Numerical Simulation of Reducing Gas Composition Impacts on DRI Shaft Furnace Operation

Samuel E. Nielson[1], Tyamo Okosun[1], Kevin Persad[2], Thomas Cash[2], Eugene Pretorius[3], Chenn Q. Zhou[1]

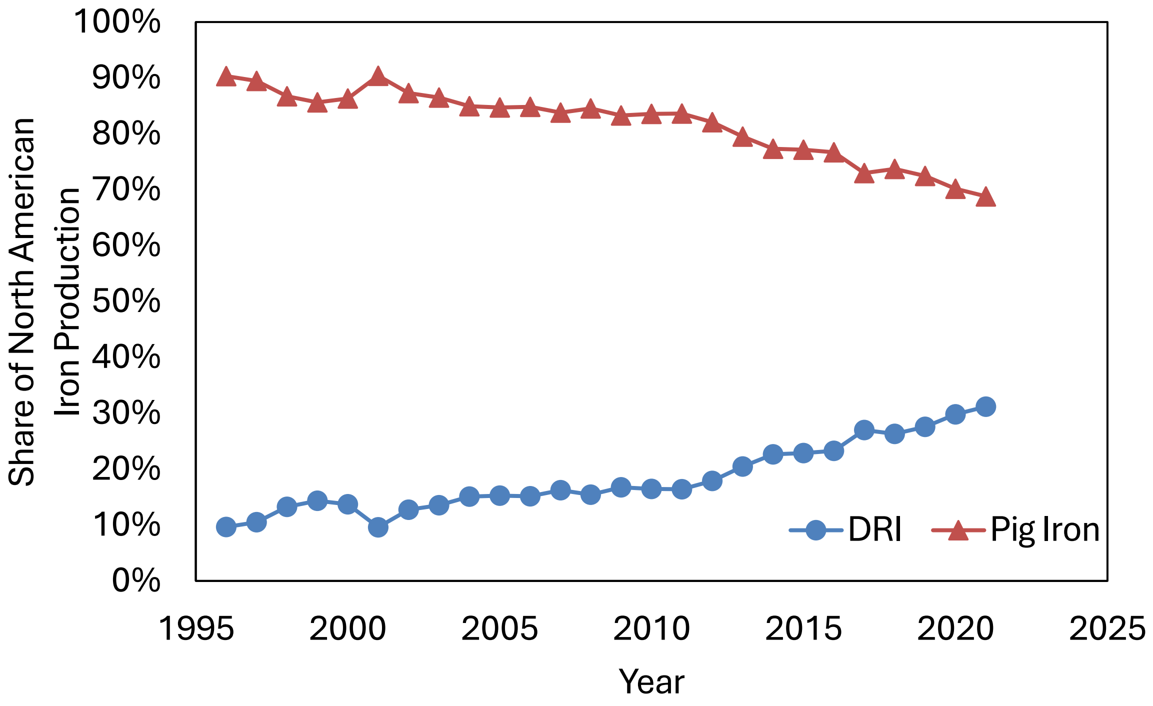
[1]Center for Innovation through Visualization and Simulation (CIVS), Purdue University Northwest, 2200 169th Street, Hammond, IN 46323, USA; Phone: 1-219-989-2665; Email: tokosun@pnw.edu

[2]Nucor Steel Louisiana, 9101 LA-3125, Convent, LA 70723

[3]Nucor Steel Berkeley, 1455 Hagan Ave, Huger, SC 29450

Introduction

- Direct Reduced Ironmaking
  - Efficient: Lower carbon emissions
  - Versatile: Feedstock for EAF or BF
  - Economical: 89% increase in annual NA production over last 25 years
- Similar physics to upper region of blast furnace
  - Gaseous reduction of ore pellets
- Differences to blast furnace
  - No smelting, no coke, limited N_2
  - Methane reforming
  - Higher pressure
  - Higher reducing gas concentration
  - Gas recycling



Introduction

- 25+ years of BF Computational Fluid Dynamics (CFD) modeling at Purdue University Northwest
- Translating BF modeling experience to DRI furnace

Center for Innovation through Visualization and Simulation **(CIVS)**

- Missions
  - Innovation **($50+ million** grants)
  - Application **($40+ million** savings from 5 out of 460+ projects)
  - Education (**2250+** research students)
- Strategies
  - **Integration** of technologies
  - Application driven
  - Partnerships (**180+** organizations)

Steel Manufacturing Simulation and Visualization Consortium **(SMSVC)**

Research Areas

1) Energy Efficiency
2) Environmental Impacts
3) Operation Efficiency
4) Raw Materials Utilization
5) Reliability and Maintenance
6) Smart Manufacturing
7) Workforce Development
8) Workplace Safety

Project Topics

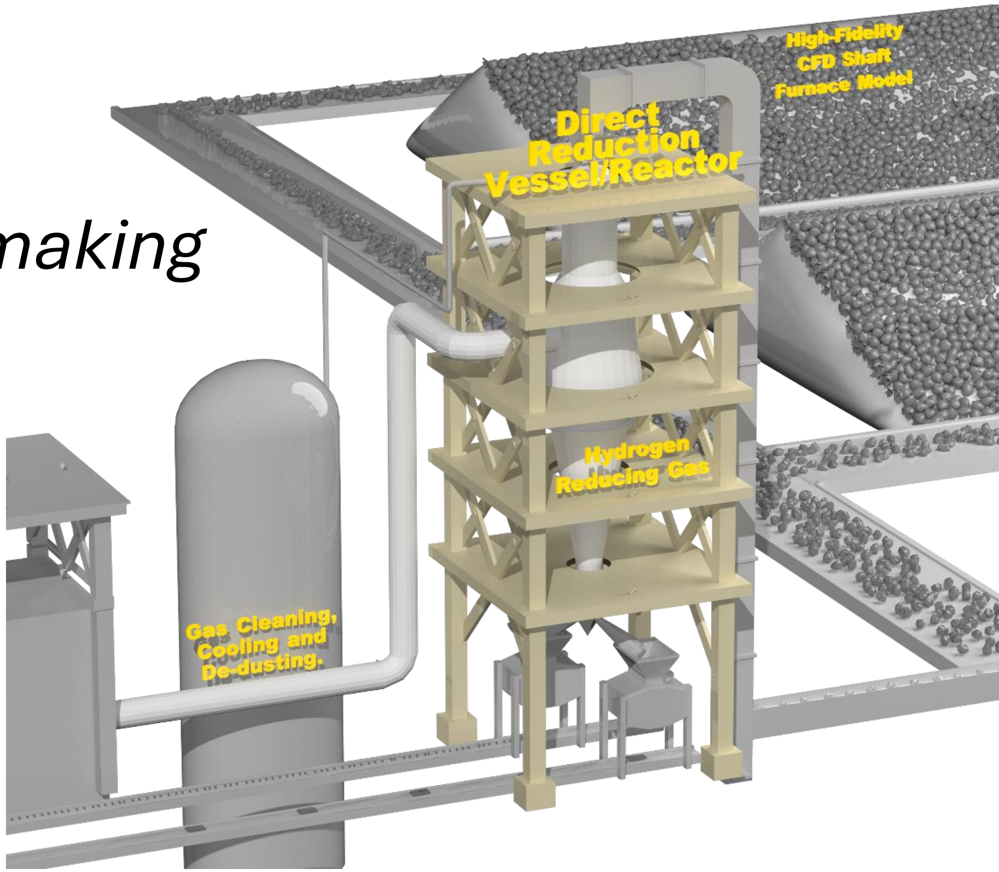
- Ironmaking
- Electric Arc Furnace
- Ladle
- Continuous Casting
- Reheating Furnace
- Safety and Training

