Advanced Gasifier Design

Advanced Reaction Systems: Task 3

2020 Gasification Project Review Meeting

September 2, 2020

NATIONAL ENERGY TECHNOLOGY LABORATORY

Computational Device Engineering Team

NETL Research and Innovation Center

MFS NETL Multiphase Flow Science
Home of the MFiX Software Suite

Advanced Gasifier Design

Supports the ARS FWP goals for next-generation modular systems

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Task 3: Advanced Gasifier Design uses NETL Simulation-Based Engineering tools – MFiX to support FE and ARS FWP goals

- Design and optimization of next generation gasification systems
  - Support Gasification Systems Major Projects – U. Alaska - Fairbanks Modular Gasification project
  - Develop and evaluate potential Coal FIRST technologies
  - Support development of next-generation oxygen separation devices
- These tools provide a SBE platform to support the ARS FWP portfolio
  - Task 4: Advanced Manufacturing and Materials
  - Task 5: Oxygen Production for Gasification
  - Task 6: Microwave Reactions for Gasification

Advanced Gasifier Design

Project Scope and Team

- ARS FWP
  - Task 3: Advanced Gasifier Design
  - Task 3.1: University of Alaska – Fairbanks Gasifier Studies
  - Task 3.2: Oxygen Separation
  - Task 3.3: Novel Coal FIRST Gasifier

Task 3: Advanced Gasifier Design


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Task 3.1: University of Alaska – Fairbanks Gasifier Studies


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Task 3.2: Oxygen Separation


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Task 3.3: Novel Coal FIRST Gasifier


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MFS NETL Multiphase Flow Science Team
Home of the MFiX Software Suite

Advanced Gasifier Design

Task Description – U. Alaska - Fairbanks Support

- Task 3: Advanced Gasifier Design
  - Task 3.1: University of Alaska – Fairbanks Gasifier Studies
  - Task 3.2: Oxygen Separation
  - Task 3.3: Novel Coal FIRST Gasifier

Support the design and optimization of the commercial gasifier for University of Alaska - Fairbanks Project [1] gasifier

- Validate the modeling approach with pilot-scale data
- Develop a prototype design representing the proposed commercial system
  - Protect commercial IP while capturing important design parameters
- Simulate plant design conditions to verify gasifier design performance
- Use model to explore other operating conditions
  - Reduced load transients
- Working in collaboration with UAF, HMI, Parsons, Sotacarbo Research Center
- Fundamental coal studies underway at ORNL (Neutron Imaging), and at NETL REACT facility
  - Data to guide model development
  - Data for code validation

[1] Making Coal Relevant for Small Scale Applications: Modular Gasification for Syngas/Engine CHP Applications in Challenging Environments, FE0031601 University of Alaska - Fairbanks

Validate Modeling Approach with Pilot Scale Data

Simulate SOTACARBO Pilot Unit with Usibelli Coal

SOTACARBO Pilot Gasifier [1]

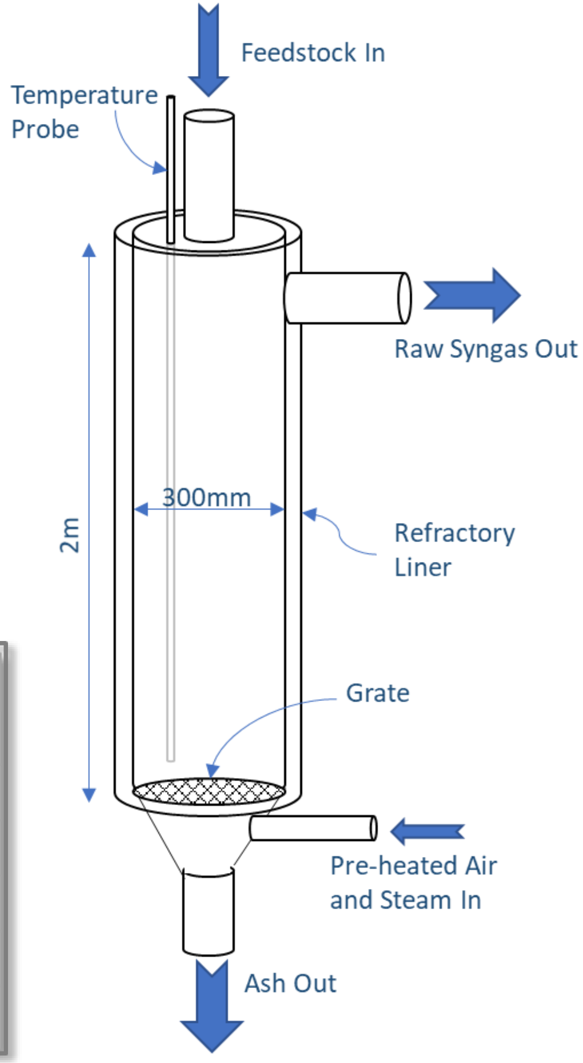
- Upflow configuration, 300mm ID x 2m height
- Refractory-lined
- Steam and Air-blown
- Variety of feedstocks fed through lock-hopper
- Micro GC and Analyzers for:
  - H_2, CO, CO_2, N_2, O_2, CH_4, H_2S, COS, C_2H_6, C_3H_8, …

Test program for Usibelli Coal

- 5-15mm particle size
- 16-hour run
  - 8 hours to stable operating condition

SOTACARBO Pilot Gasifier

SOTACARBO SUSTAINABLE ENERGY RESEARCH CENTRE



Proximate Analysis		Ultimate Analysis (by weight)	
Fixed Carbon	31.34	C	48.56
Moisture	17.64	H	5.96
Volatiles	41	N	0.50
Ash	10.02	S	0.18
		O	17.14
Bulk Density (kg/m³)	800	Moisture+Ash	17.64+10.02

[1] Frau, C., Ferrara, F., Orsini, A., Pettinau, A., 2015, Characterization of Several Kinds of Coal and Biomass for Pyrolysis and Gasification, Fuel, 152, pp. 138-145

Validate Modeling Approach with Pilot Scale Data

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Modeling techniques for demanding gasifier simulations

Industrial gasifier simulations are very demanding applications

- Gasifiers require extended time to go from light-off to stable operation
- Industrial-scale systems are computationally demanding – lots of particles to track!
- Chemical reactions and heat transfer increase the complexity of the calculations

To reduce particle number – use Coarse-Grained DEM approach

- Lump small particles into slightly larger particles to reduce the count

To deal with long start up transients – use a reduced order model to accelerate the calculations

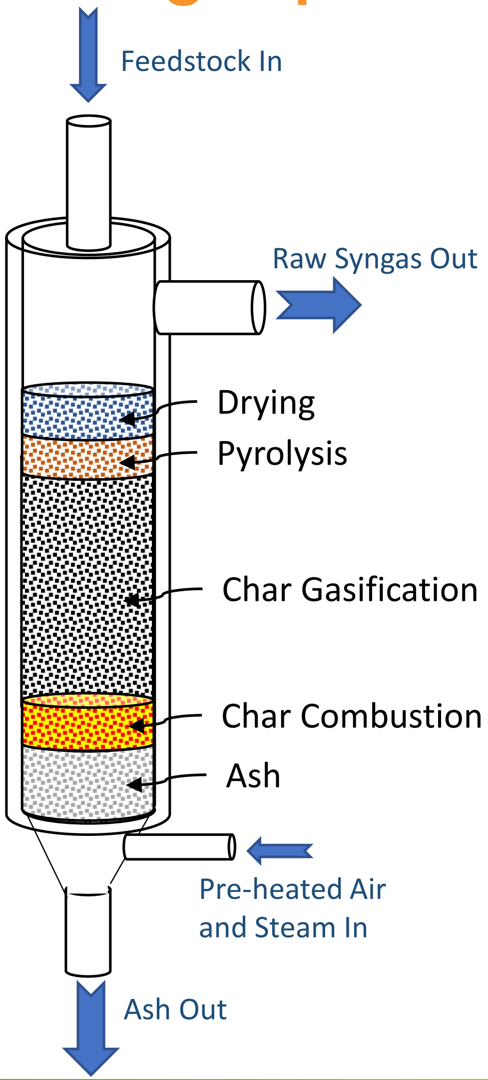
- Quasi 1-D model runs quickly to develop a good initial condition (i.e. a good "guess" on where to start the 3-D model)
- Then run the full 3-D model to get to stable operation and more accurate results

Coal Particles assumed to shrink as they react

- Shrink in proportion to mass loss from reactions

Validate Modeling Approach with Pilot Scale Data

Solids and gas phase reactions

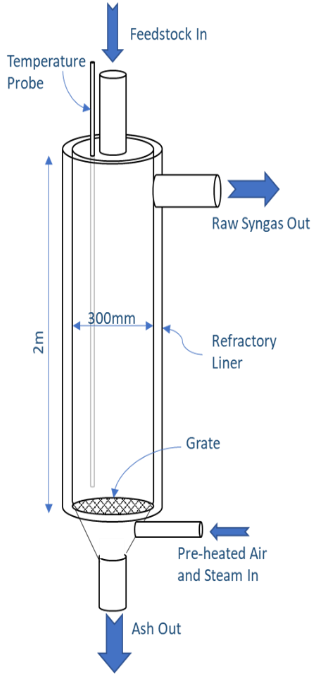


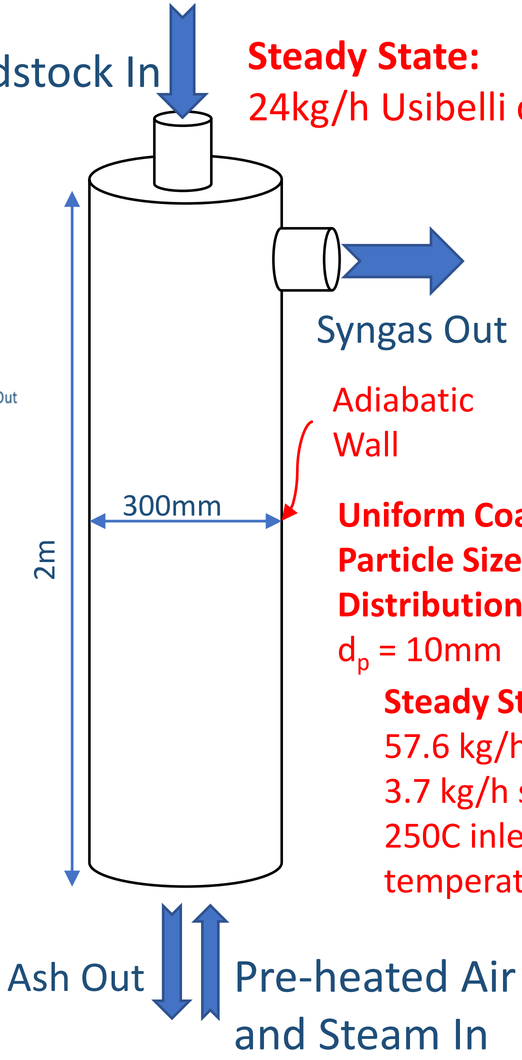
Categories	Forward reaction	Backward reaction
	Reactions	
Drying	Moisture(coal) $\rightarrow H_2O$(gas)	
Pyrolysis	**Volatiles** --> 0.212783 **CO** + 0.080835 **CO_2** + 0.313279 **CH_4** + 0.090044 **H_2** + 1.25472 **H_2O** + 0.011148 **H_2S** + 0.07535 **TAR** + 0.619475 **C**	
Gasification	$Char + H_2O \rightarrow CO + H_2$	$CO + H_2 \rightarrow Char + H_2O$
	$Char + CO_2 \rightarrow 2CO$	$2CO \rightarrow Char + CO_2$
	$Char + 2H_2 \rightarrow CH_4$	$CH_4 \rightarrow Char + 2H_2$
	$Char + O_2 \rightarrow CO_2$	
Gas phase reactions	$CO + \frac{1}{2}O_2 \rightarrow CO_2$	
	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	
	$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	
	$CO + H_2O \rightarrow CO_2 + H_2$	
	$CO_2 + H_2 \rightarrow CO + H_2O$	

