

# From Pilot Data to Full-Scale Digital Gasifier: A Data- Informed CPFD Story

SCALING INNOVATIVE GASIFIER TECHNOLOGY  
USING ADVANCED DATA MODELING

# End-to-End Modeling Story

2023



- Pilot Plant Model Set-up
- Validation of process parameters with Case-1
- Effect of pressure analyzed with Case-2

2024



- Submitted to EnergyWerx Program
- Model refinement
  - Effect of bed material properties

2025



- Commercial scale Model Set-up
- Baseline model assessment
- Fluidized bed behavior verified
- Reaction Kinetics refinement required



# From Pilot Validation to Commercial Scale Model

## **Reducing Risk and Accelerating Deployment**

The digital modeling approach reduces development risks and accelerates deployment of low-carbon renewable fuel technologies.

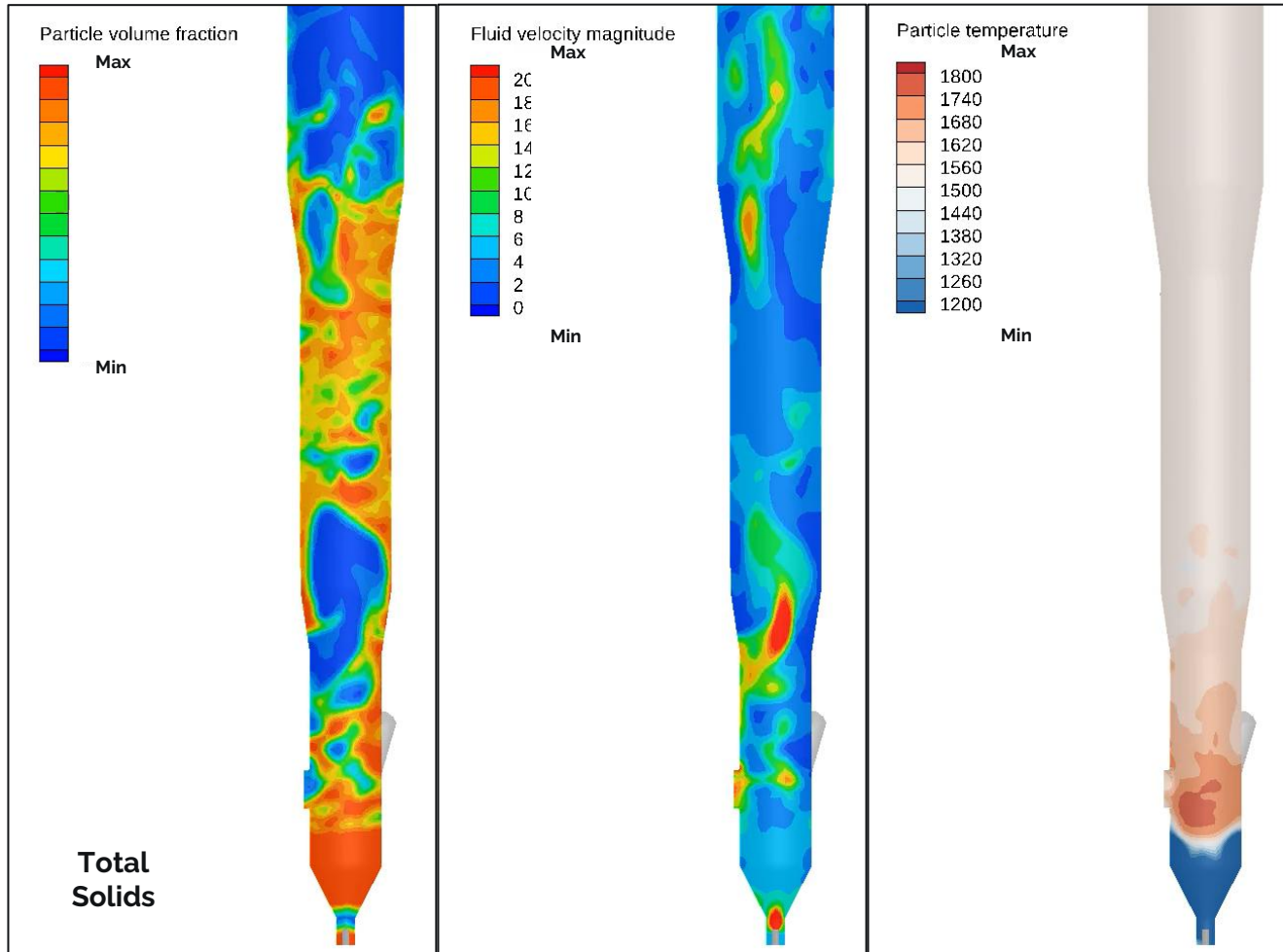
## **Data-Informed Modeling Approach**

The approach combines physics-based modeling with **real operational data** to validate pilot-scale model