(6 project technical committees with **200+** industry participants)

- Focused Areas:
  - **Smart Manufacturing:** Digital Twin, AI, Multi-physics Modeling, Simulation & Visualization
  - **Energy,** environment, productivity, quality
  - **Workforce Development:** Virtual training simulators for processes and safety

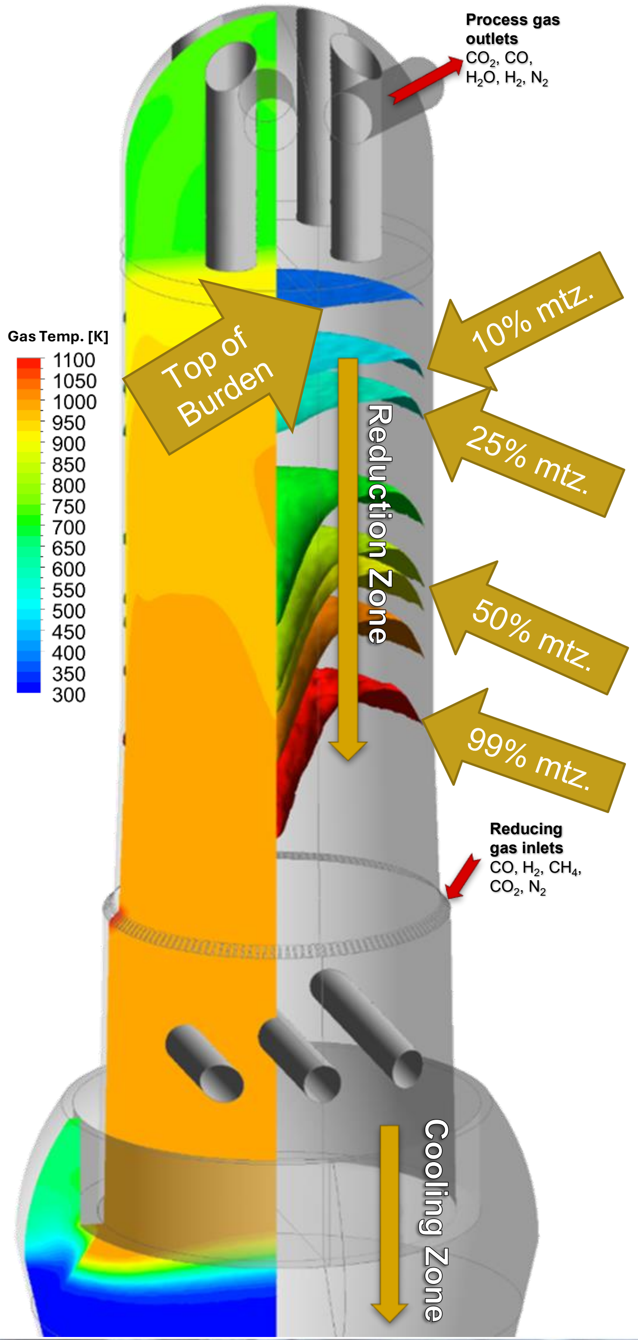
Introduction

- Project: *Scaling Hydrogen-Direct Reduced Iron Pathways to Decarbonize Iron and Steelmaking*
  - Supported by U.S. Department of Energy
    - Award number DE-EE0010842
  - Project led by Carnegie Mellon University
    - Dr. Chris Pistorius, Dr. Valerie Karplus
  - Standard DRI shaft furnaces use CO/H_2 reducing gas mixture
  - **100% H_2 reducing gas** would eliminate CO_2, but **H_2 reduction presents new challenges**
  - Experimental, LCA/TEA, CFD Modeling for 100% H_2 DRI process
  - Developing a CFD model to simulate existing industrial DRI processes & compare with high-H_2 and 100% H_2 operations



Motivation

- Investigate operation of a DRI furnace with nearly 100% H_2 reducing gas
  - Maintain pellet carbon content near 4.3 wt%
  - Control reduction speed to limit encapsulation risk
  - Simplify process gas scrubbing cycle by reducing need for CO_2 removal
- Limitations
  - Impacts on remainder of plant process not considered
  - Encapsulation risk not yet included in modeling approach
    - "Wustite reserve zone" size can be used as a proxy
    - More rapid reduction rates in modeling might indicate higher likelihood for encapsulation in real world
  - Simplified SMR kinetics for conventional baseline case
  - WGSR and Dry Methane reactions reforming absent in baseline case



DRI Modeling Approaches

- CFD-DEM
  - High computational expense
  - Captures phase interaction with most detail
- Eulerian multiphase/porous zone CFD
  - Good balance of detail and speed
  - 2D or 3D geometry
  - <u>Current method employed for this project</u>
- Plug flow & 1D models
  - Relies on many simplifications and assumptions
  - Low computational expense