Cau, G., Tola, V., Pettinau, A., 2015, A Steady State Model for Predicting Performance of Small-scale, Up-draft coal Gasifiers, Fuel, 152, pp. 3-12

Validate Modeling Approach with Pilot Scale Data

Gasifier 3-D steady flow

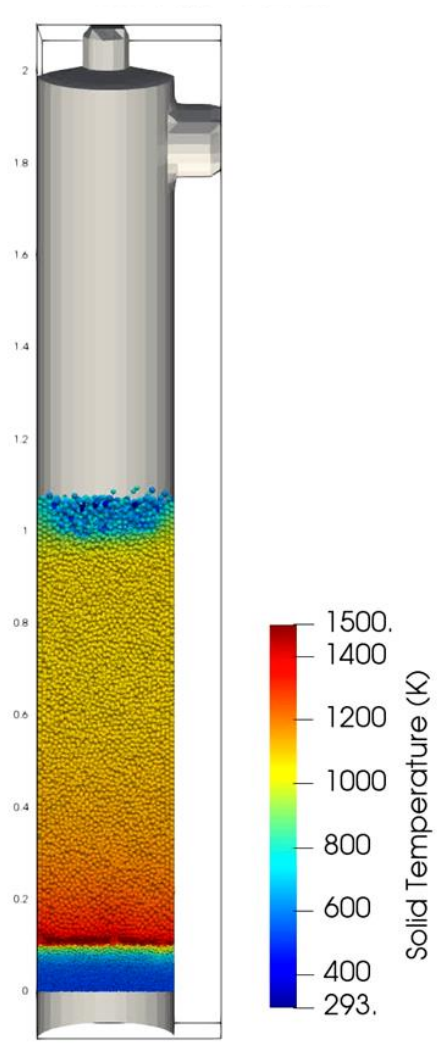


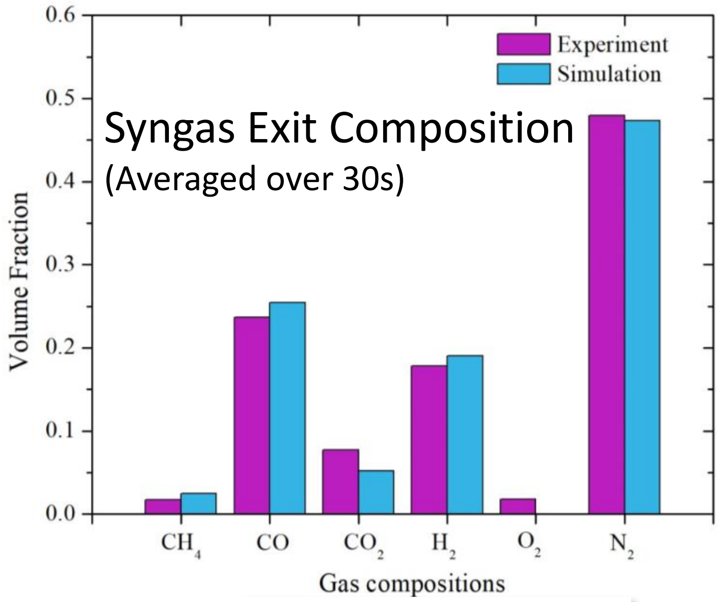


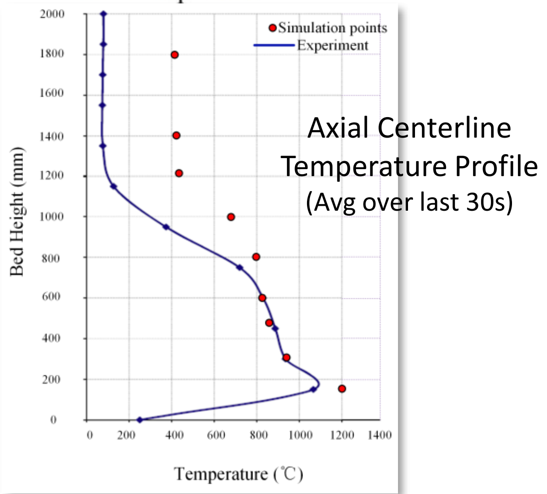
Steady State:
24kg/h Usibelli coal

Uniform Coal Particle Size Distribution
d_p = 10mm

Steady State:
57.6 kg/h air
3.7 kg/h steam
250C inlet temperature







Yu, J., Lu, L., Gao, X., Xu, Y., Shahnam, M., Rogers, W., 2020, Coupling Reduced-Order Modeling and Coarse-Grained CFD-DEM to Accelerate Coal Gasifier Simulation and Optimization, (*in Press*) AIChE Journal.

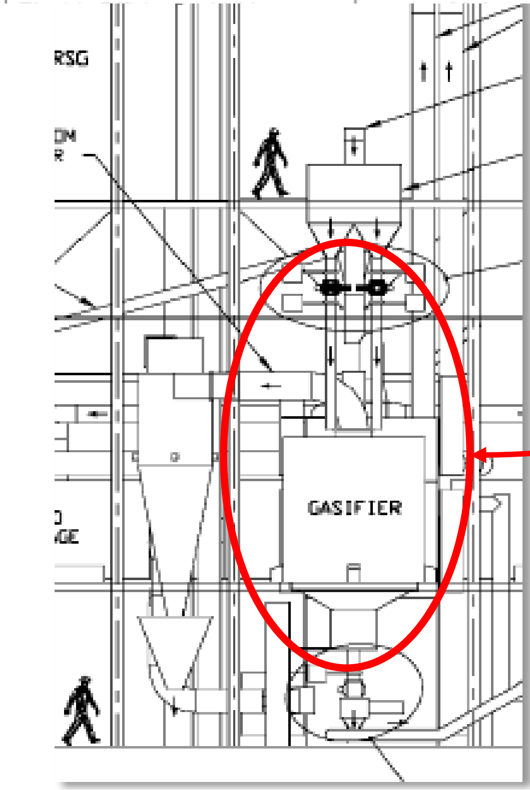
Develop a Commercial-Scale Prototype

UAF FEED study guides design geometry

Develop Prototype Gasifier Design – FEED Data and Geometric Scaling of HMI Design

Exhibit 1-2: Modular Design of HMI Gasifier/Jenbacher Engine Power System

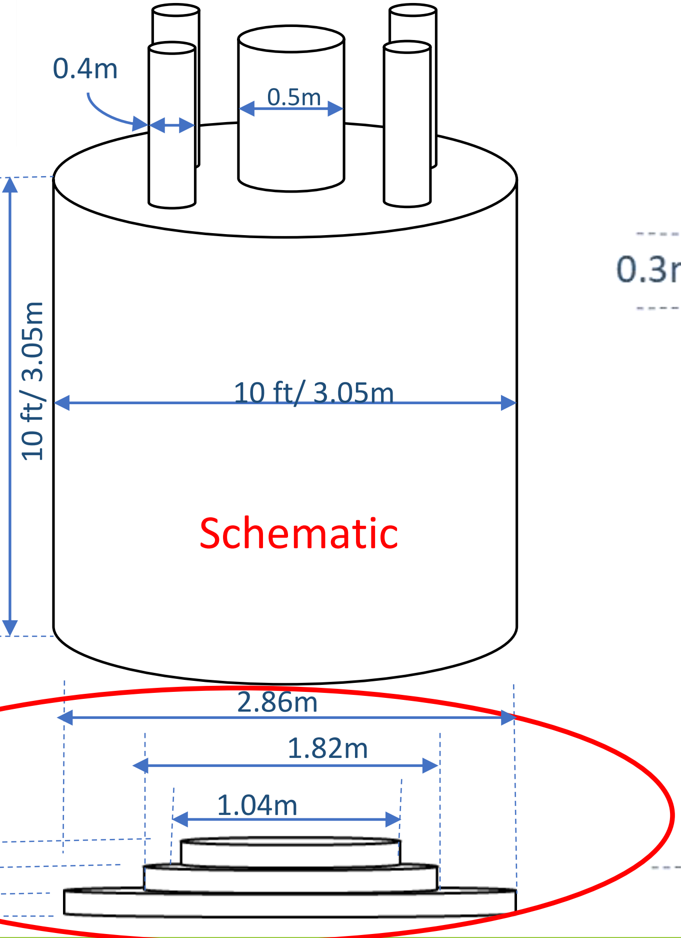
Plant Size, MWe	2	7	21
No. HMI Gasifiers	1 @ 6-foot ID	1 @ 10-foot ID	2 @ 12 foot-3 inch ID
No. Jenbacher Engines	1	3	9

