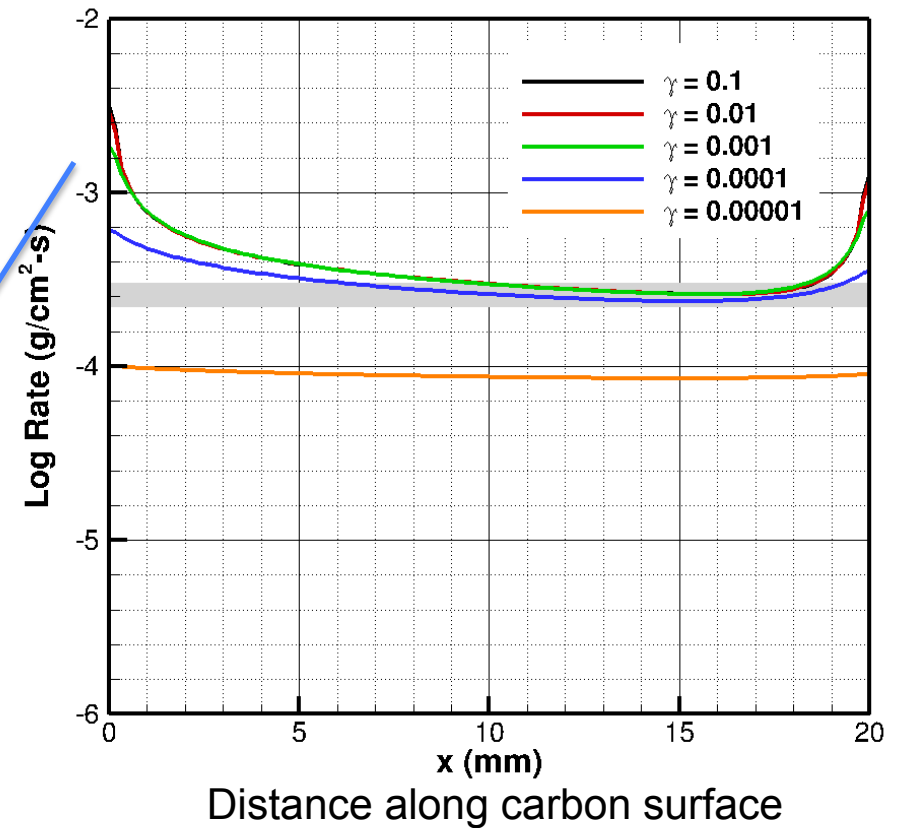


Distance across channel at $x = 10$ mm

Helium Case 2: $\text{Log PO}_2 = 4.9$



Simulation results for C loss rate



- Also slightly high
- Issues with diffusion model?

Summary and Next Steps

- CFD simulations are needed to understand flow in DNE-TGA
- Approximately bracket Ar and N₂ data with $\gamma \sim 10^{-3}$
- Simulations predict excessive reaction for He:
 - Diffusion models are critical
 - Role of flow speed?
- Simulate full DNE-TGA geometry
- Establish bounds on $\text{C(s)} + \text{O}_2 \rightarrow \text{CO}_2$ rate
- Design a DNE-TGA with less dependence on diffusion rates:
 - Larger flow speeds
 - Thinner boundary layers

MURI: Scientific Accomplishments / Breakthroughs

- N_4 , O_4 , N_2O_2 potential energy surfaces at relevant conditions
- Novel potential energy surface fitting approaches
- Parallelization and upgrades of ANT trajectory code
- Shock-layer radiation emission measurements at flight conditions
- ReaxFF modeling of graphite gas-surface interaction
- CFD analysis of Dynamic Nonequilibrium TGA
- Molecular beam measurements of UHTCs and graphite at high T
- Sensitivity of shock layer flows to detailed rate processes
- Potential universal carbon oxidation mechanism