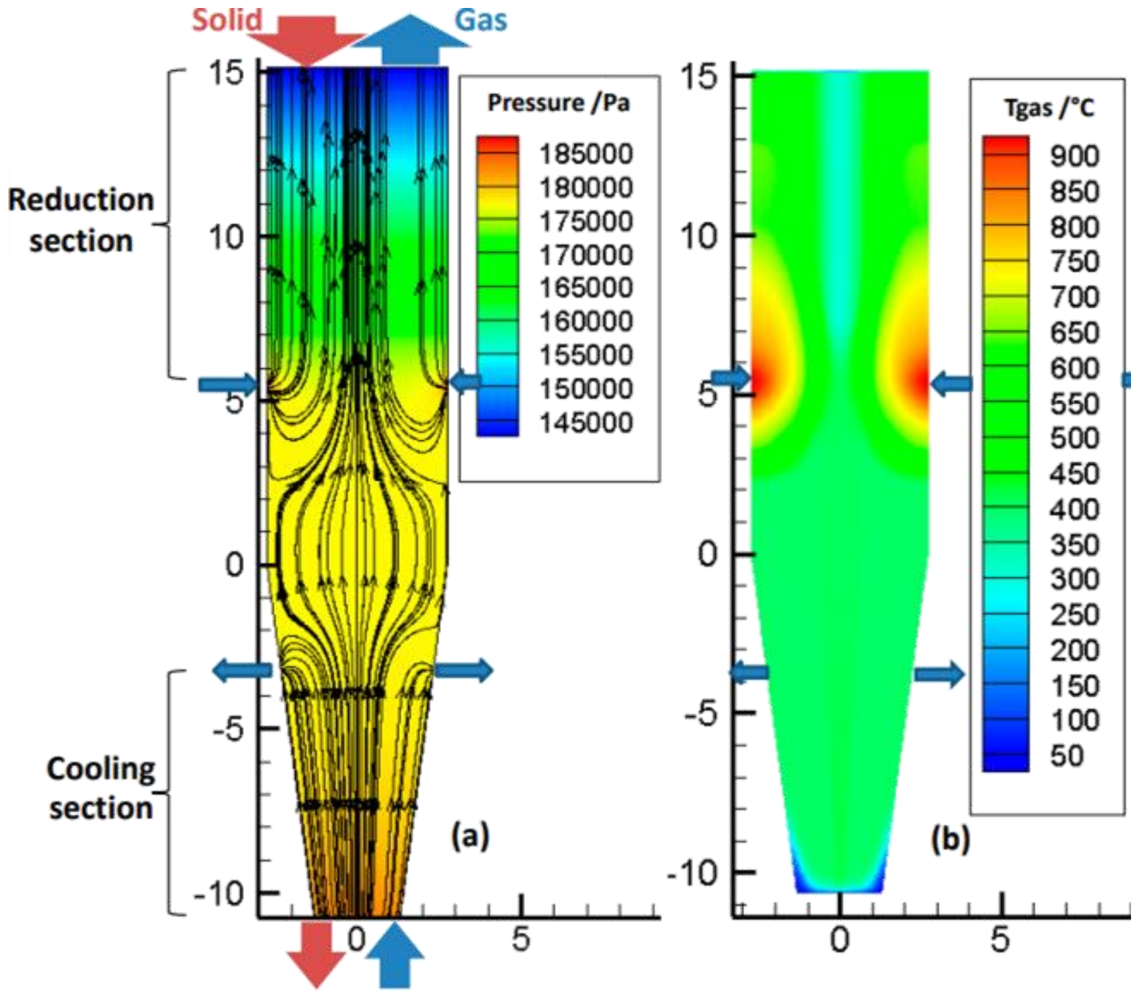
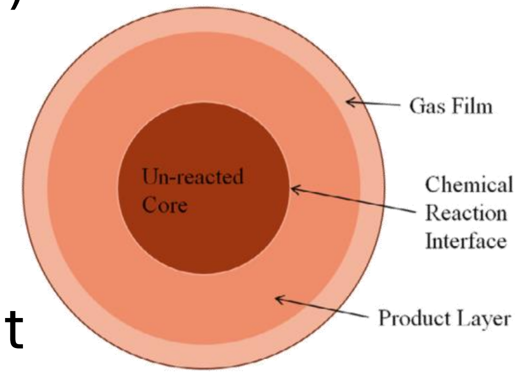


Image Source: Detailed modeling of the direct reduction of iron ore in a shaft furnace, Hamadeh H. et. al. *Materials* 2018.

Model Description

- Commercial Solver (Fluent)
- 3D steady-state
- Eulerian multiphase
  - Gas: Fluent solver
  - Ore: single phase Fluent
- K-ε turbulence model
  - Realizable, Per-phase tracking
- Unreacted Shrinking Core model for reduction
- Oxygen balance production rate mode
- Finite-rate for homogeneous gas reactions
- Interphase heat transfer:
  - Ranz-Marshall



DRI Model Reactions

Reduction Reactions

1) $3\ Fe_2O_3 + H_2 \rightarrow 2\ Fe_3O_4 + H_2O$
2) $3\ Fe_2O_3 + CO \rightarrow 2\ Fe_3O_4 + CO_2$
3) $Fe_3O_4 + H_2 \rightarrow 3\ FeO + H_2O$
4) $Fe_3O_4 + CO \rightarrow 3\ FeO + CO_2$
5) $FeO + H_2 \rightarrow Fe + H_2O$
6) $FeO + CO \rightarrow Fe + CO_2$