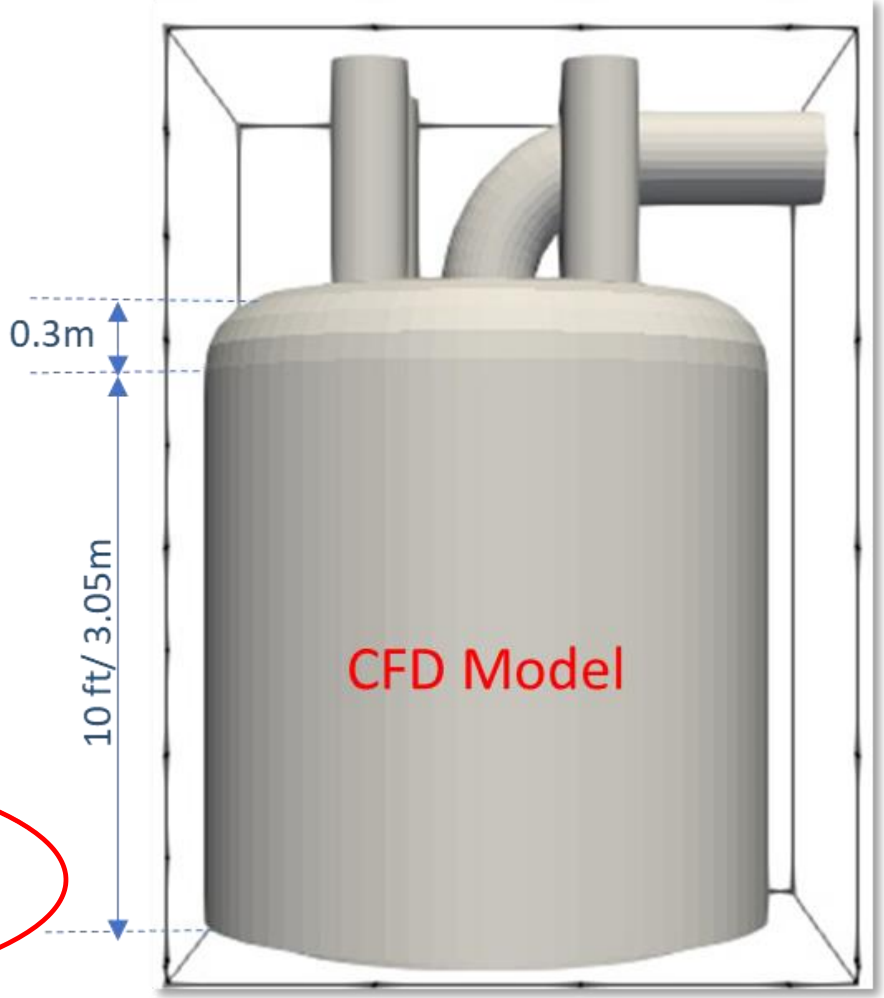


Diameter is specified

Scale the height and piping diameters from FEED drawings

Scale the grate geometry from the HMI 5MW system at Sotacarbo

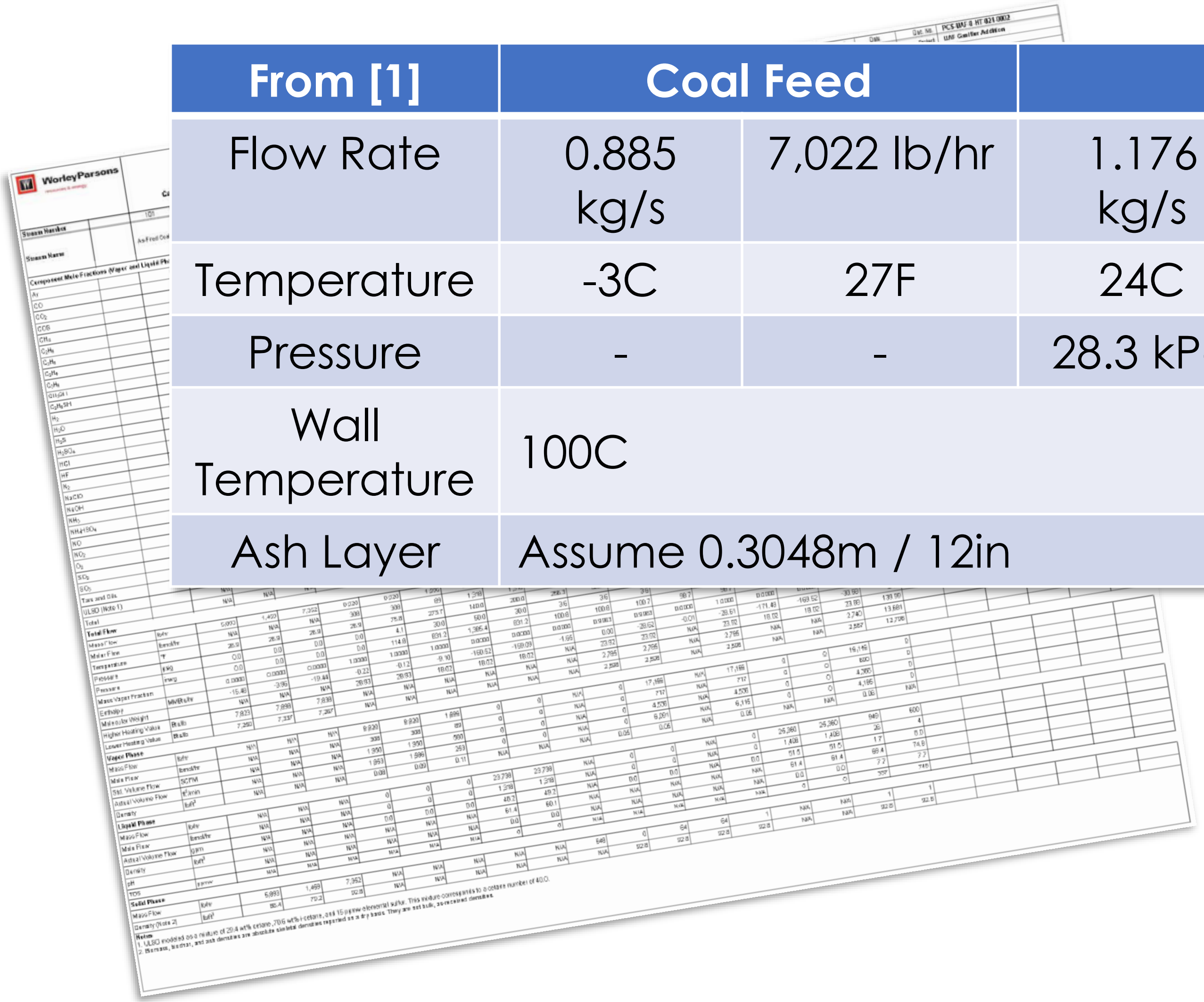




[1] Final Report: Making Coal Relevant for Small Scale Applications: Modular Gasification for Syngas/Engine CHP Applications in Challenging Environments, DOE-FE0031446- Small Scale Modularization of Gasification Technology Components for Radically Engineered Modular Systems 2019, UAF.

Simulate Plant Design Conditions

FEED Study provides the simulation conditions – flows, pressures, temperatures



From [1]	Coal Feed		Air		Steam	
Flow Rate	0.885 kg/s	7,022 lb/hr	1.176 kg/s	9,336 lb/hr	0.211 kg/s	1,671 lb/hr
Temperature	-3C	27F	24C	76F	134C	273F
Pressure	-	-	28.3 kPa	4.1 psig	207 kPa	30 psig
Wall Temperature	100C					
Ash Layer	Assume 0.3048m / 12in					

Proximate Analysis		Ultimate Analysis (by weight)	
Fixed Carbon	31.34	C	48.56
Moisture	17.64	H	5.96
Volatiles	41	N	0.50
Ash	10.02	S	0.18
		O	17.14
Bulk Density (kg/m^3)	800	Moisture+Ash	17.64+10.02

[2] Frau, C., Ferrara, F., Orsini, A., Pettinau, A., 2015, Characterization of Several Kinds of Coal and Biomass for Pyrolysis and Gasification, Fuel, 152, pp. 138-145

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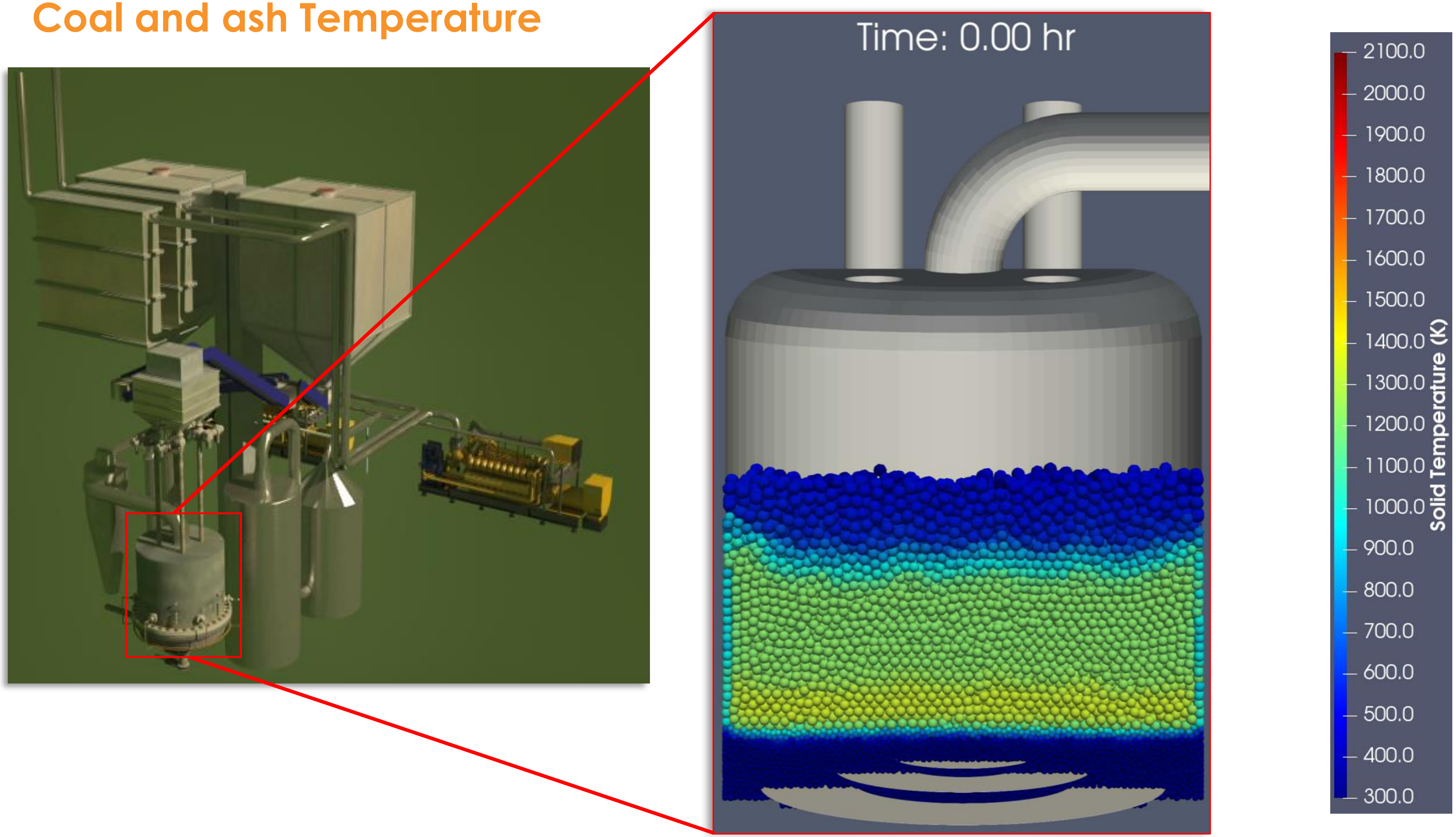
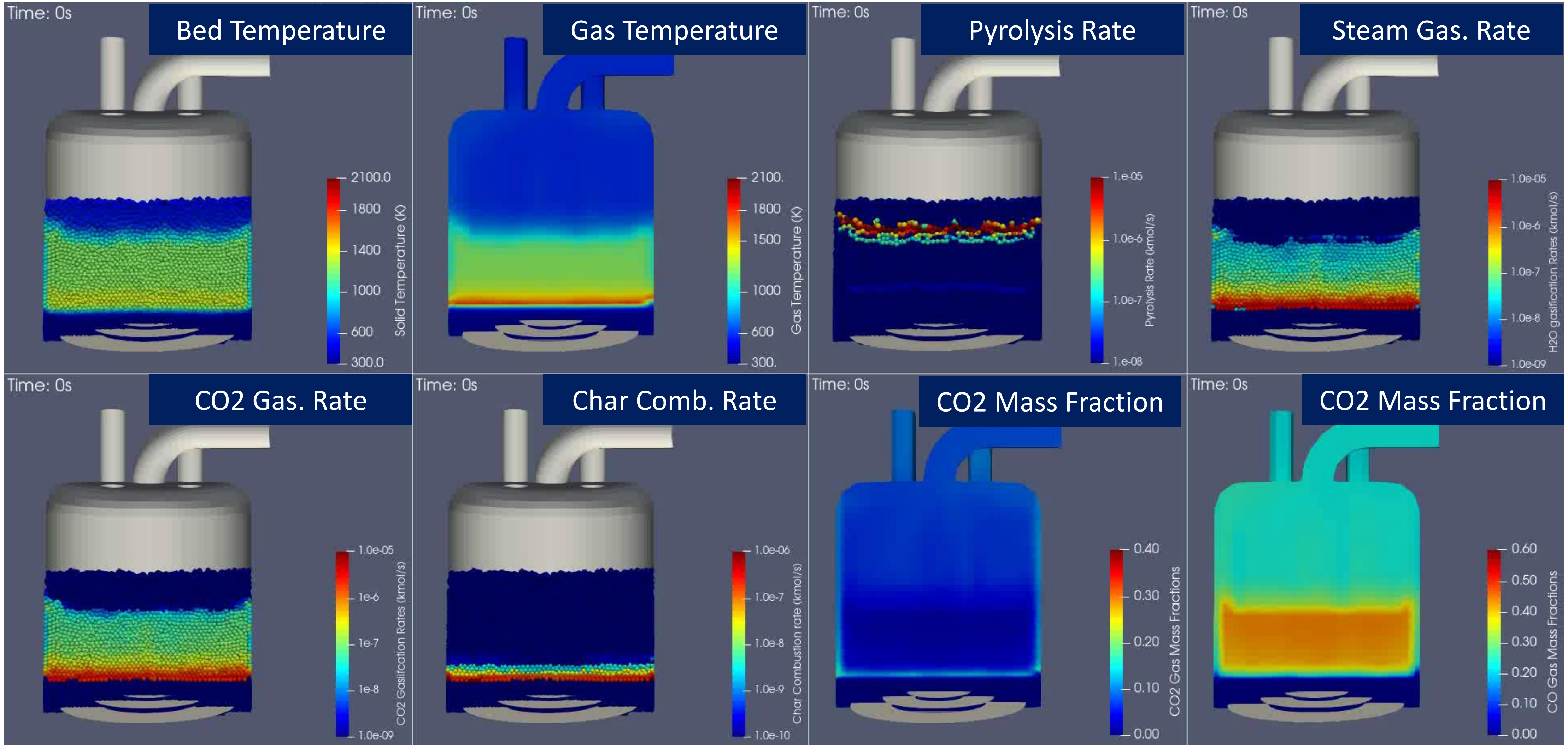
Simulate Plant Design Conditions