## **Scale-Up from Pilot to Full-Scale**

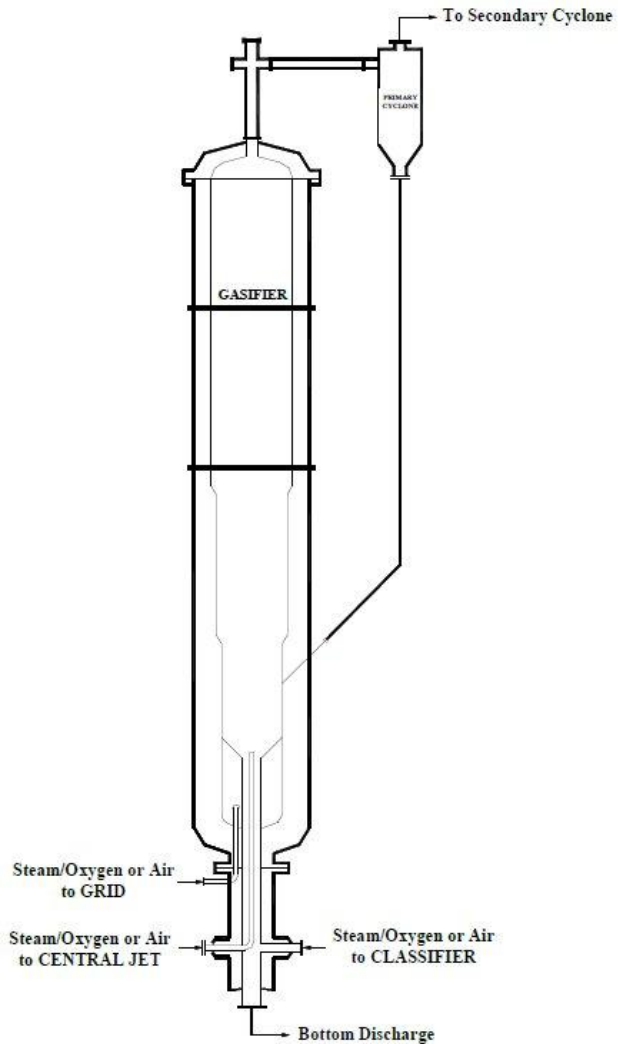
Modeling maturity builds iteratively, bridging pilot experiments to credible commercial-scale digital gasifier representations.

# Why Modeling Matters for Biomass Gasification



- **Complexity of Biomass Gasifiers**
  - Biomass gasifiers involve complex turbulent gas-solid flows and multi-phase chemical reactions challenging traditional design methods
- **Benefits of CFPD Modeling**
  - CFPD modeling visualizes internal gasifier conditions like fluidization behavior and thermal profiles to reduce uncertainty
- **Modeling as Decision Support**
  - Modeling complements experiments to inform design tradeoffs, accelerate deployment and improve operational stability

# Step 1: Pilot-Scale Modeling Approach



## Pilot-Scale Model Development

The CPFD model was developed for a smaller-scale U-Gas pilot plant with quality experimental data.

## Simulation and Validation

Transient 3D simulation validated internal hydrodynamics and temperature profiles against measured data.

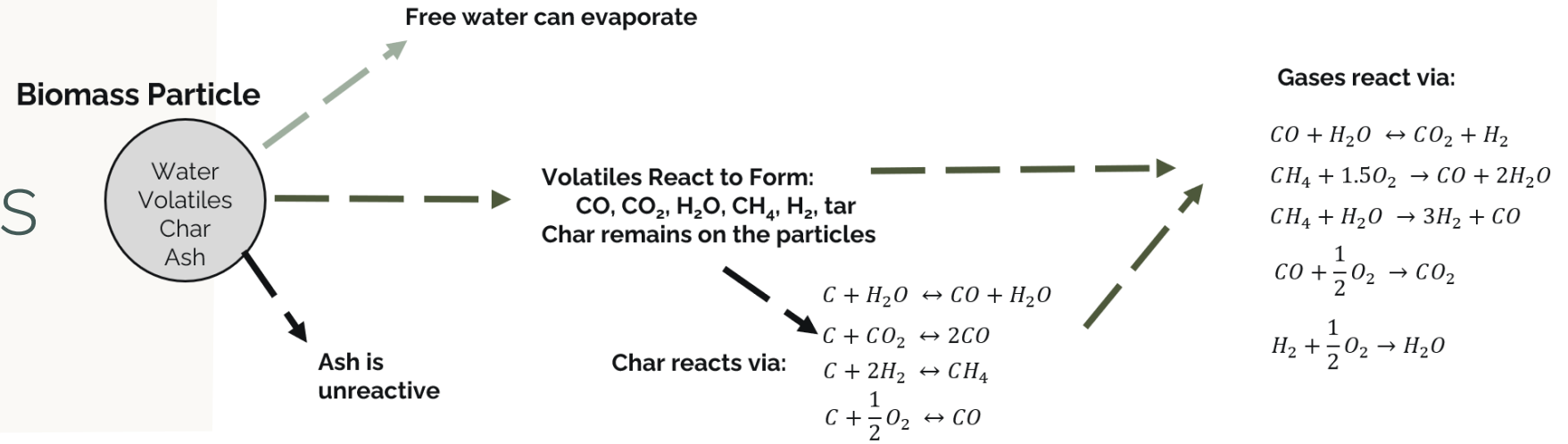
## Model Calibration

Calibration used multiple operating conditions to reflect realistic physical behavior, not just a single scenario.

## Foundation for Scale-Up

The pilot-scale model serves as a foundational step to guide future scale-up and refinement efforts.

# Data-Informed Reaction Kinetics Framework



## Plug-Flow Model Regression

A plug-flow model was used to regress kinetic parameters against pilot plant outlet data for consistency with observed performance.