Carburization Reactions

7) $Fe + CH_4 \rightarrow Fe_3C + 2\ H_2$
8) $Fe + 2CO \rightarrow Fe_3C + CO_2$

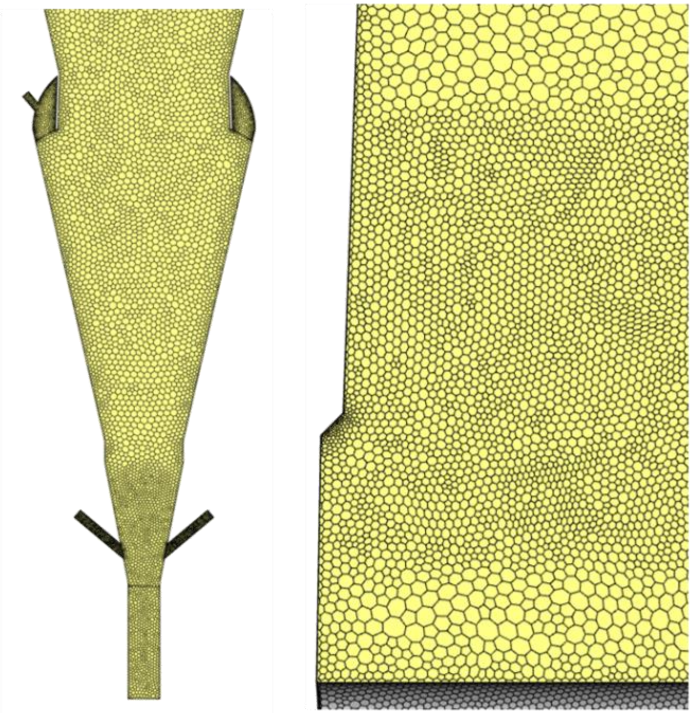
Homogenous Gas Phase Reactions

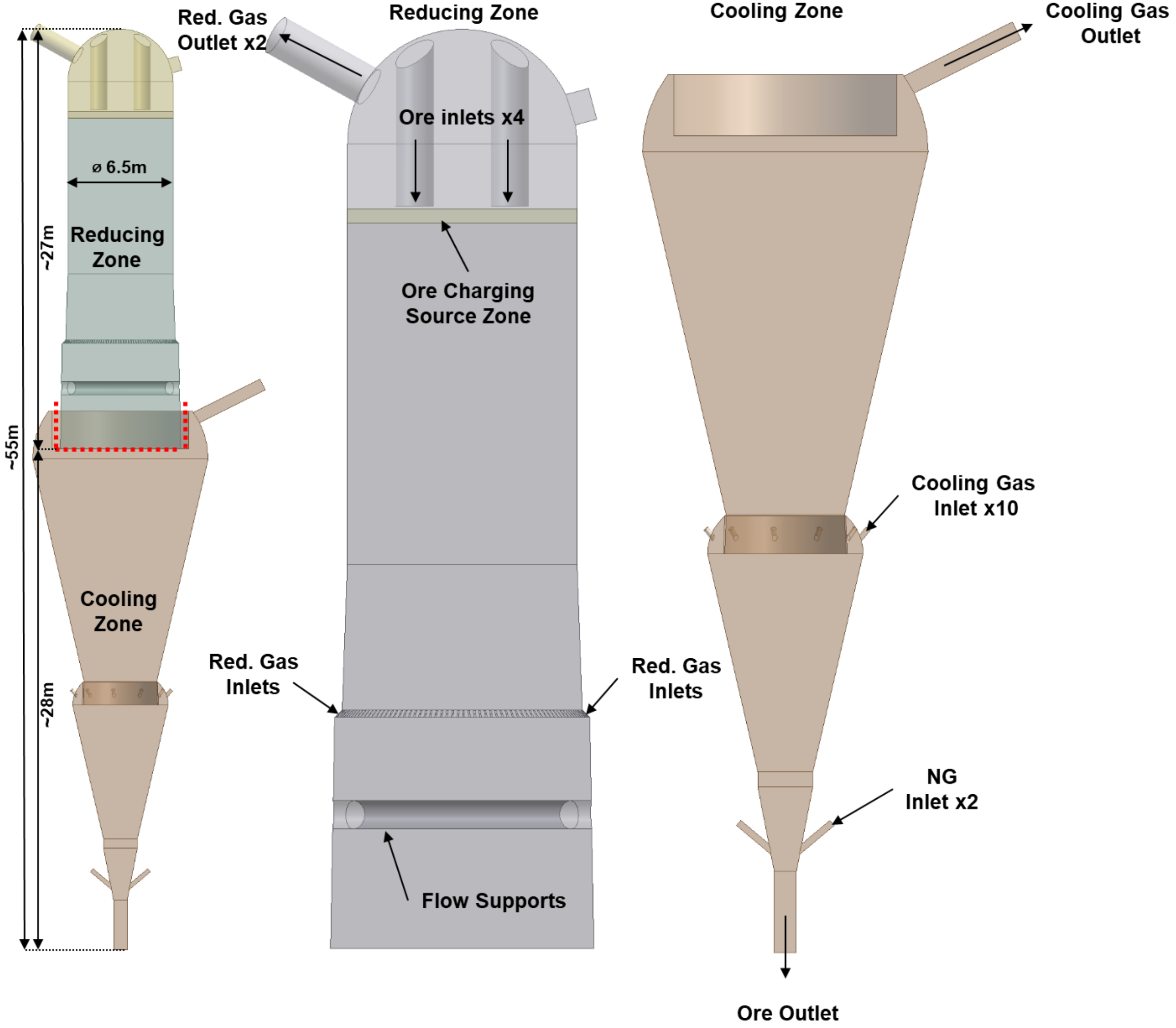
9) $CH_4 + H_2O \rightarrow CO + 3\ H_2$
10) $CH_4 + CO_2 \rightarrow 2\ CO + 2H_2$
11) $CO + H_2O \leftrightarrow CO_2 + H_2$

Yet to be implemented in red

Computational Geometry

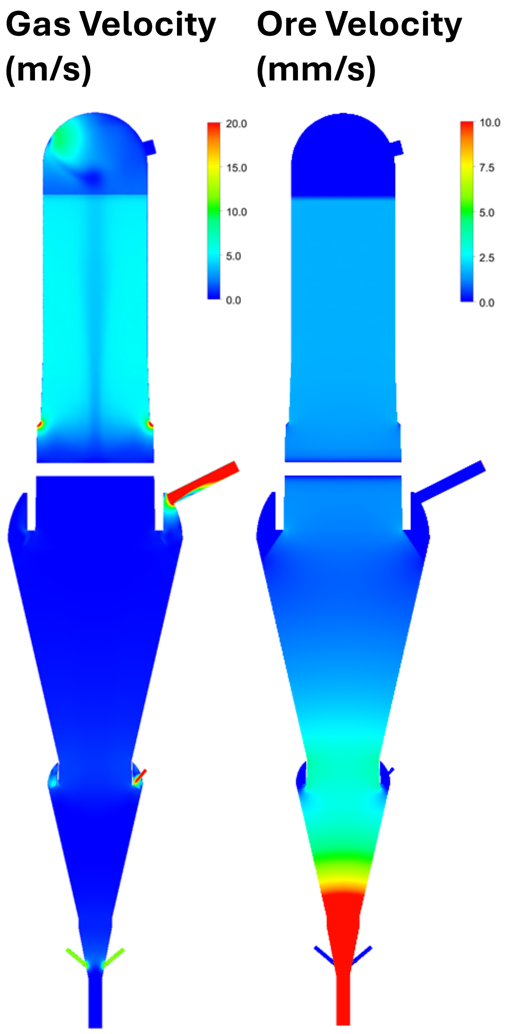
- Polyhedral mesh:
  - 1.54 million cells
  - Single symmetry plane
  - Local refinement





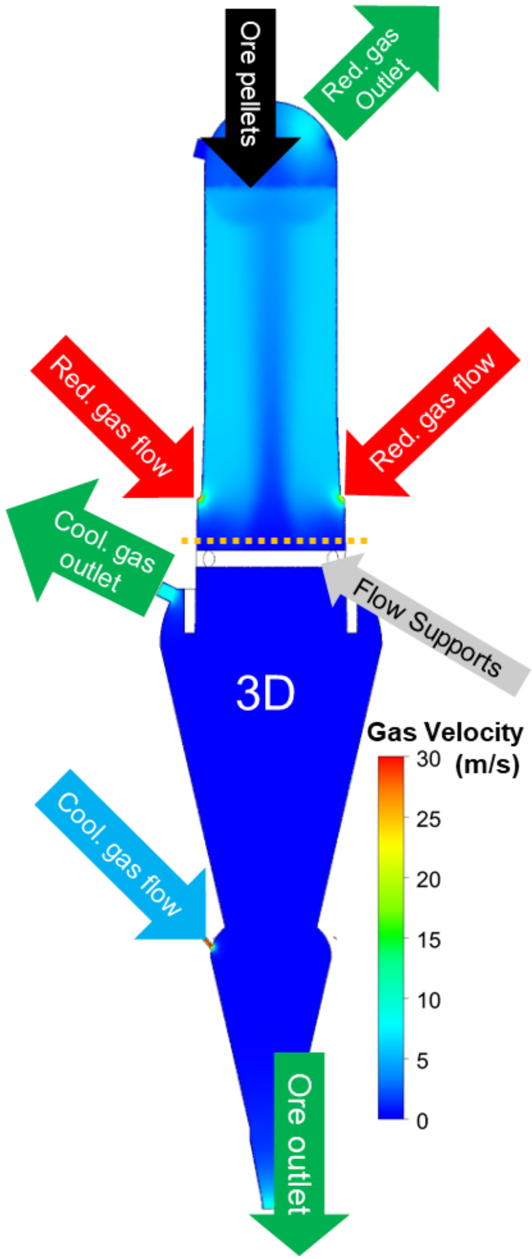
Multiphase Flow Modeling

- Eulerian multiphase
  - Transient → automatic solution of ore flow → very slow solution
  - Steady state → frozen ore flow → fast solution
- Ore flow:
  - Single phase model to calculate ore velocity field
  - Velocity field frozen and mapped to multiphase model
- Gas flow
  - Handled by Fluent
  - Outflows adjust pressure to hit target mass flow rate
    - Adjusts to account for variable interphase mass transfer with carburizing and reduction reactions
    - User sets expected mass exchange between zones
  - Tracks impacts of chemistry and temperature changes on flow field