Coal and ash Temperature



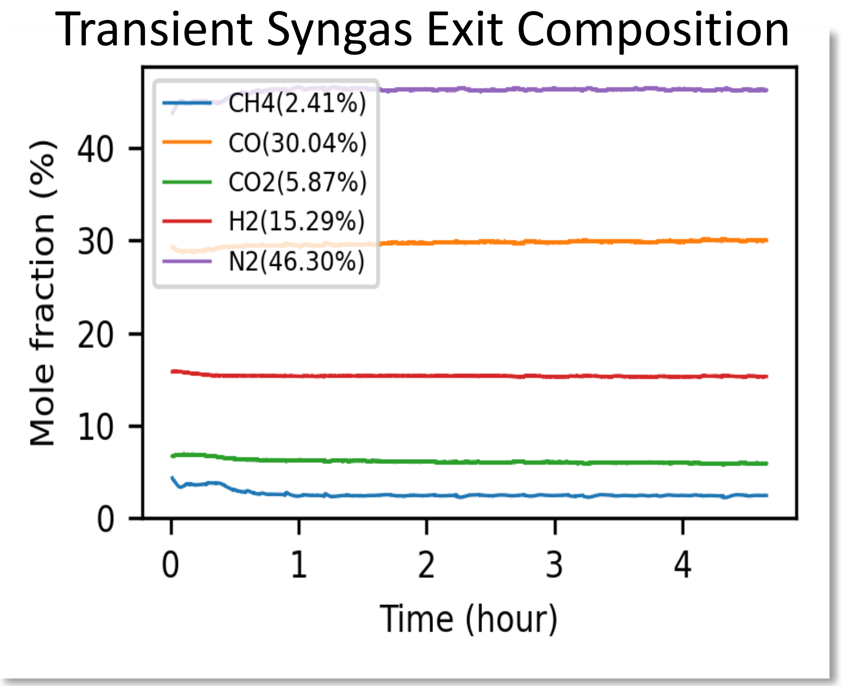
Simulate Plant Design Conditions

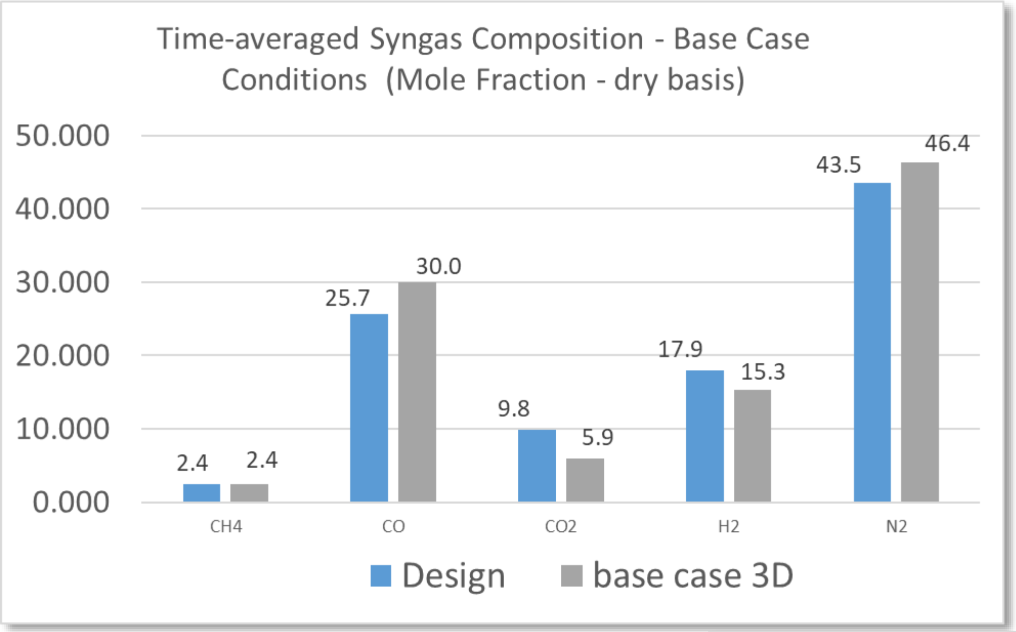
Key operating parameters to guide design

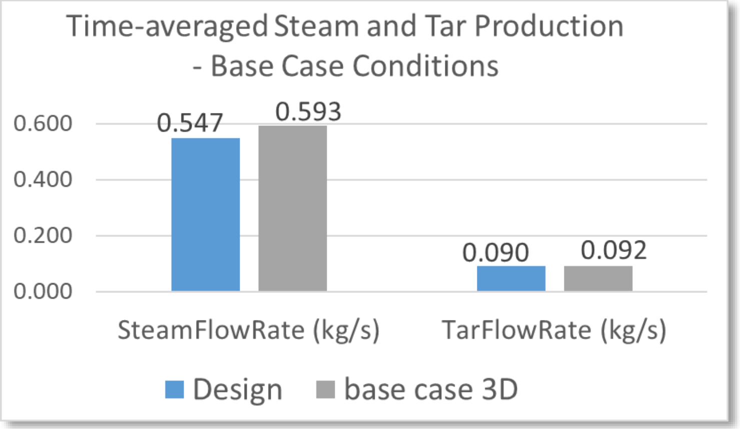


Simulate Plant Design Conditions

Syngas composition at gasifier exit







Steady operating condition was obtained

Predicted performance compares well to the FEED design

Explore A Range of Operating Conditions

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Use the model to evaluate gasifier performance

UAF gasifier will experience fluctuating plant loads

- Plant will share the grid with local wind generation

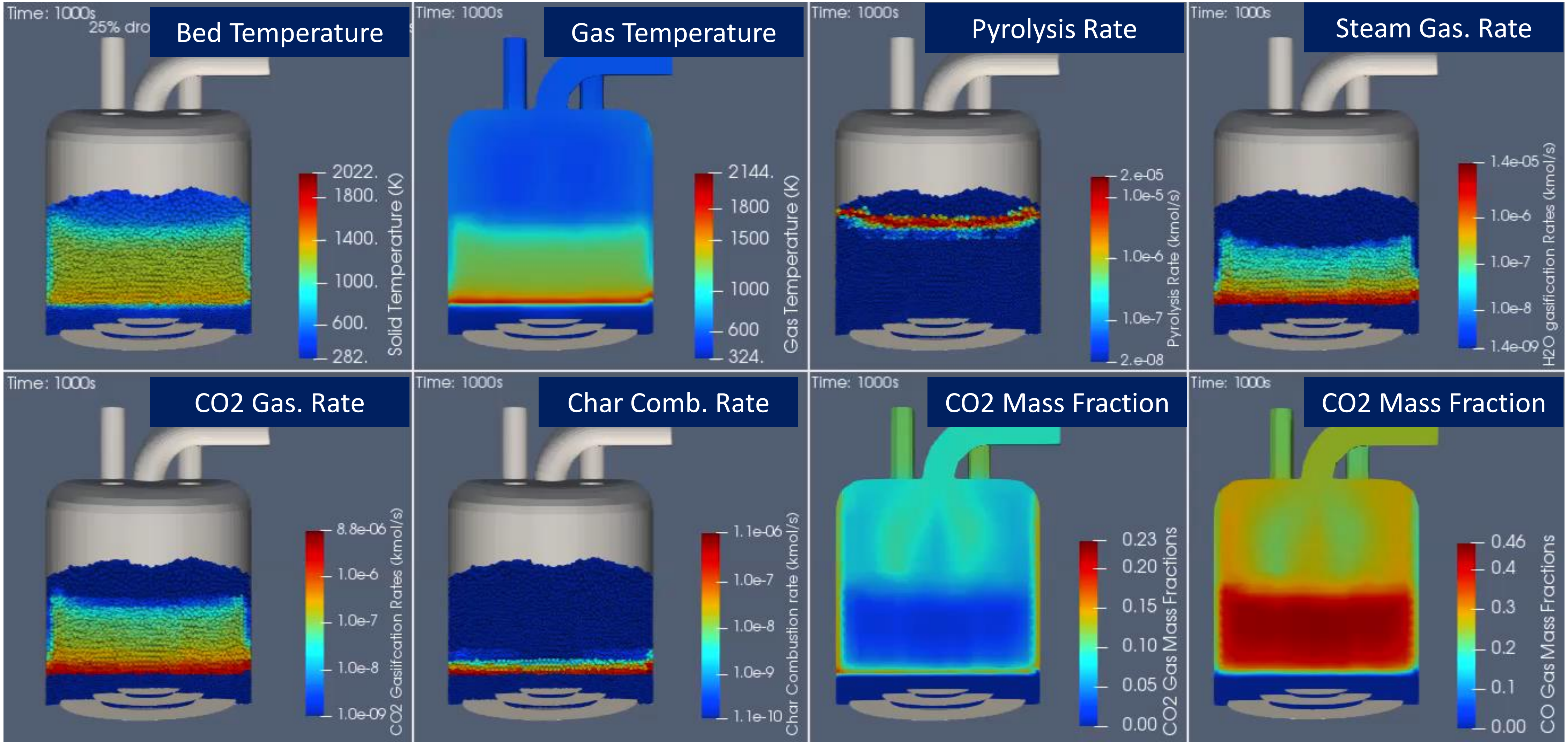
- Simulate a 25% instantaneous drop in design condition inlet flows
  - Operate at 75% for 1.5 hours
  - Follow with instantaneous increase to 100% design condition inlet flows
  - Evaluate effects on syngas flow rate, composition, bed performance

- Simulate a 50% instantaneous drop in design condition inlet flows
  - Operate at 50% for 1.5 hours
  - Follow with instantaneous increase to 100% design condition inlet flows
  - Evaluate effects on syngas flow rate, composition, bed performance