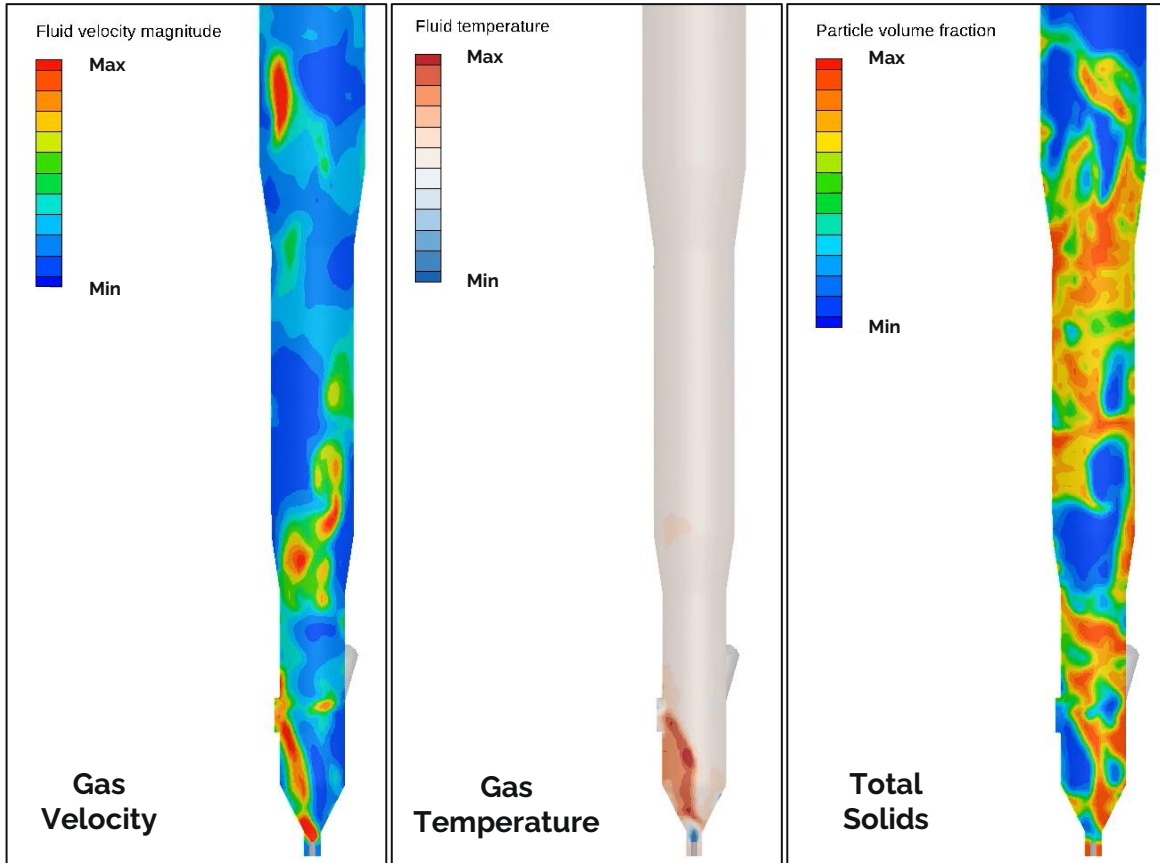
## Comprehensive Reaction Network

The kinetics incorporated char oxidation, steam and CO<sub>2</sub> gasification, methane reforming, and water-gas shift reactions in the simulation.

## Model Transferability and Reliability

Anchoring kinetics to real data enhanced model predictability and scalability, reducing arbitrary tuning significantly.

# Pilot-Scale Validation Results



## Model Validation Accuracy

Simulated outlet gas compositions closely matched experimental data, confirming model reliability.

## Axial Species Profiles

Axial profiles of H<sub>2</sub>, CO, CO<sub>2</sub>, and CH<sub>4</sub> revealed dominant reaction zones along the reactor.

## Temperature Prediction Alignment

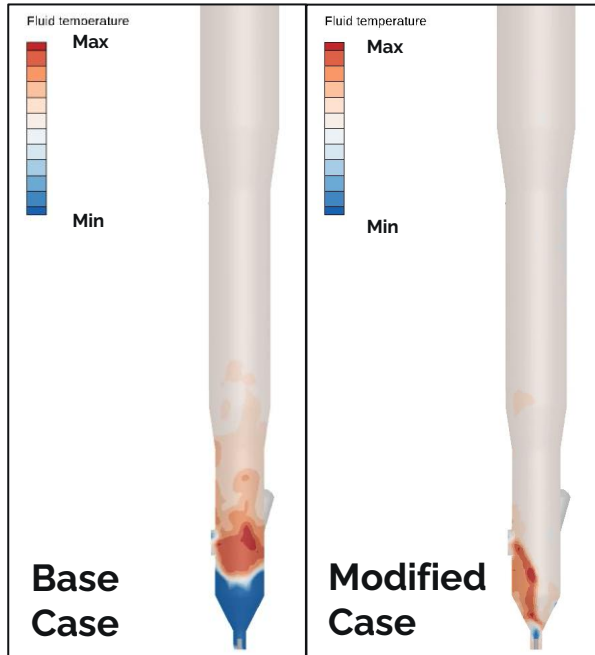
Predicted temperature trends matched measured data, showing interaction of mixing and heat release.

## Model Confidence for Scale-Up

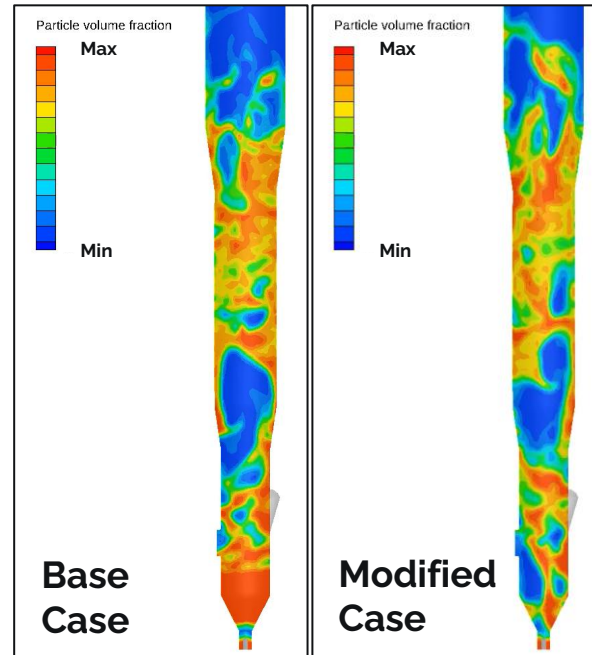
Validation results enabled confident use of pilot model as a reference for scale-up decisions.

# Key Insight: Hydrodynamics and Mixing

## Fluid Temperature



## Total Solids



- **Impact of Hydrodynamics**

- Hydrodynamics and mixing strongly influence reactor performance by affecting solids circulation and temperature distribution.