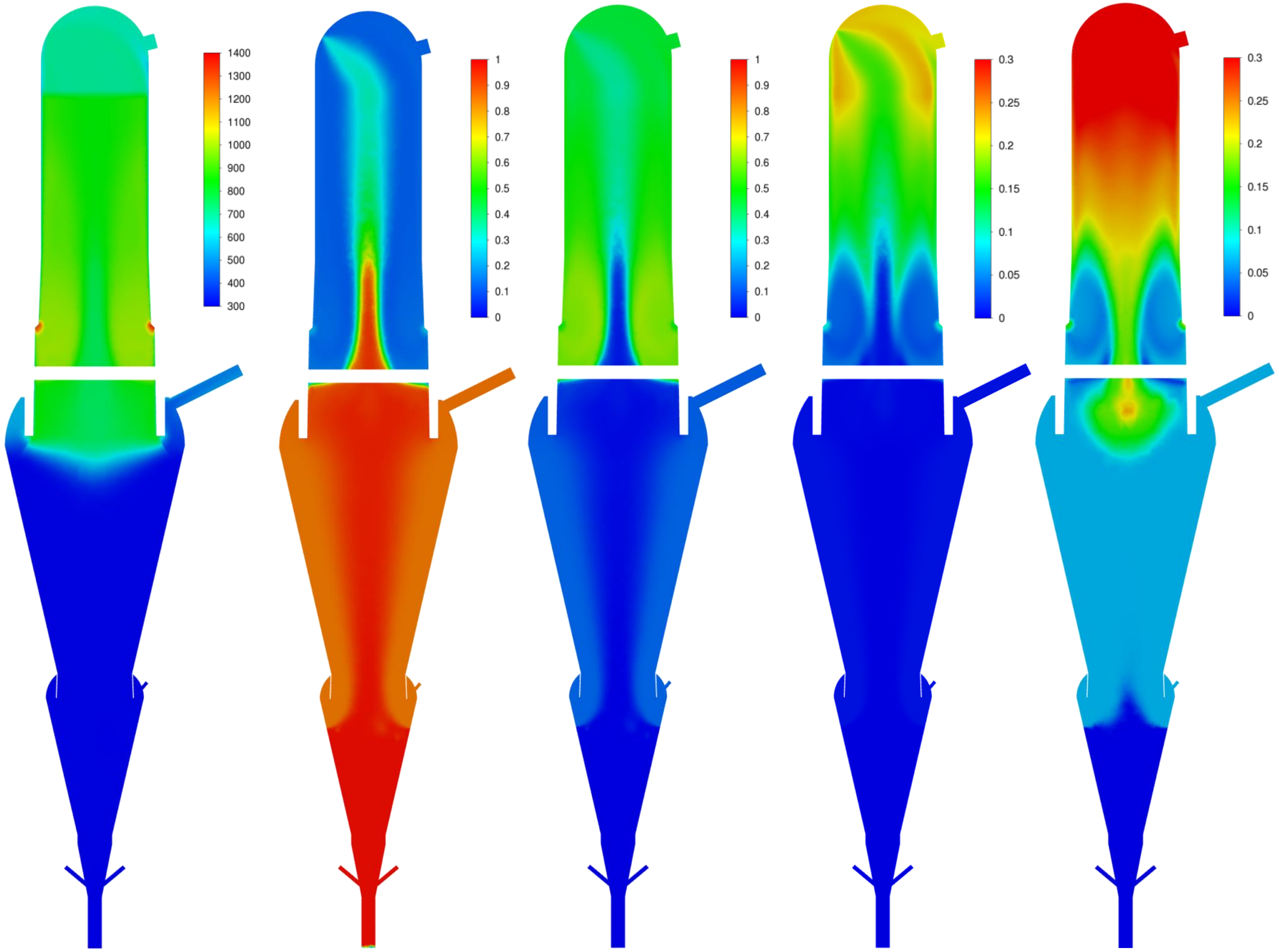
Boundary Conditions

- Production rate fixed at 312 tph
  - 2.5% gangue in final product
- Cooling zone remains unchanged
  - Primarily CH_4 as cooling gas
    - Source of carbon for pellets
  - 7.5% of total flow rate is drawn into reduction zone
    - Aligns with other estimates in literature
    - Improved model stability vs no gas exchange
- High pressure of zero reformer process maintained (~7 bar)



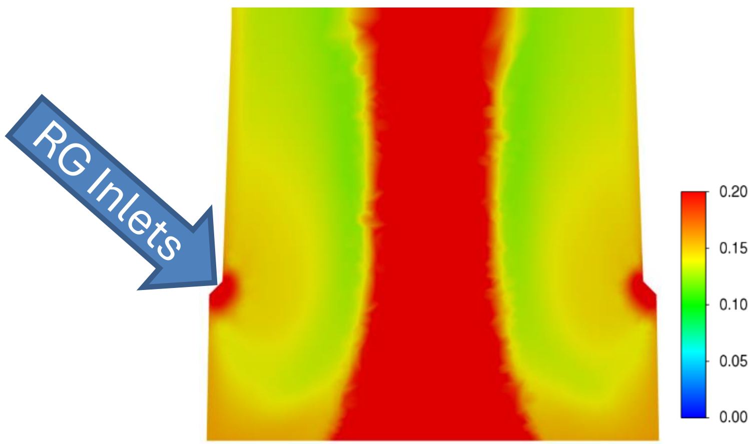
Gas Phase Results – Baseline

Gas Temp. [K] | CH_4 Vol. Fract. | H_2 Vol. Fract. | H_2O Vol. Fract. | H_2 Util.