- The model maintains constant bed height by controlling ash discharge

Explore A Range of Operating Conditions

25% Instantaneous drop in load –> Operate 1.5 hours -> Jump to 100% load



Explore A Range of Operating Conditions

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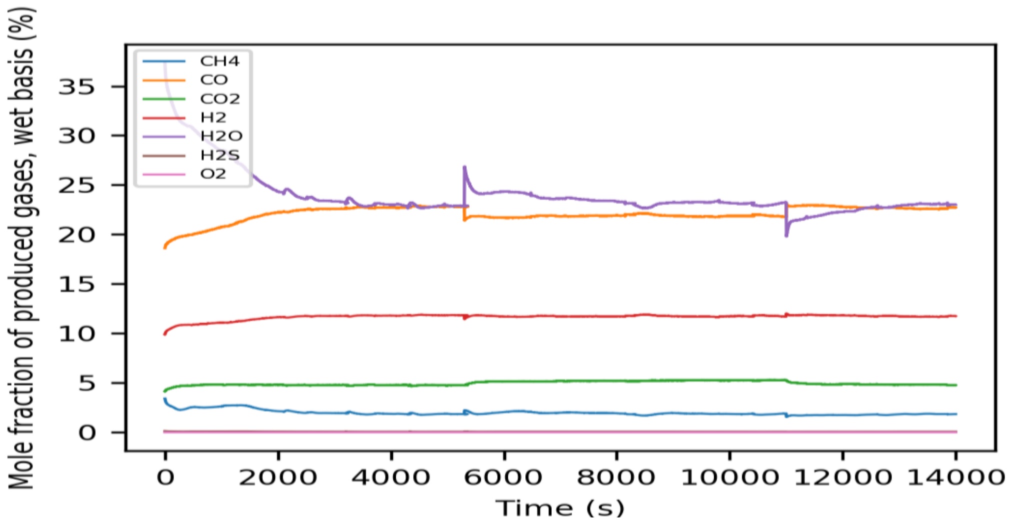
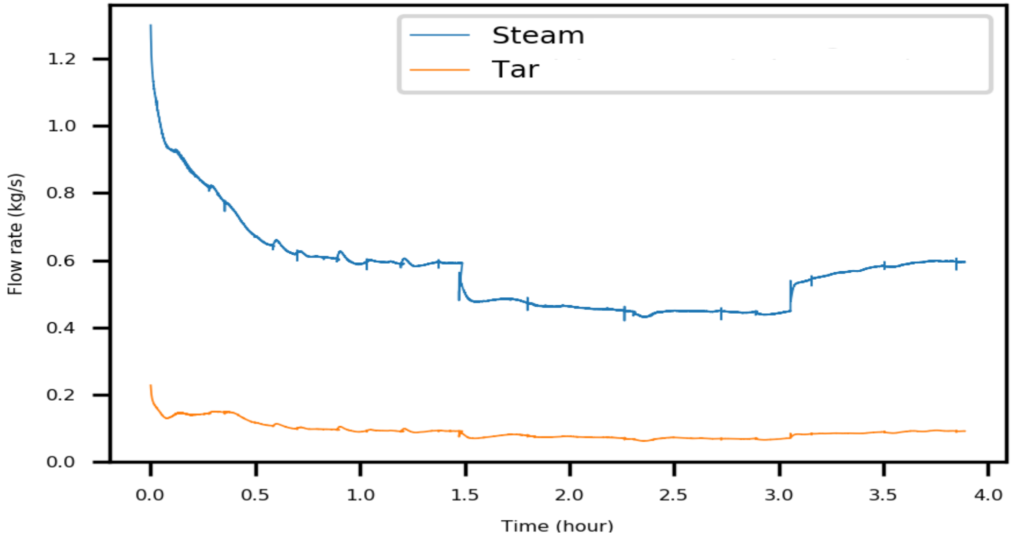
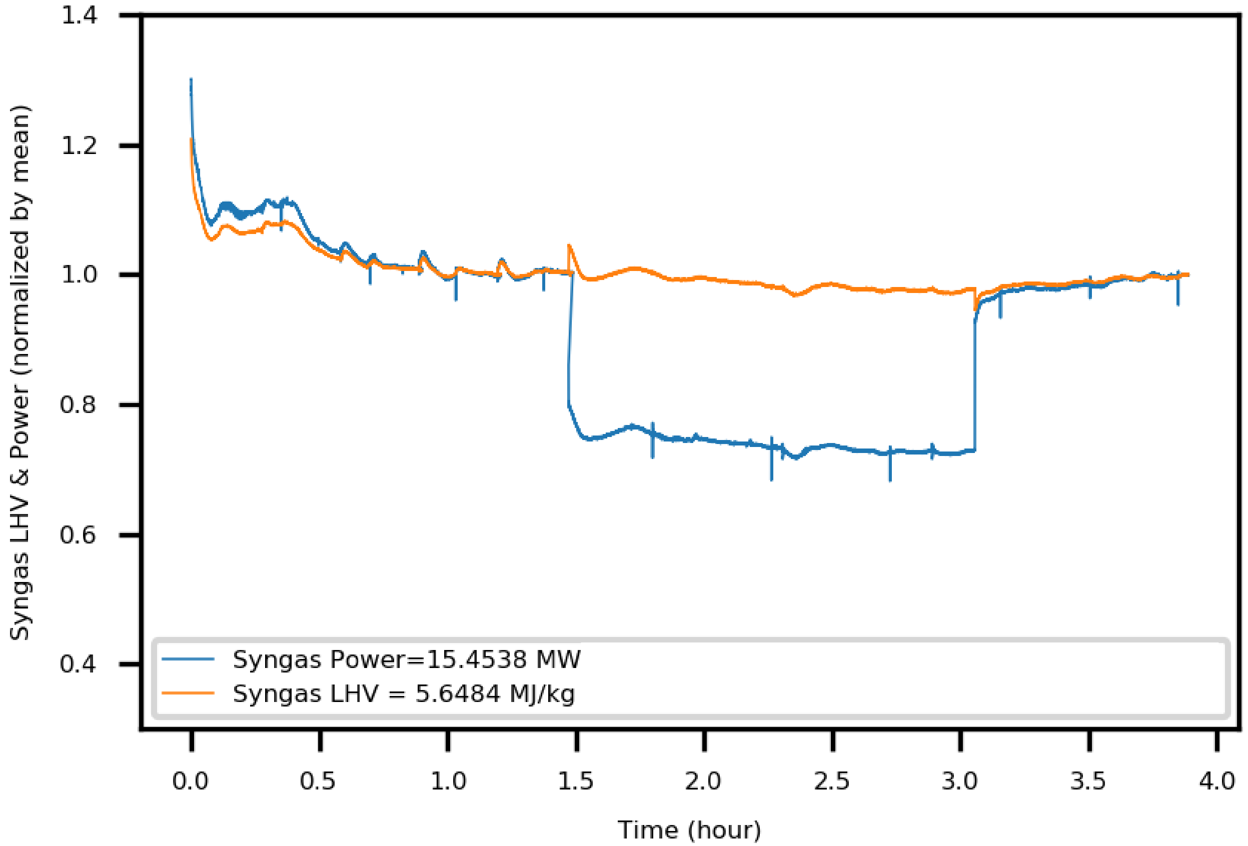
Transient Behavior for 25% load reduction







Explore A Range of Operating Conditions

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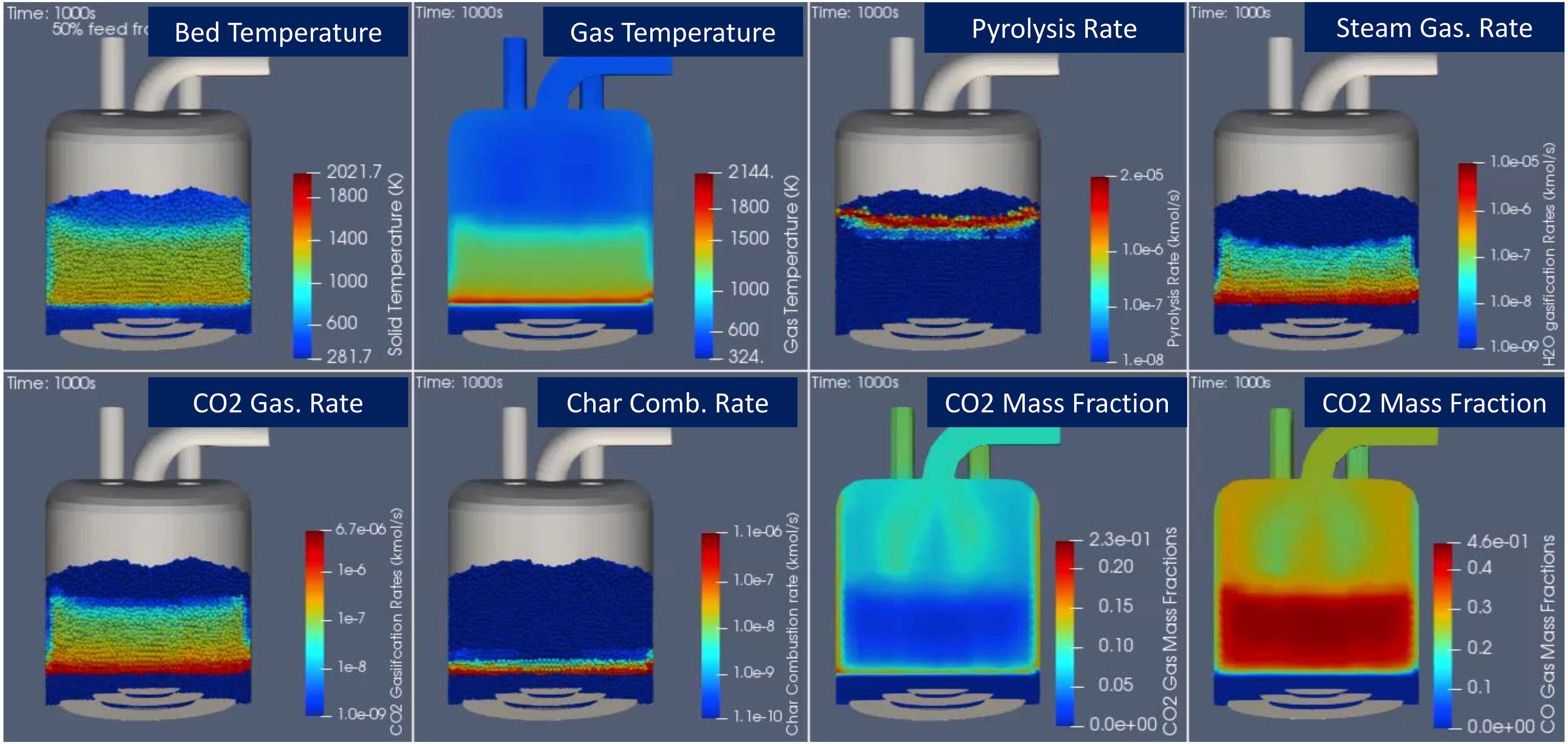
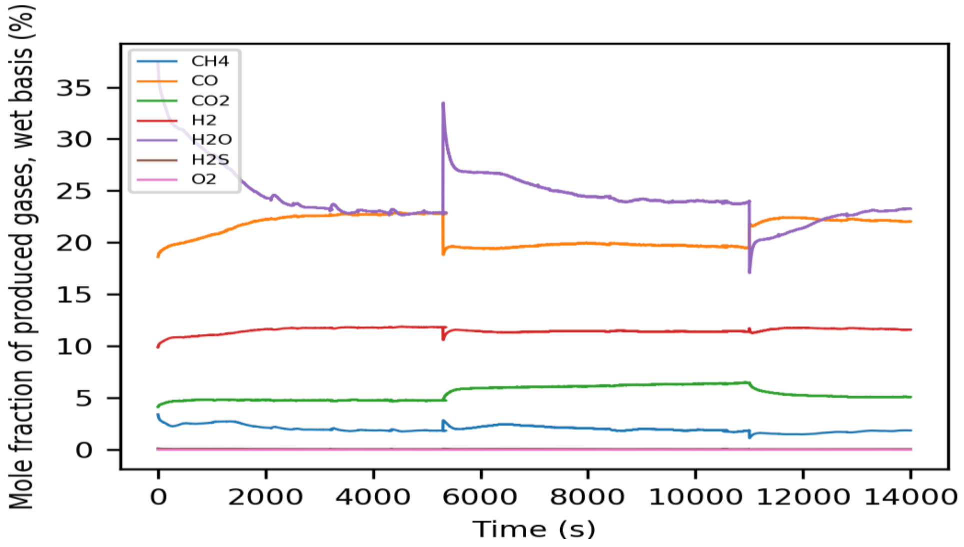
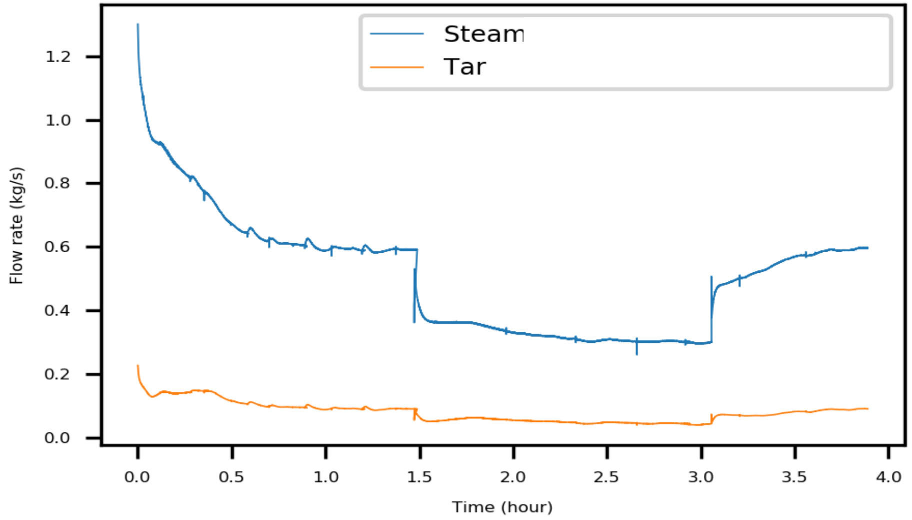
50% Instantaneous drop in load –> Operate 1.5 hours -> Jump to 100% load