- **Stagnant Solids Zones**

- Stagnant solids near the reactor bottom reduce temperature and conversion efficiency, limiting reaction rates.

- **Gas Velocity Variability**

- Gas velocity fields exhibit spatial variability with fast bubbles and jets alongside slower regions, impacting mixing.

- **Design Focus Shift**

- Understanding hydrodynamics led to design improvements focusing on solids circulation and avoiding poor mixing.

# Key Insight: Particle Size Distribution Effects

## **Reactor Behavior Sensitivity**

Reactor behavior is highly sensitive to variations in particle size distribution affecting overall performance.

## **Impact on Mixing and Dispersion**

Different particle sizes dramatically influence solids mixing and carbon dispersion within the reactor bed.

## **Temperature Uniformity Improvement**

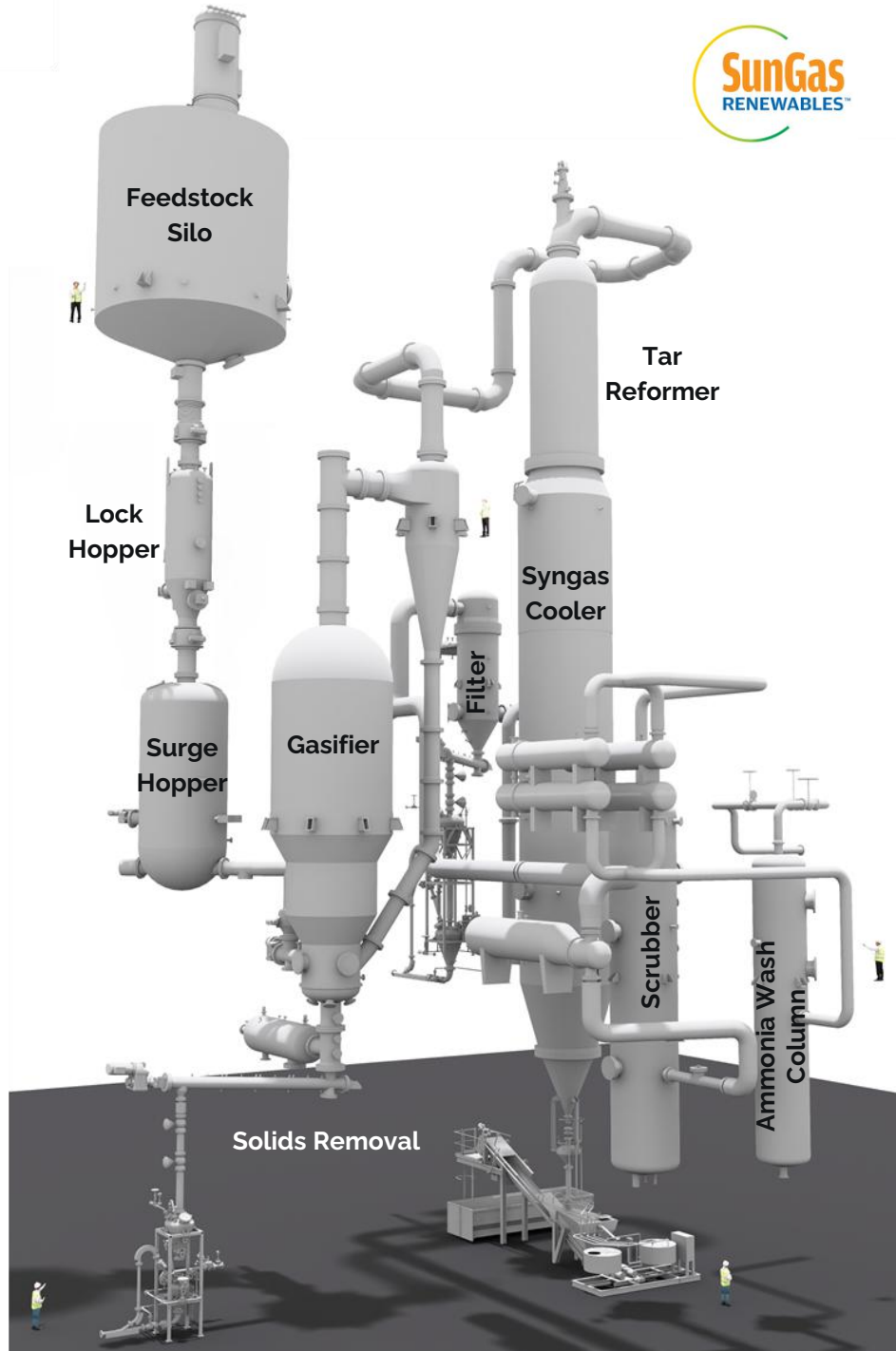
Appropriate particle size distributions reduce temperature gradients by enhancing turbulence and eliminating packed regions.

## **PSD as a Design Variable**

Particle size distribution is a key design variable critical for model assumptions and further sensitivity analysis.



# SunGas S-1000™ Overview



## Integrated Subsystems

SunGas System 1000 integrates gasification, tar reforming, syngas cleanup, and fuel synthesis subsystems for efficient biomass processing.

## Feedstock Flexibility

The system processes various biomass feedstocks and produces multiple energy products like methanol, renewable natural gas, and sustainable aviation fuel.