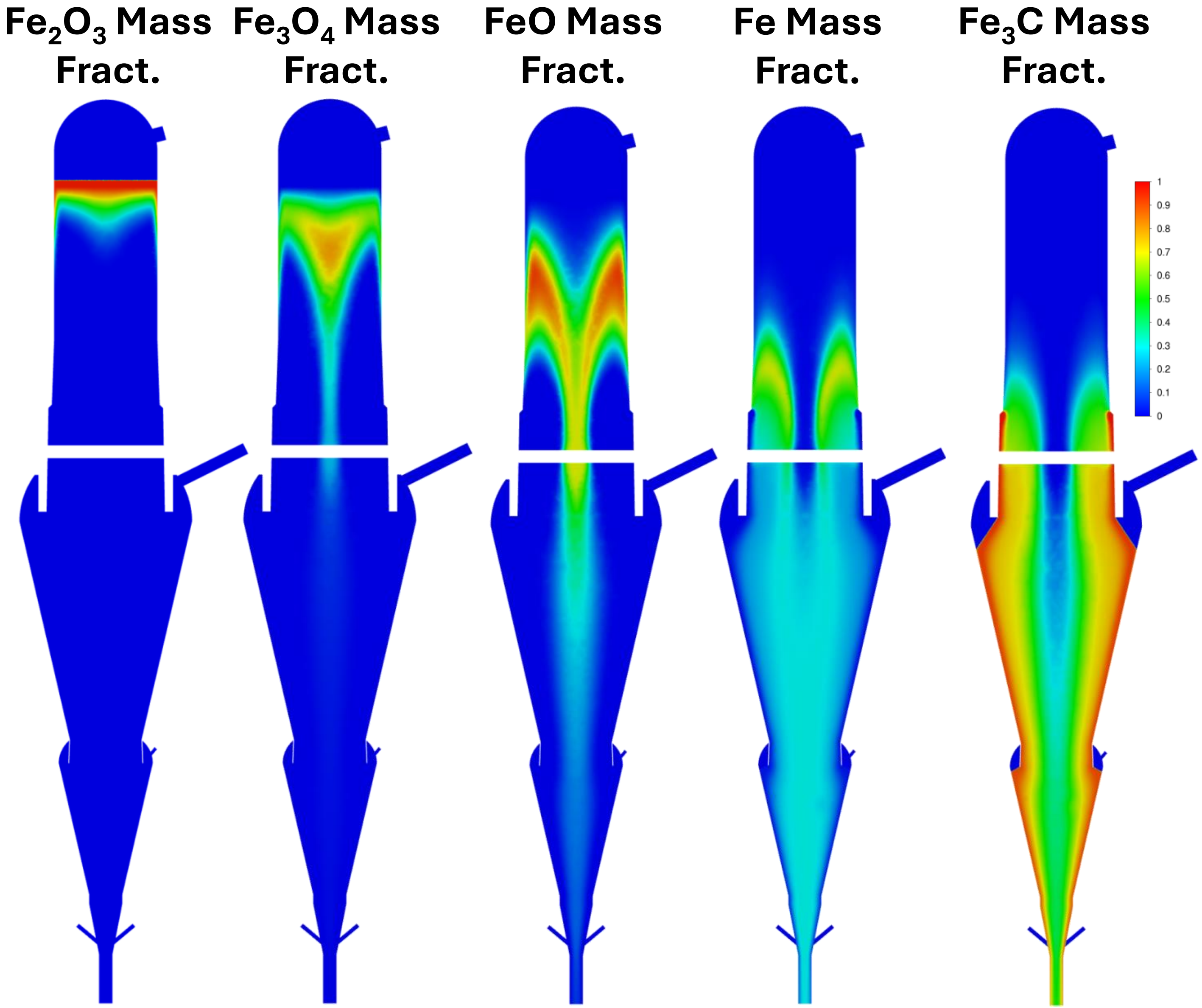


- Boundary conditions derived from industrial plant
- Production rate: 312 tph
- SMR & CH_4 decomposition rapidly cool gas

CH_4 Vol. Fract. Detail View



Ore Phase Results – Baseline

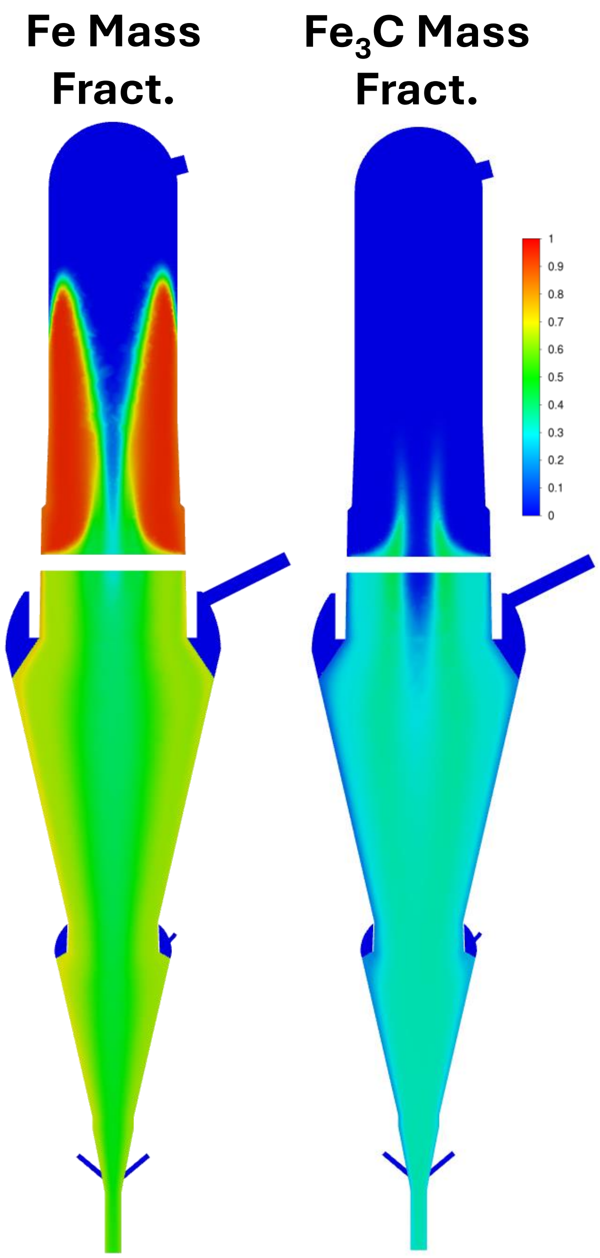


- Unreduced wustite remains at furnace center
- Slight over production of metallization and gas utilization
- Peak carburization near walls

Parameter	Target	Conv. DRI
H_2 util.	36.2%	39.5%
CO util.	43.2%	45.5%
Mtz.	94.5-96%	96.7%
RG outlet Y_{CH4}	19.0%	17.7%
Pellet wt% C	3.0-4.5%	4.5%

Initial Test Results

- Case Conditions:
  - 100% H_2 @ 120 Nm/s, T_{RG} 1338K
  - Similar H_2 flow rate to baseline after SMR reactions complete
- Findings
  - Carburization was very low
    - 1.5-2.5% average at outlet
    - Poor carburization near walls
  - Increasing $\dot{m}_{RG}$ had little impact on carburization
    - Poor gas penetration at lower rates
    - Higher reducing gas flow rates drove metallization high in shaft
- Tests with 50-50 H_2-N_2 (mass basis) blends showed similar high metallization height and poor carburization



Inlet Conditions

- Small amount of methane added to boost carburization near wall
  - Generates additional H_2 for reduction
  - Reduces gas temperature to control metallization height
  - CH_4 cracking in gas supply system not considered
    - Modified gas injection equipment may be needed
- Additional test cases for impact of RG injection temperature to control metallization height and carburization