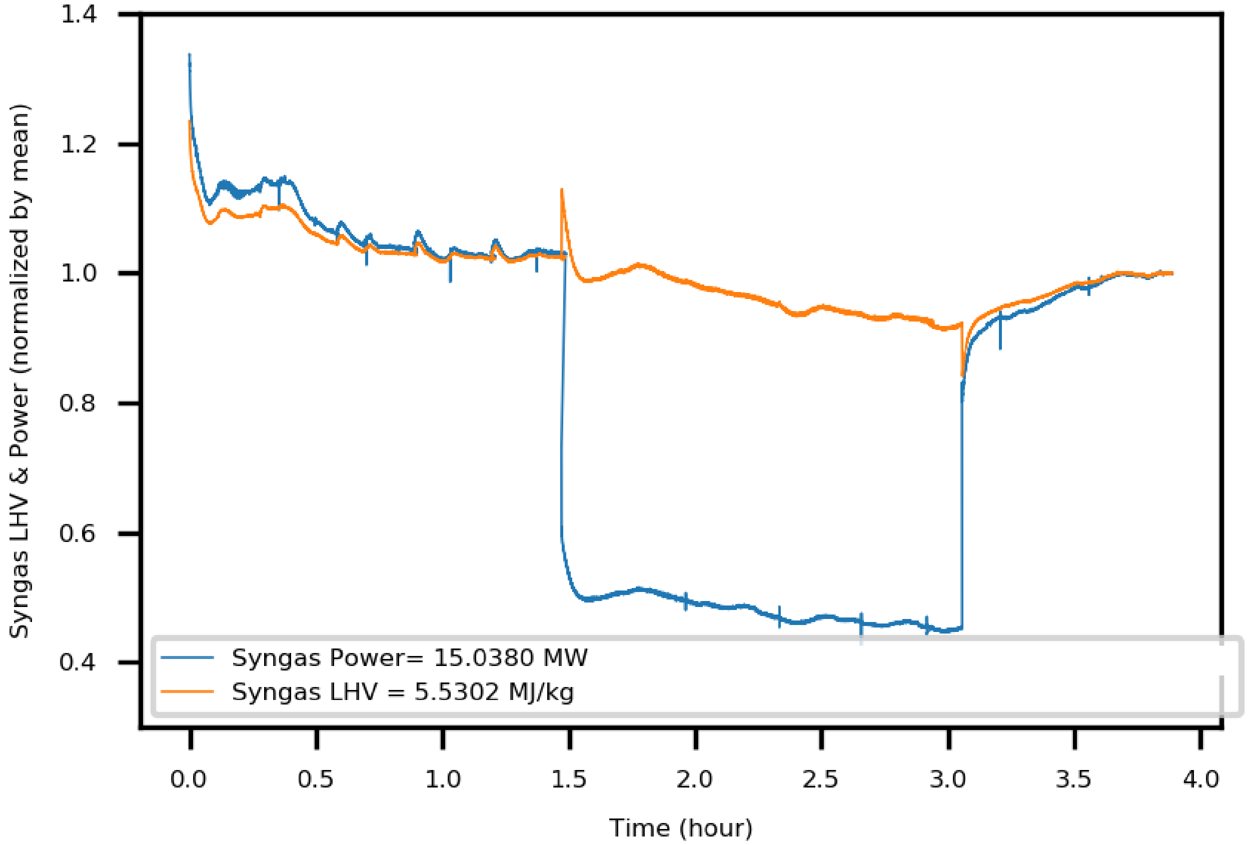


Explore A Range of Operating Conditions

Transient Behavior for 50% load reduction







Explore A Range of Operating Conditions

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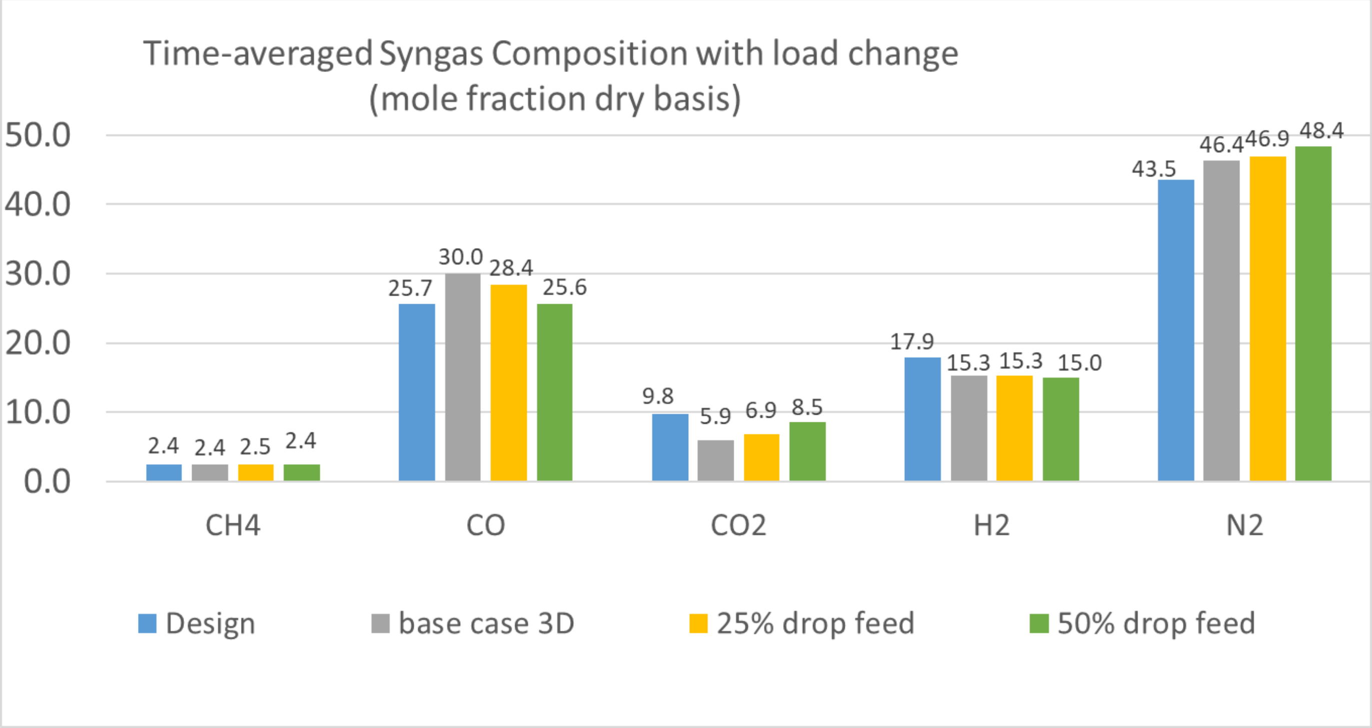
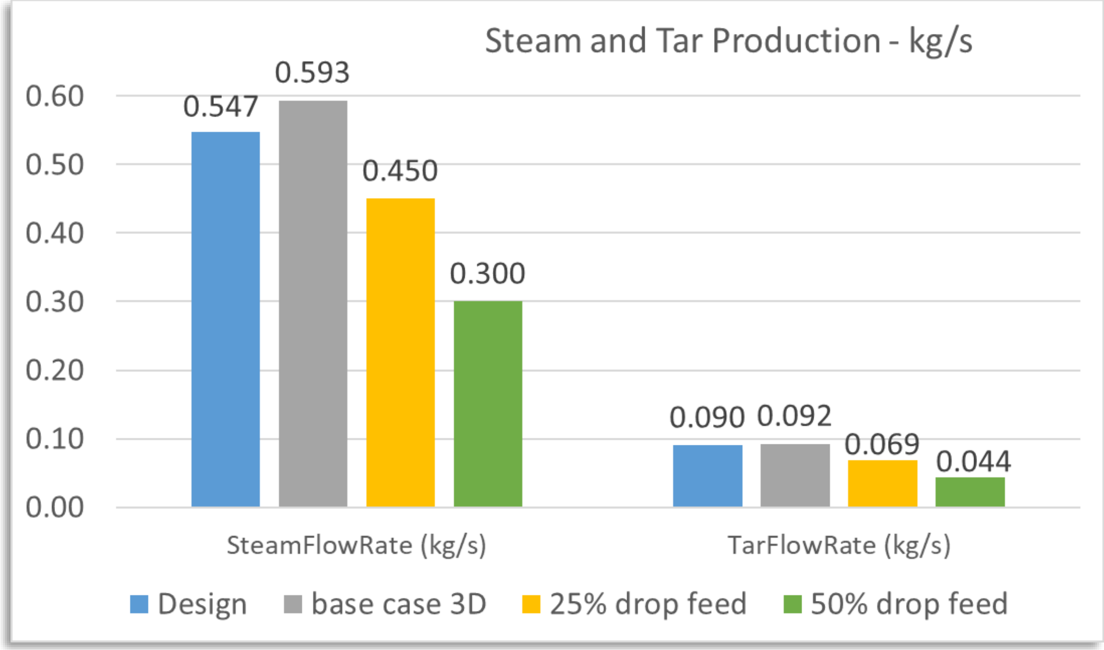
Syngas composition at gasifier exit





Gasifier responds well to large step changes in load

- Syngas composition can be maintained
- Bed Level can be controlled

Advanced Gasifier Design

Task Description – Perovskite-based Oxygen Separation

Task 3: Advanced Gasifier Design

Task 3.1: University of Alaska – Fairbanks Gasifier Studies

Task 3.2: Oxygen Separation

Task 3.3: Novel Coal FIRST Gasifier

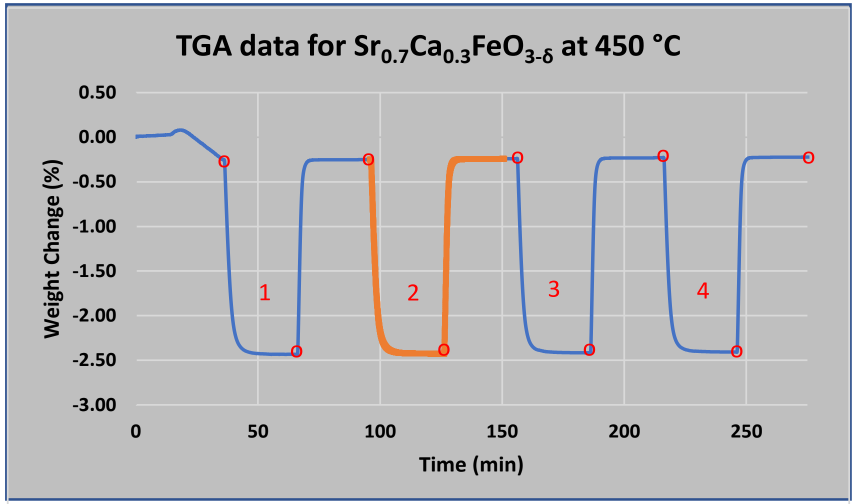
Develop and exercise models to support development of perovskite-based fixed-bed oxygen separation devices

- Supports ARS FWP Task 5 [1]
- Use Lab scale data to develop and validate kinetics, material and transport properties
  - Adsorption
  - Desorption
  - Heat of reaction
  - Material properties
- Model Bench Scale systems to validate scale-up, heat transfer
- Perform pilot and commercial scale simulations of prototype systems

[1] Oxygen Production for Gasification, NETL FWP 1022405, Task 5.1
Jonathan Lekse, NETL-RIC