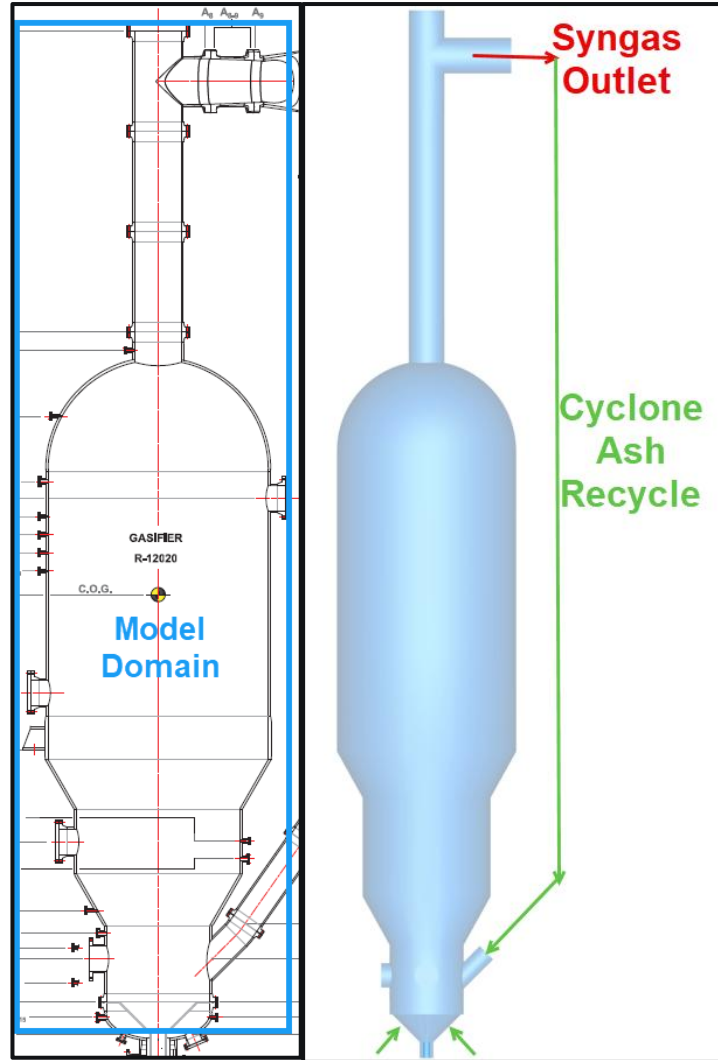
## Sustainability Focus

Designed to enable significant carbon reductions by using biogenic carbon and incorporating carbon capture and sequestration technologies.

## Modeling and Optimization

Accurate modeling of gasifier hydrodynamics, temperature, and gas composition improves overall system performance and economics.

# Transitioning from Pilot to Full Scale



- **Validated Modeling Framework**
  - The pilot-scale effort produced a validated modeling framework trusted for accurate predictions and analysis.
- **Carrying Forward Key Elements**
  - Full-scale modeling builds on established kinetics and critical parameters identified in pilot studies.
- **Structured Scale-Up Approach**
  - Scale-up is a structured extension of prior learning, avoiding leaps of faith with added complexity as needed.

# Step 2: Full-Scale Baseline CPFD Model

## Development of Full-Scale Model

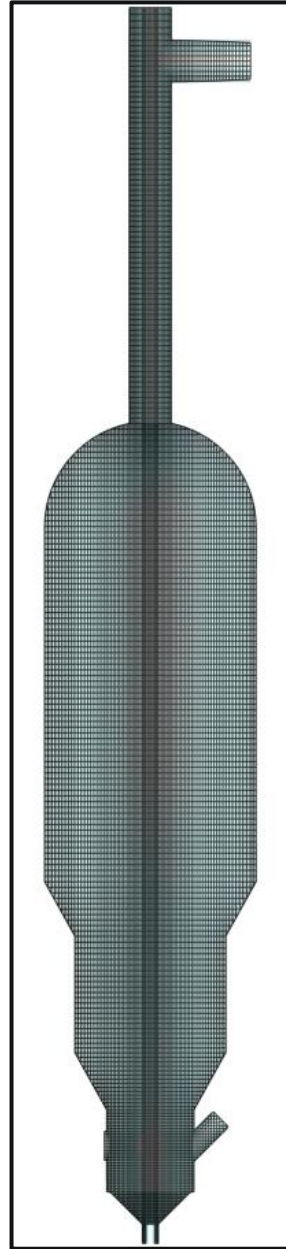
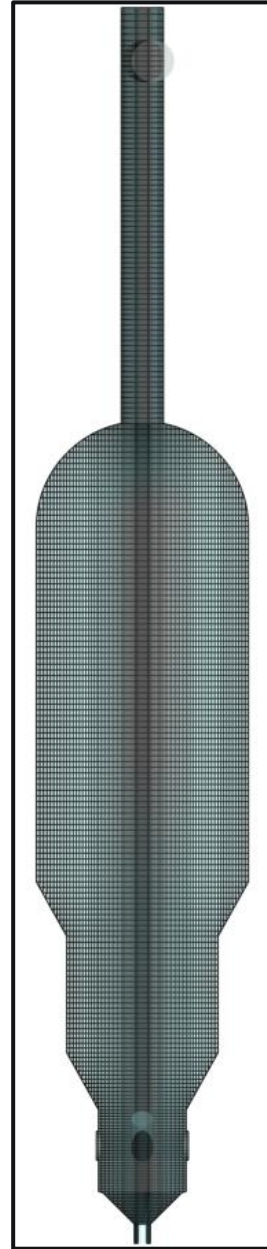
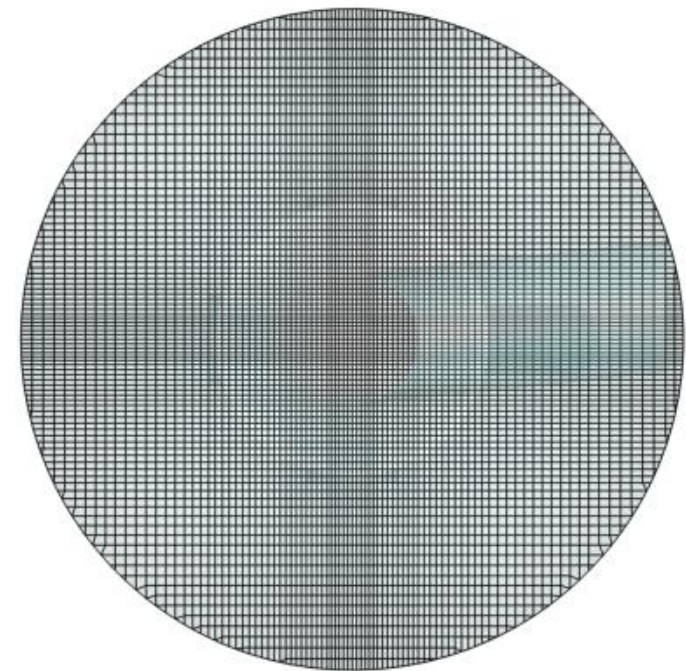
A comprehensive 3D digital model of the commercial SunGas gasifier was developed using engineering data and pilot-scale framework.