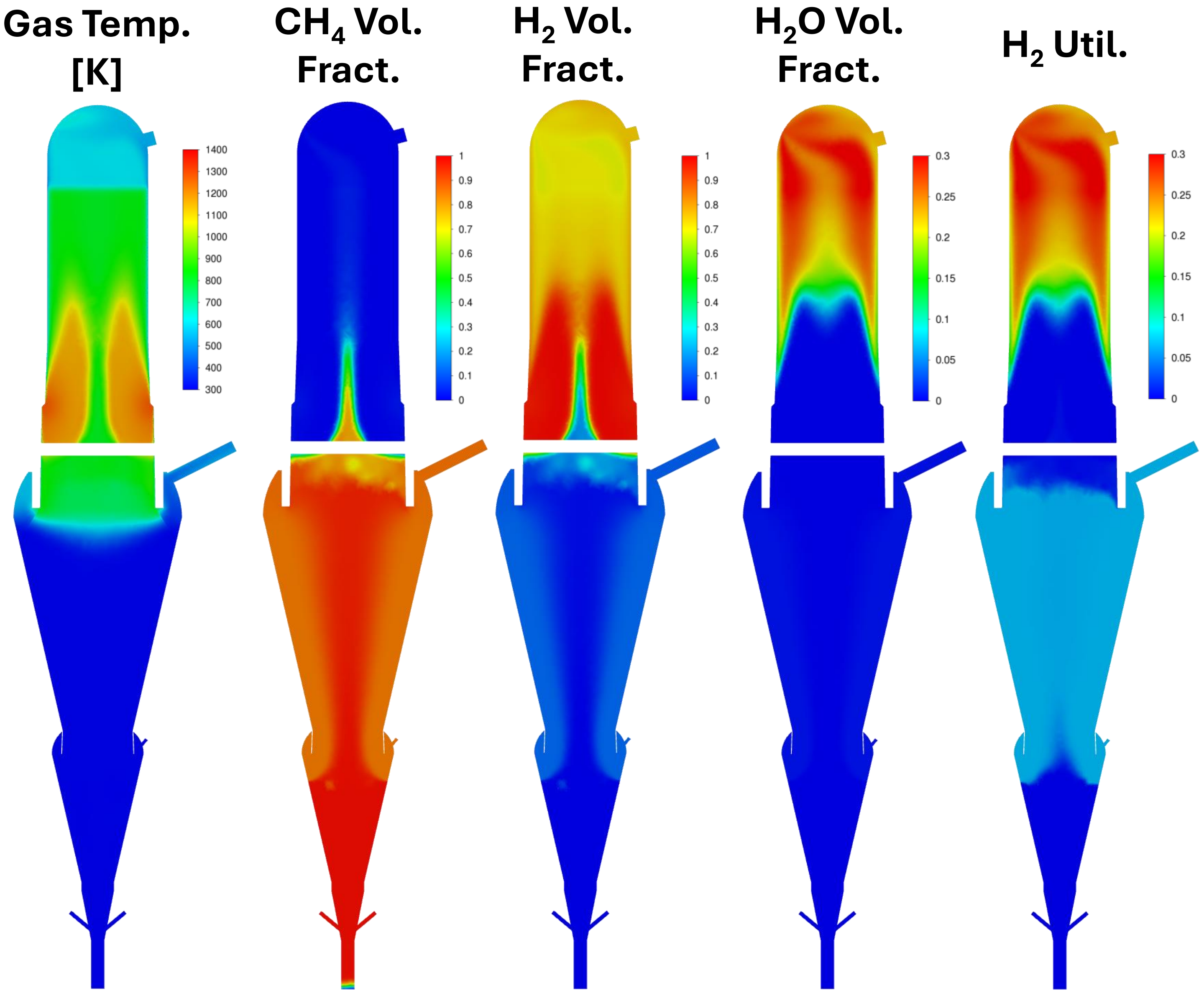
Parameter		Conv. DRI	H_2 DRI
RG ṁ [kg/s]		45.88	9.0
RG volumetric flow [Nm/s]		174.3	161.1
% vol.	CH_4	24.1%	3.6%
	CO_2	1.5%	0.0%
	CO	12.6%	0.0%
	H_2O	10.6%	0.0%
	H_2	48.0%	96.4%
	N_2	3.1%	0.0%
RG Temp. [K]		1338K	1280K

Major Findings

- Without SMR heat demand lower reducing gas temperature can realize similar carburization and reduction degree
- Significantly worse H_2 utilization
  - 27% vs industrial measurement of 36.2%
  - CO utilization not relevant for High H_2 case
- Complete metallization with high H_2 RG
  - Potential for encapsulation remains
- Blend of H_2-N_2-CH_4 may improve utilization by using N_2 as sensible heat carrier to replace unreacted H_2

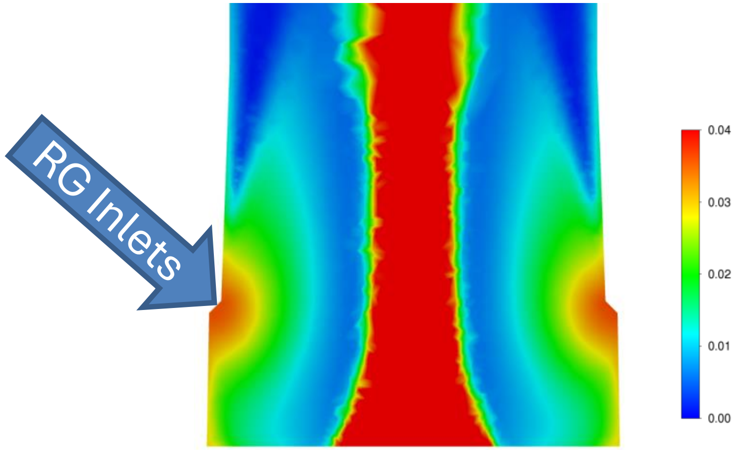
Parameter	Target	Conv. DRI	H_2 DRI
H_2 util.	36.2%	39.5%	27.1%
CO util.	43.2%	45.5%	-
Mtz.	94.5-96%	96.7%	100%
RG outlet Y_{CH4}	19.0%	17.7%	1.2%
Pellet wt% C	3.0-4.5%	4.5%	4.4%