Modeling Oxygen Separation with Perovskite Beds

Translating TGA data to Numerical model



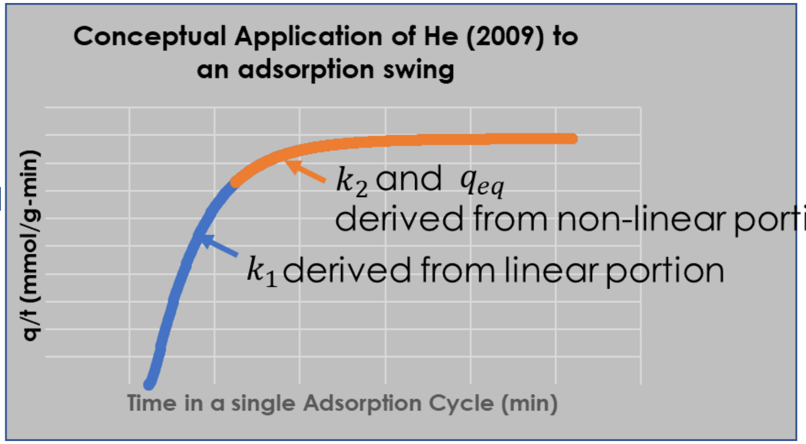
He (2009) suggests that each adsorption/desorption step can be characterized by a two-component calculation:

A linear component: $q_{O_2} = k_1 t$

A non-linear component: (Lagergren equation)

$$\frac{t}{q_{O_2}} = \frac{1}{k_2 q_{eq}^2} + \frac{1}{q_{eq}} t$$

q_{O_2} = Oxygen capacity (mmol/g)
q_{eq} = Equilibrium oxygen capacity (mmol/g)
k_1 = Linear rate coefficient (mmol/g-min)
k_2 = Diffusive rate coefficient (mmol/g-min)
t = Time (min)



Mass in-flow
- Air for adsorb swing
- N_2 for desorb swing

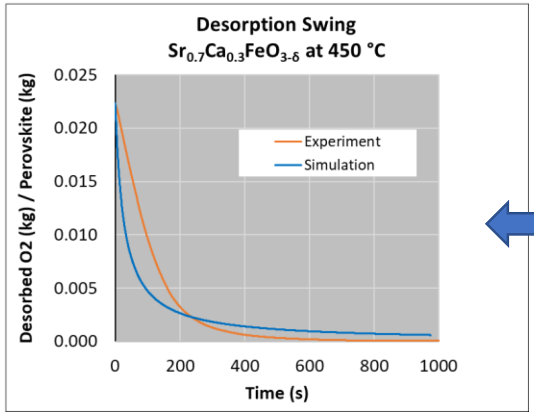
Tube:
Diameter = 0.021 m
Height = 0.559 m

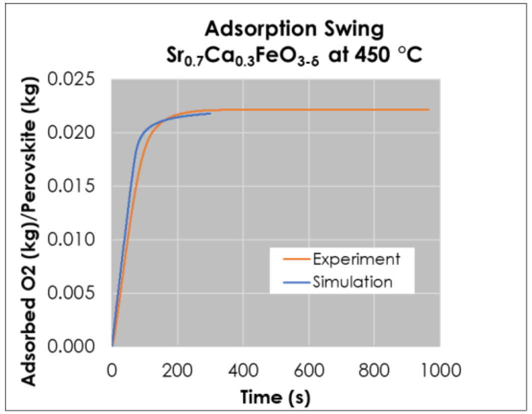
Particles:
Diameter = 0.0031 m
(300 g total)

Mesh: 4 x 60 x 4

Isothermal

Pressure out-flow





He, Y., Zhu, X., Li, Q., Yang, W., "Perovskite Oxide Absorbents for Oxygen Separation," AIChE Journal, Vol 55, No 12, Dec 2009, pp. 3125-3133

Advanced Gasifier Design

Task Description – Novel Coal FIRST Gasifier

- Task 3: Advanced Gasifier Design
  - Task 3.1: University of Alaska – Fairbanks Gasifier Studies
  - Task 3.2: Oxygen Separation
  - Task 3.3: Novel Coal FIRST Gasifier

Evaluate Novel Gasifier Technologies to Address Coal FIRST Initiative

- Model transient response to load variations
- Model oxygen-blown systems for potential carbon capture
- Model gasifier performance with coal-biomass co-feed

Novel Coal FIRST Gasifier

The Moving Bed Gasifier has much potential for Coal FIRST application

- High efficiency (40+% HHV); maintain over the load range
- ✓ Modular Design (proposed UAF plant is modular)
- ✓ Small Scale 50 – 350 MW (scalable and modular)
- ✓ Near-zero emissions (CO_2 Capture, biomass blending)
- ✓ High ramp rate capable (demonstrated in UAF simulations)
- Minimum load commensurate with 2050 renewable penetration
- ✓ Integration with energy storage (tar-liquids storage for use in generation)
- Minimum water consumption
- ✓ Reduced design, construction, and commissioning schedules (low pressure, proven design)
- Reduce maintenance and forced outages
- ✓ Integration with other plant value streams (tar-liquids production)
- ✓ Capable of natural gas co-firing (integrate NG with syngas)

Novel Coal FIRST Gasifier

Use the model to evaluate gasifier performance for Coal FIRST application

- High ramp rate capable (demonstrated in UAF simulations)
  - Simulate 25% and 50% instantaneous drop in design condition inlet flows, step change back to 100%
    - Stable output and good control of bed height
- Near-zero emissions (CO_2 Capture, biomass blending)
  - Study Oxygen enrichment performance
    - Replace 60% of inlet air with O_2 and steam
    - Replace 100% of inlet air with O_2 and steam
    - Replace 100% of inlet air with O2 and CO_2

Novel Coal FIRST Gasifier

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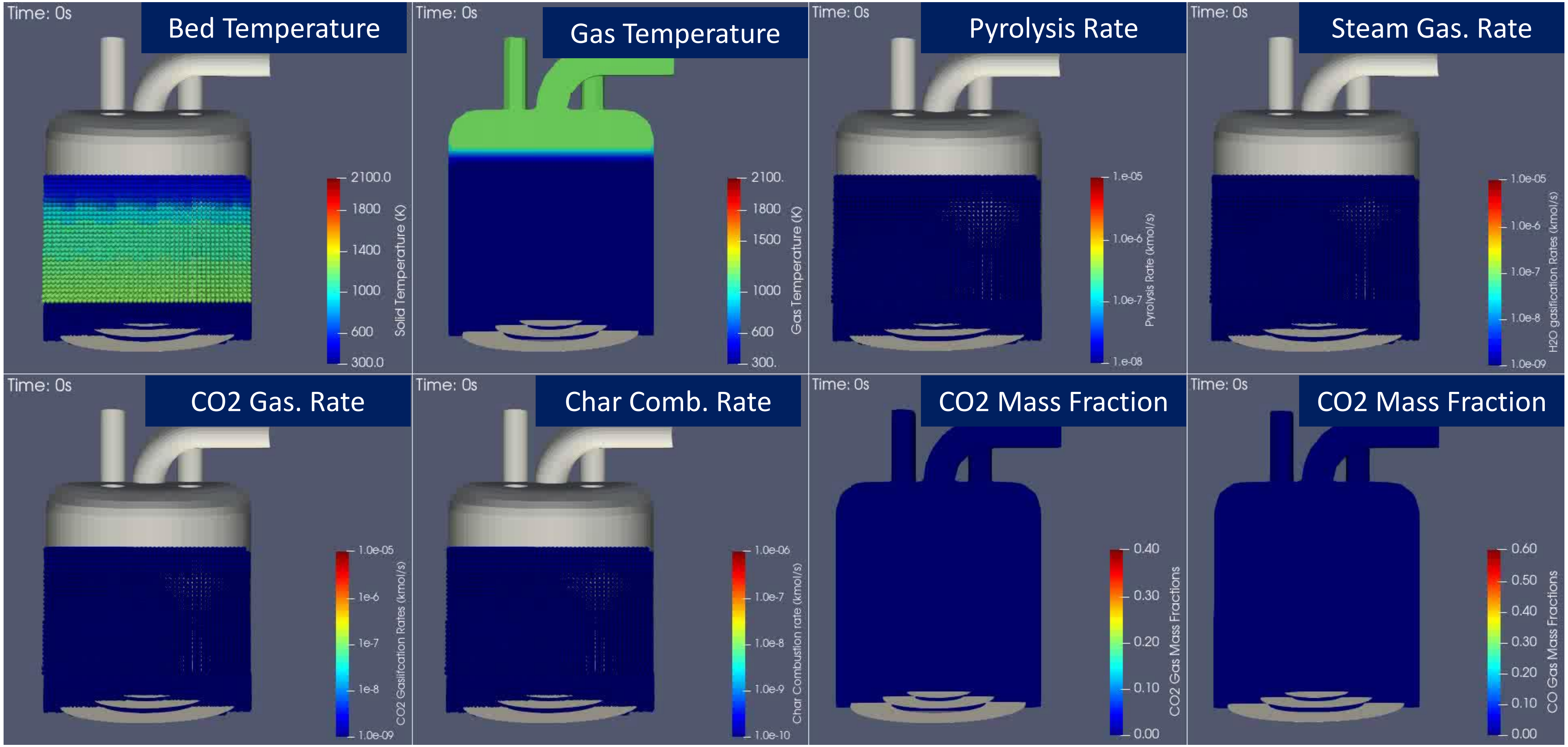
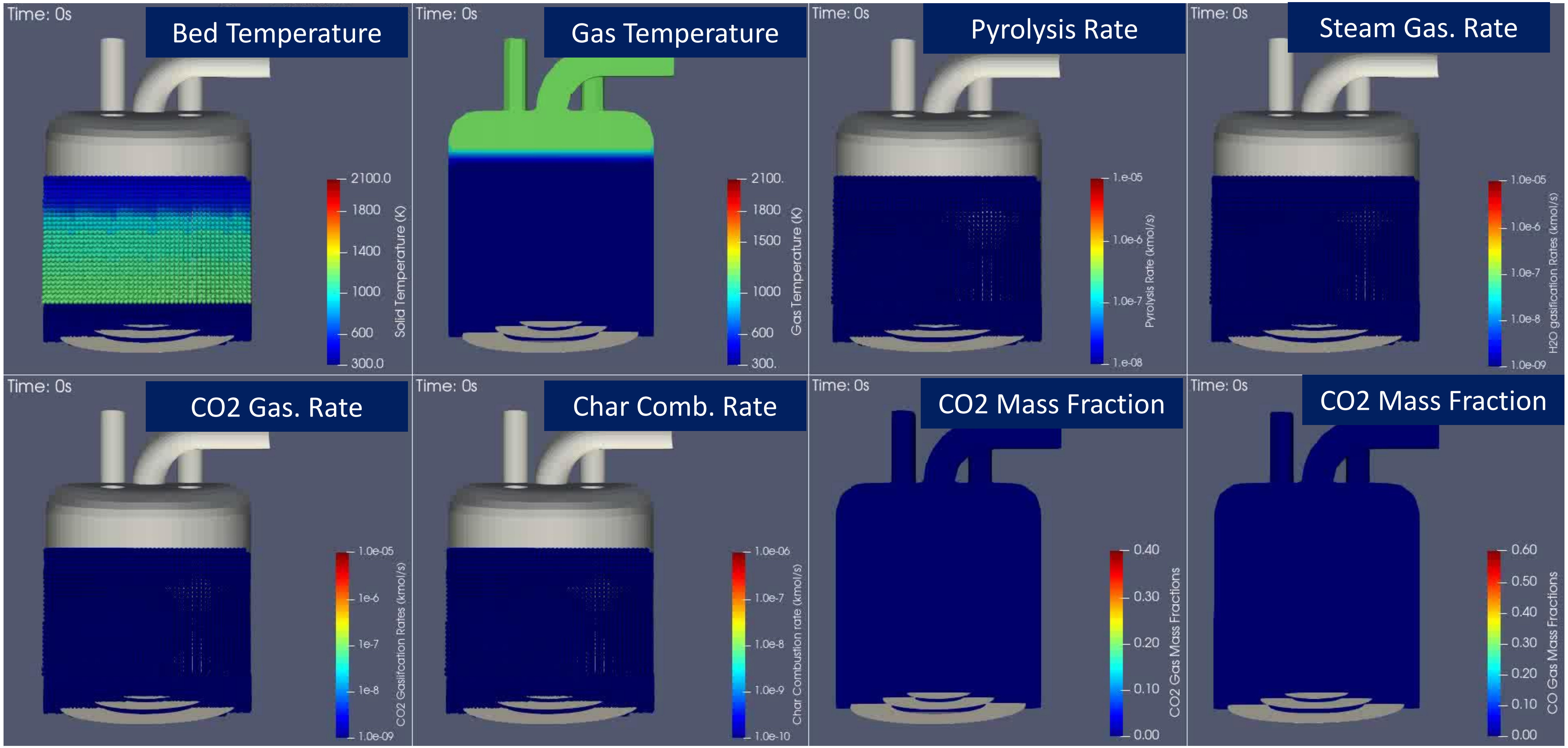
Replace 60% of inlet air with O_2 and steam