## High Resolution Computational Grid

The model incorporated nearly one million computational cells to accurately represent the full reactor geometry and internal components.

## Model as Calibration Baseline

This baseline model serves as a starting point for future calibration and virtual testing, not as a final design.



# What Carried Over from the Pilot Model

## Reuse of Reaction Kinetics

The full-scale model reused the reaction kinetics framework from the pilot study ensuring consistent chemical processes.

## Consistent Assumptions

Volatile composition assumptions and initial PSD concepts developed at pilot scale were maintained in the full-scale model.

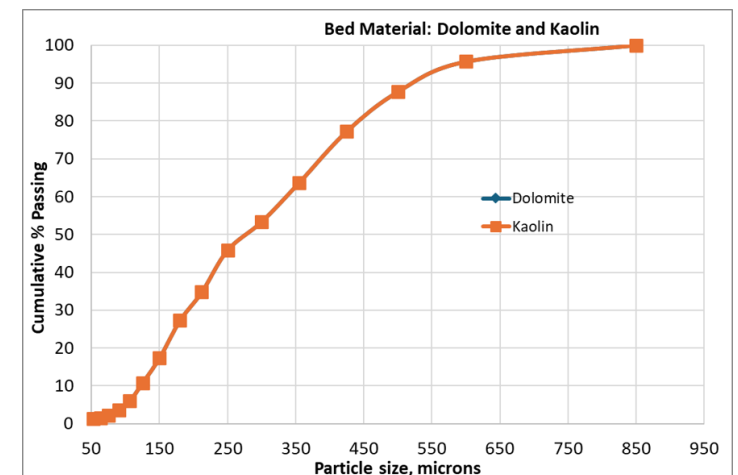
## Reliable Scale Comparison

Consistency across scales allowed attribution of differences to geometry and operation, not model assumptions.

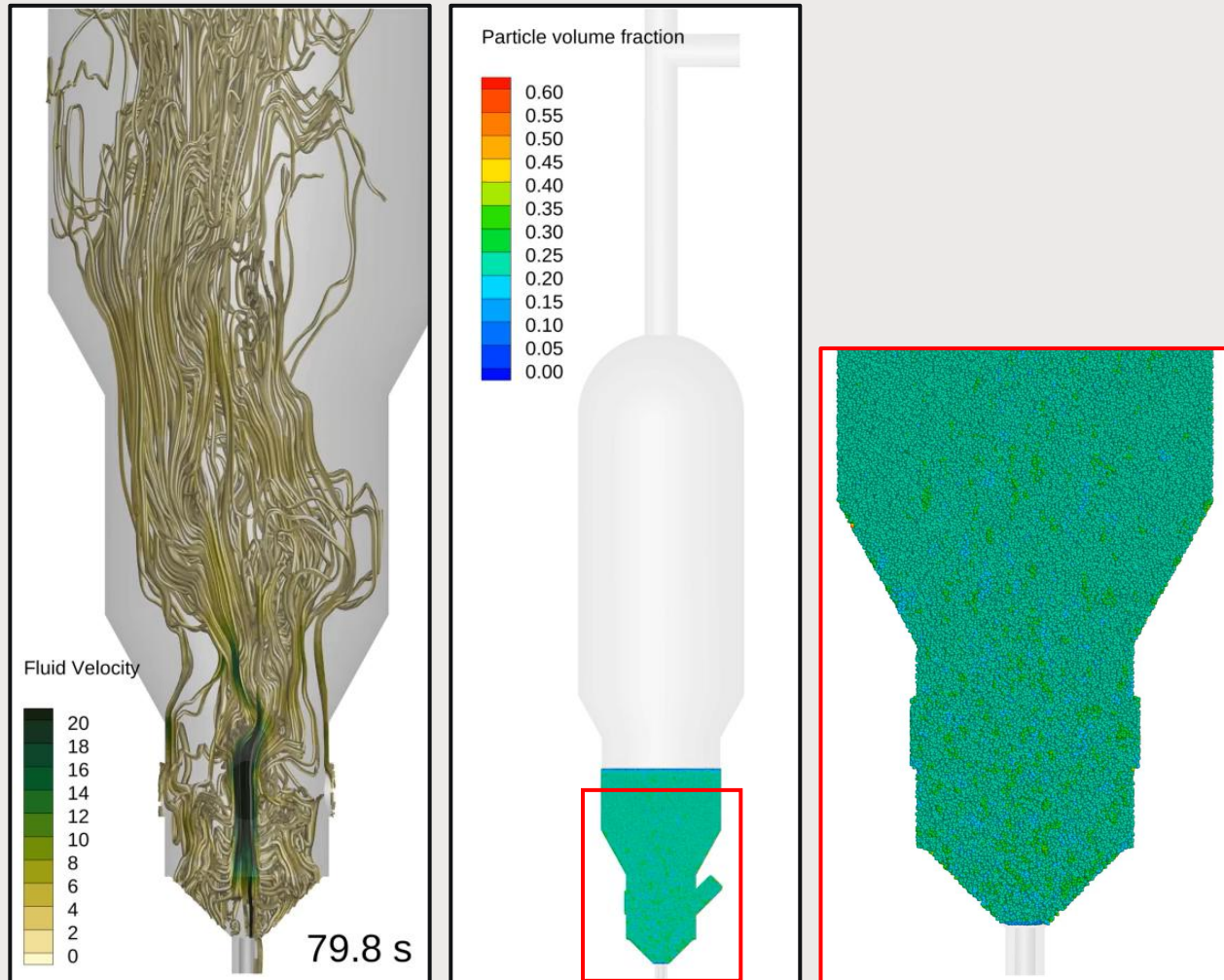
## Pilot Model as Backbone

The validated pilot model became the backbone of the commercial-scale digital twin, reinforcing model reliability.