Gas Phase Results – High H_2 RG

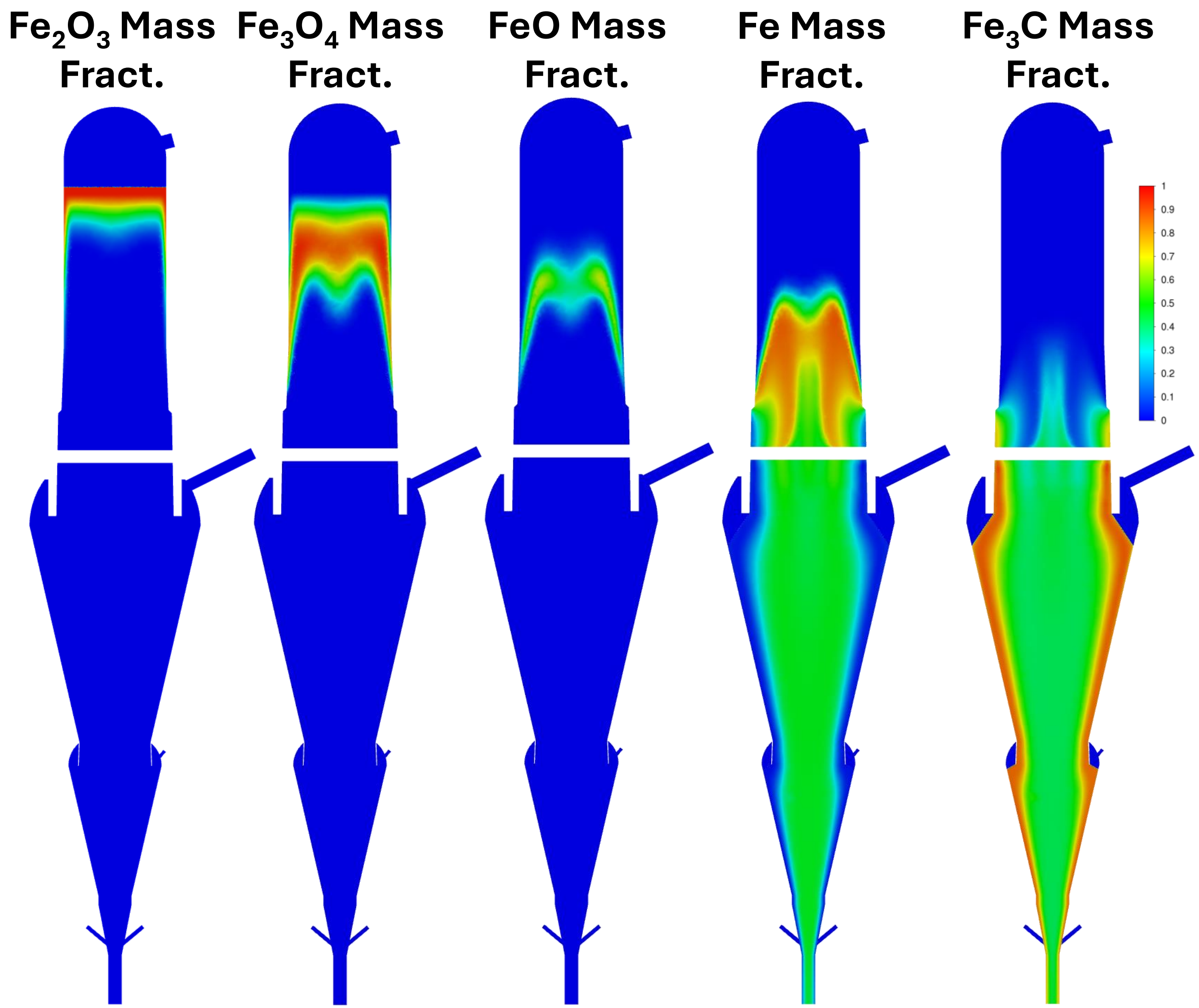


- Rapid CH_4 consumption in front of RG inlets
- CH_4 drawn into RZ from CZ consumed by carburizing reactions

CH_4 Vol. Fract. Detail View

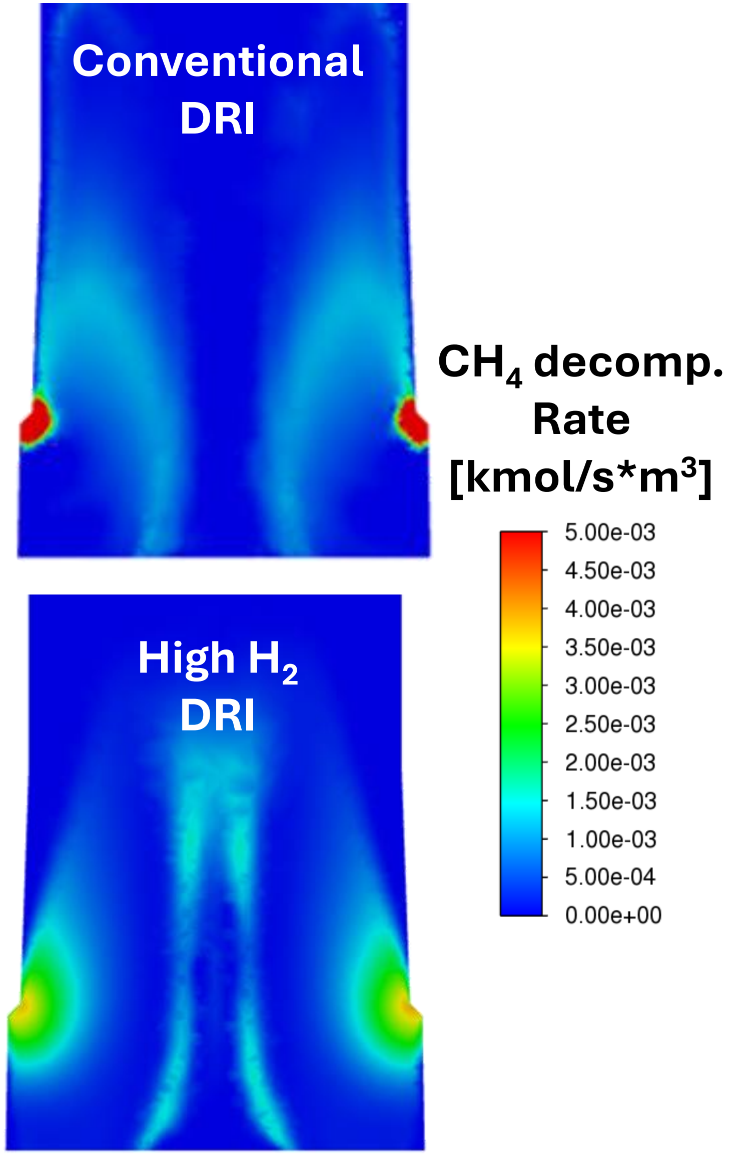


Ore Phase Results – High H_2 RG



- Rapid reduction to magnetite
- Much smaller "wustite reserve zone" than conventional case
- More uniform radial carbon deposition
- Wustitite reduction is rapid
  - Potential for encapsulation

Reaction Rates



- CH_4 carburizing reaction:
  - Higher CH_4 content in conventional DRI produces higher peak intensity
  - Endothermic effect of SMR prevents large region of carburization reaction
- Steam methane reforming:
  - High H_2 case requires H_2O from ore reduction before SMR can occur
  - Conventional DRI: 0.2366 kmol/s
  - H_2 DRI: 0.0446 kmol/s
- CO_2 emissions from top gas:
  - Baseline: 102.0 kg CO_2/tonne of product
  - High H_2: 11.8 kg CO_2/tonne of product

Conclusions

- Operation with only H_2 or H_2-N_2 blend shows poor carburization and high metallization height
- Addition of a small amount of NG to reducing gas may be able to provide carburization near walls
- Temperature of reducing gas can be used to control carburization degree
- Rapid reduction of wustite remains a concern
  - Potential to encapsulate unreacted magnetite
- 8x reduction in CO_2 in top gas

Thank You

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