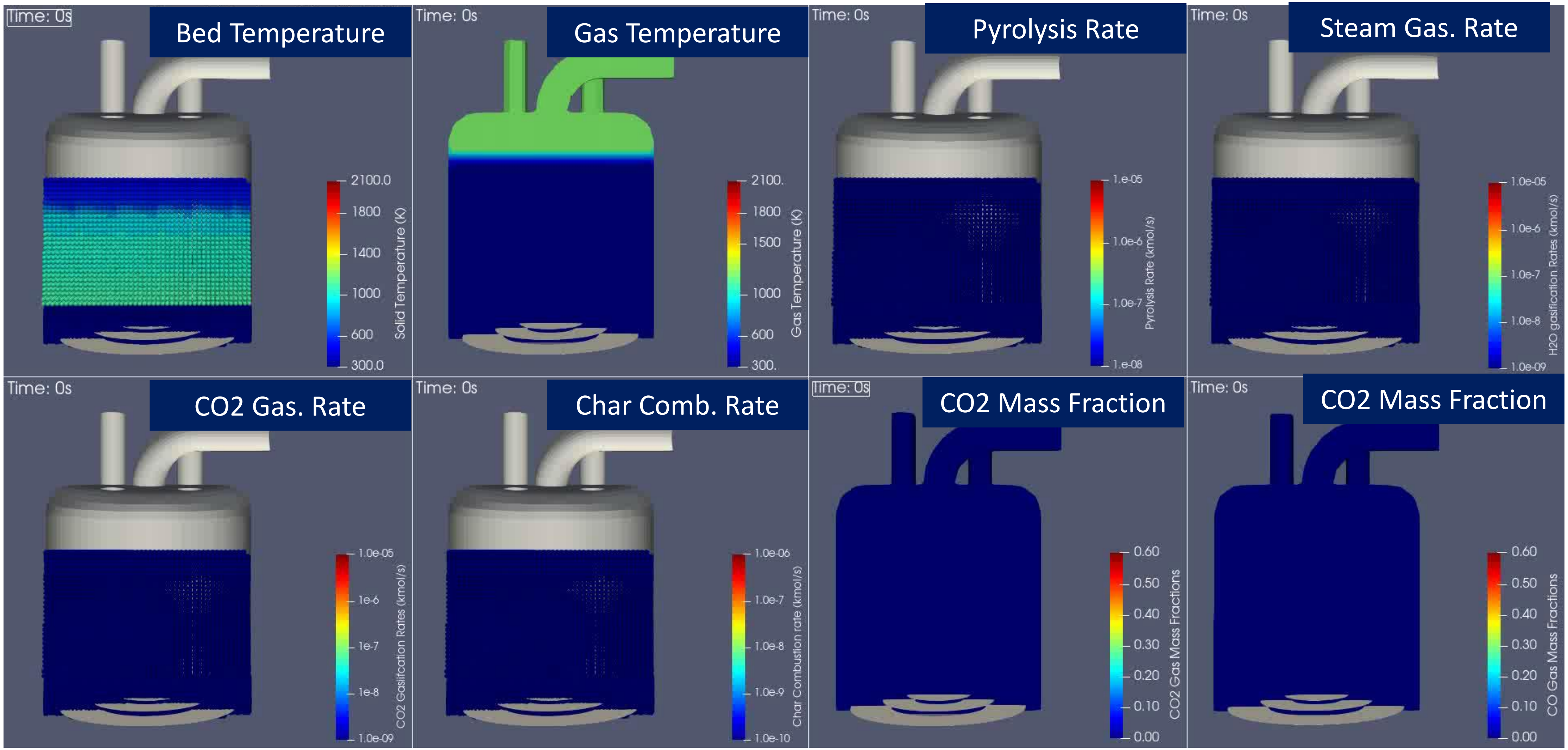
Novel Coal FIRST Gasifier

Replace 100% of inlet air with O_2 and steam



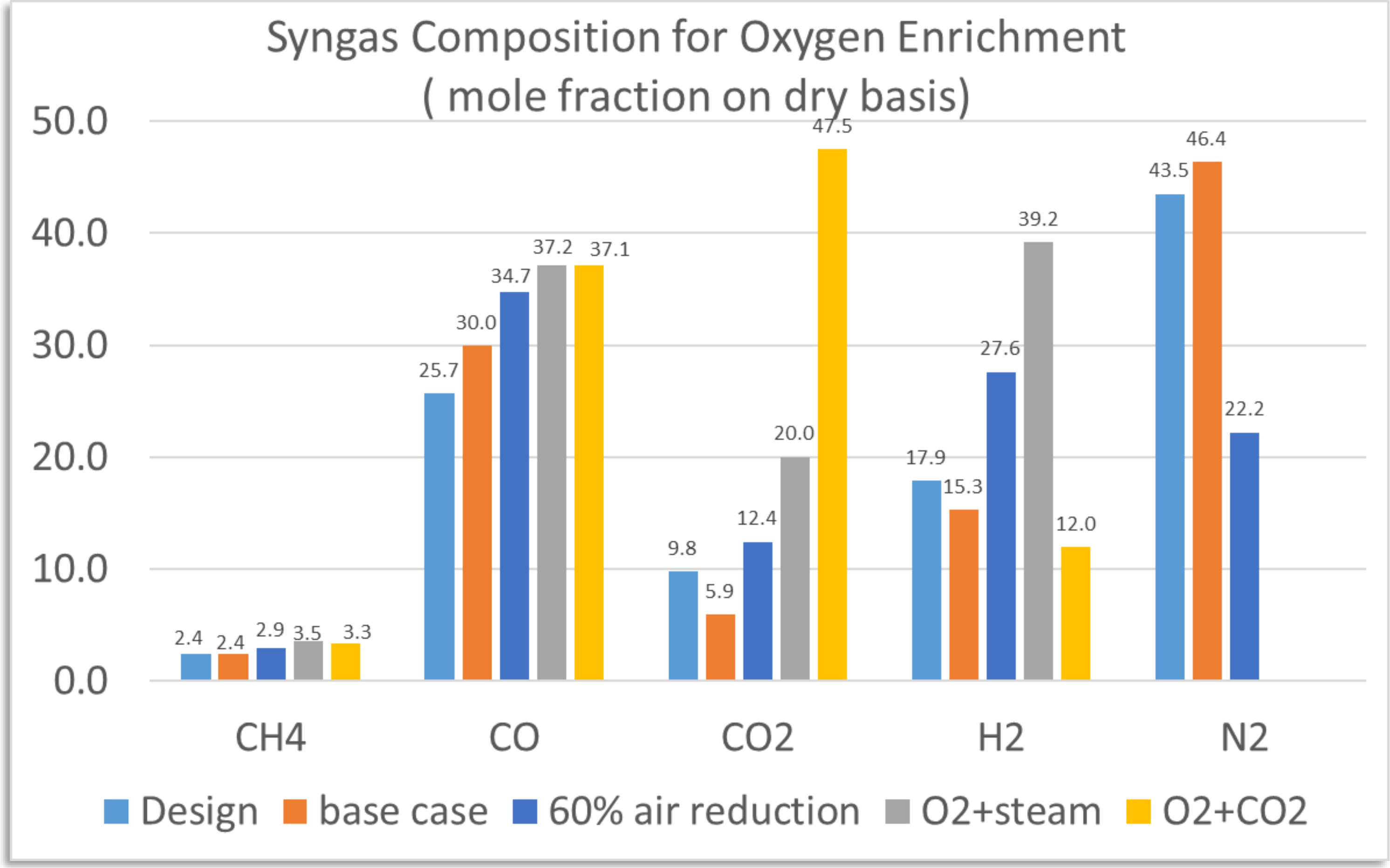
Novel Coal FIRST Gasifier

Replace 100% of inlet air with O_2 and CO_2



Novel Coal FIRST Gasifier

Syngas Exit Composition with Oxygen Enrichment



- Oxygen-blown with steam produces higher H_2 as expected
- Steam and CO_2 diluents can be adjusted for specific syngas applications

Summary and Next Steps

NATIONAL ENERGY TECHNOLOGY LABORATORY

Novel commercial-scale moving bed prototype has been developed

A prototype 22.5MW_{th} moving bed gasifier has been extensively studied for application in the proposed UAF plant

- Prototype is scaled-up from an existing HMI commercial design
- Model kinetics validated with data from Sotacarbo Research Center
- Predicted gasifier performance agrees closely with UAF FEED study design conditions
- Additional studies verified that gasifier responds well to large fluctuations in load
  - Syngas composition is stable; Bed level can be controlled

Next Steps – Validation of sub-models and further application to support the UAF Program

- In-situ neutron imaging work at ORNL [1] will provide data on particle morphology changes and coal bed dynamics during drying, pyrolysis and gasification of Usibelli coal
- NETL REACT facility will provide transient data on syngas and tar composition for Usibelli coal in TGA and fixed bed systems
- Apply model to operating conditions of interest to the UAF team to help guide design and operations

[1] Experimental Validation of Coal Gasification with Neutron Imaging, FWP-FEAB325 James Parks II, Oak Ridge National Laboratory (ORNL)

Summary and Next Steps

Novel commercial-scale moving bed prototype for Coal FIRST application

Robust gasifier performance to load changes may be suitable Coal FIRST application

- Gasifier performance was studied over a range of oxygen enrichment conditions
    - Gasifier was stable over full range of conditions, bed temperatures were controllable
    - Syngas composition changed with stoichiometry as expected

Next Steps

- Evaluate gasifier performance with biomass-coal co-feed
    - Air and oxygen-enriched systems
    - Evaluate load response

Summary and Next Steps

Commercial-scale fixed perovskite beds for oxygen generation

Small-scale models of perovskite beds have been developed

- Adsorption and Desorption kinetics have been validated with TGA data
- Preliminary studies at lab scale are underway

Next Steps

- Validate fixed bed models at the lab scale
  - Small-scale systems including heat transfer
- Simulations to explore scale-up to pilot and commercial

Acknowledgements

- **FE Program**
  - Regis Conrad
  - Bhima Sastri
  - Jai-Woh Kim
  - K. David Lyons
  - Diane R. Madden
- **Experimental**
  - ARS Perovskite Team
    - Jonathan Lekse
    - Eric Popczun
    - Sittichai Natesakhawa
  - ARS REACT Team
    - Dushyant Shekhawat
    - Mark Smith
- **Computational**
  - ARS Multiphase Flow Science
    - Mehrdad Shahnam
    - MaryAnn Clarke
    - Deepthi Chandramouli
    - Liqiang Lu
    - Jia Yu
    - Yupeng Xu

- **Collaborators**
  - UAF Team
    - Brent Sheets
    - Rolf Maurer
    - Alberto Pettinau
    - David Thimsen
    - Harvey Goldstein
  - ORNL
    - James Parks
    - Charles Finney
    - Costas Tsouris

Thank you
Questions?

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