No.	Reaction	Description
1	$d[\text{Volatile(S)}]/dt = -1 \cdot k_{10}$	Volatile consumption
2	$d[\text{CO}_2]/dt = -0.167259 \cdot d[\text{Volatile(S)}]/dt$	CO <sub>2</sub> production
3	$d[\text{CO}]/dt = -0.468326 \cdot d[\text{Volatile(S)}]/dt$	CO production
4	$d[\text{H}_2\text{O(v)}]/dt = -0.142034 \cdot d[\text{Volatile(S)}]/dt$	H <sub>2</sub> O production
5	$d[\text{H}_2]/dt = -0.017487 \cdot d[\text{Volatile(S)}]/dt$	H <sub>2</sub> production
6	$d[\text{CH}_4]/dt = -0.128333 \cdot d[\text{Volatile(S)}]/dt$	CH <sub>4</sub> production
7	$d[\text{C}_{10}\text{H}_8]/dt = -0.076561 \cdot d[\text{Volatile(S)}]/dt$	Tar production



# Hydrodynamics at Commercial Scale



## Jet-Driven Recirculation

Jet-driven recirculation acts as the main mixing mechanism, moving solids upward and creating circulation loops.

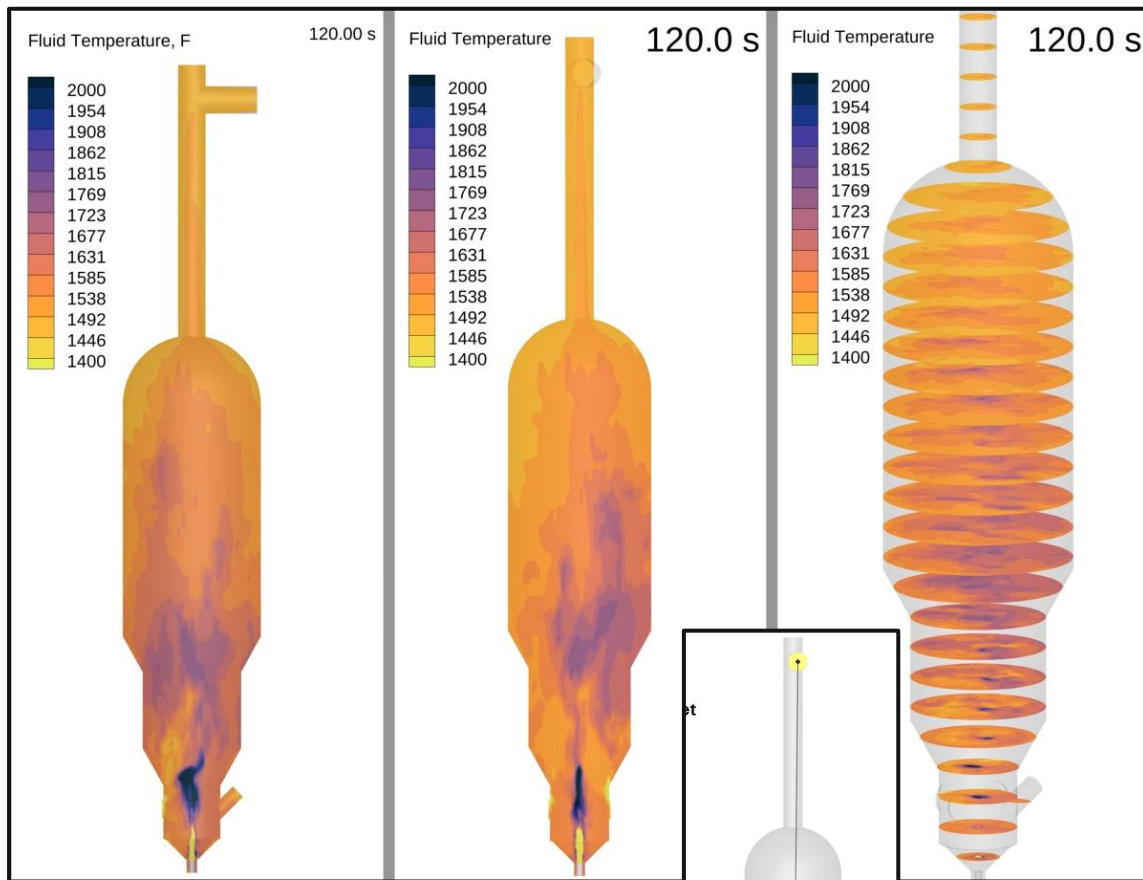
## Solids Movement Dynamics

Solids rise rapidly in reactor core and descend along the walls, demonstrating rapid mixing of gas and solids.

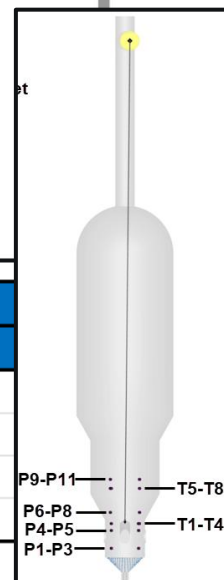
## Scaling Validation

Full-scale observations confirmed pilot-scale hydrodynamic behaviors and revealed new spatial flow details unique to larger setup.

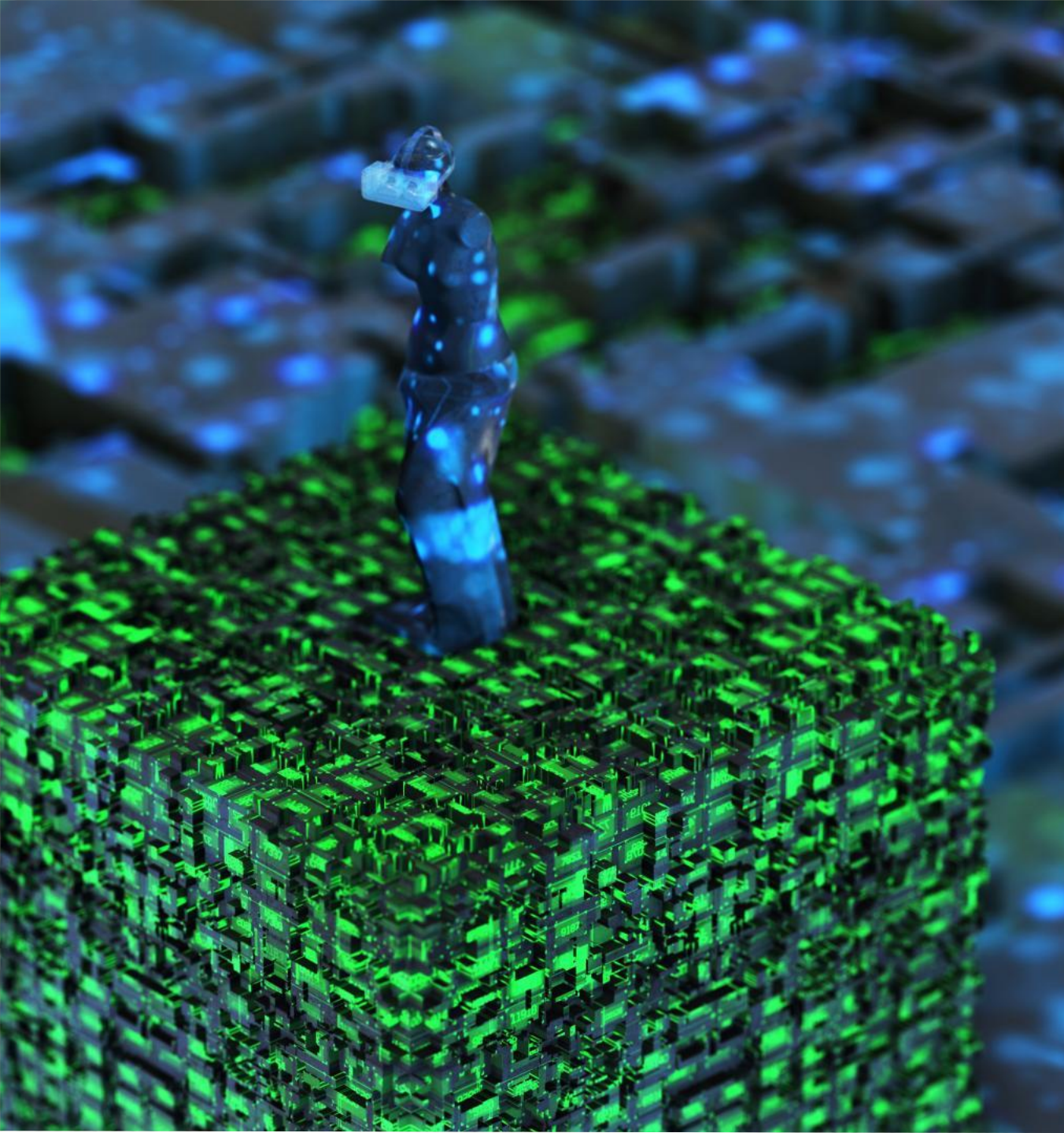
# Reaction Zones and Temperature Structure



Data points: Temperature (F)	
Notation	Value
T1 to T4	1549
T5 to T8	1558
T9 to T12	1550
Outlet Temperature, F	1487
Expected Bed Temperature, F	1560



- **Oxidation Hot Spots**
  - Oxidation reactions create hot spots near the jet, showing localized high temperature zones in the reactor.
- **Reforming and Water-Gas Shift Reactions**
  - Downstream regions are dominated by reforming and water-gas shift reactions, influencing temperature and gas composition.
- **Uniform Freeboard Conditions**
  - The freeboard area shows cooler temperatures and uniform gas compositions due to lower oxygen levels.
- **Modeling Consistency Across Scales**
  - Consistent reaction and temperature patterns in pilot and full-scale models validate the reaction-mixing interplay.



# Remaining Gaps and Sensitivities

## **Alignment with Pilot Insights**

Sensitivities identified in the full-scale study closely match pilot work findings, validating early detection efforts.

## **Model Uncertainties**

The baseline model has unresolved uncertainties related to reaction kinetics, particle transient conditions (e.g. representation of attrition and cohesion).

## **Future Modeling Agenda**

Explore better representation of transient particle conditions to improve model accuracy and sensitivity check for key process conditions



# Final Takeaways: Why the Connection Matters

## **Pilot-Scale Model Insights**

The pilot-scale CPFD model provided critical insights into hydrodynamics, mixing, and sensitivity drivers for full-scale assumptions.

## **Risk Reduction & Optimization**

Using a data-informed framework helped reduce scale-up risk and enabled virtual testing and optimization of processes.

## **Cumulative Modeling Benefits**

Early investment in validated pilot-scale models yields dividends in transitioning to commercial low-carbon energy technologies.