

Design Study for Bio-Oil Production from Biomass using a Dual Fluidized-Bed Reactor

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Introduction

- The goal of the CFD modeling study is investigate the catalytic fast pyrolysis (CFP) of biomass (e.g. wood chips) into bio-oil.
- Bio-oil with reduced oxygen content (CFP oil, 10-20w%O) could be co-processed with Vacuum Gas Oil (VGO) in a conventional refinery¹.
- A dual-fluidized bed pilot plant is available at West Biofuels in Woodland California.
- A reconfiguration from gasification to pyrolysis is guided by the results of the CFD study.

¹[M. Talmadge et al., "A Perspective on oxygenated species in the refinery integration of pyrolysis oil," Green Chemistry \(2014\).](#)

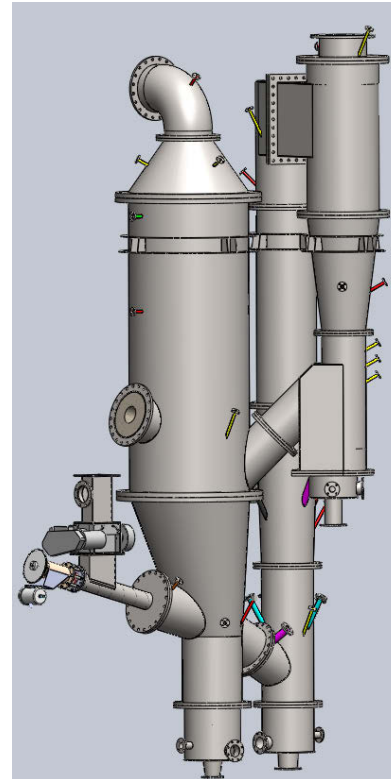
Previous Configuration as Gasifier

5 ton/day Pilot Plant



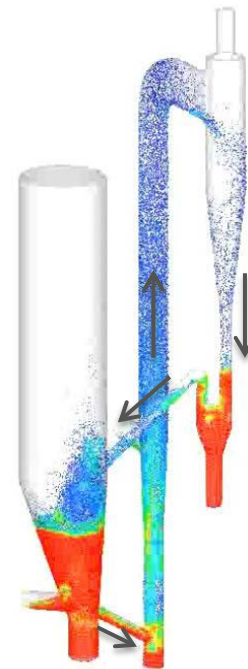
West Biofuels, LLC

CAD Model of Reactor



8.5 m

Internal Geometry



Front-side views

Original design by [H. Hofbauer et al., "The FICFB-Gasification Process" In: Developments in Thermochemical Biomass Conversion \(1997\).](#)

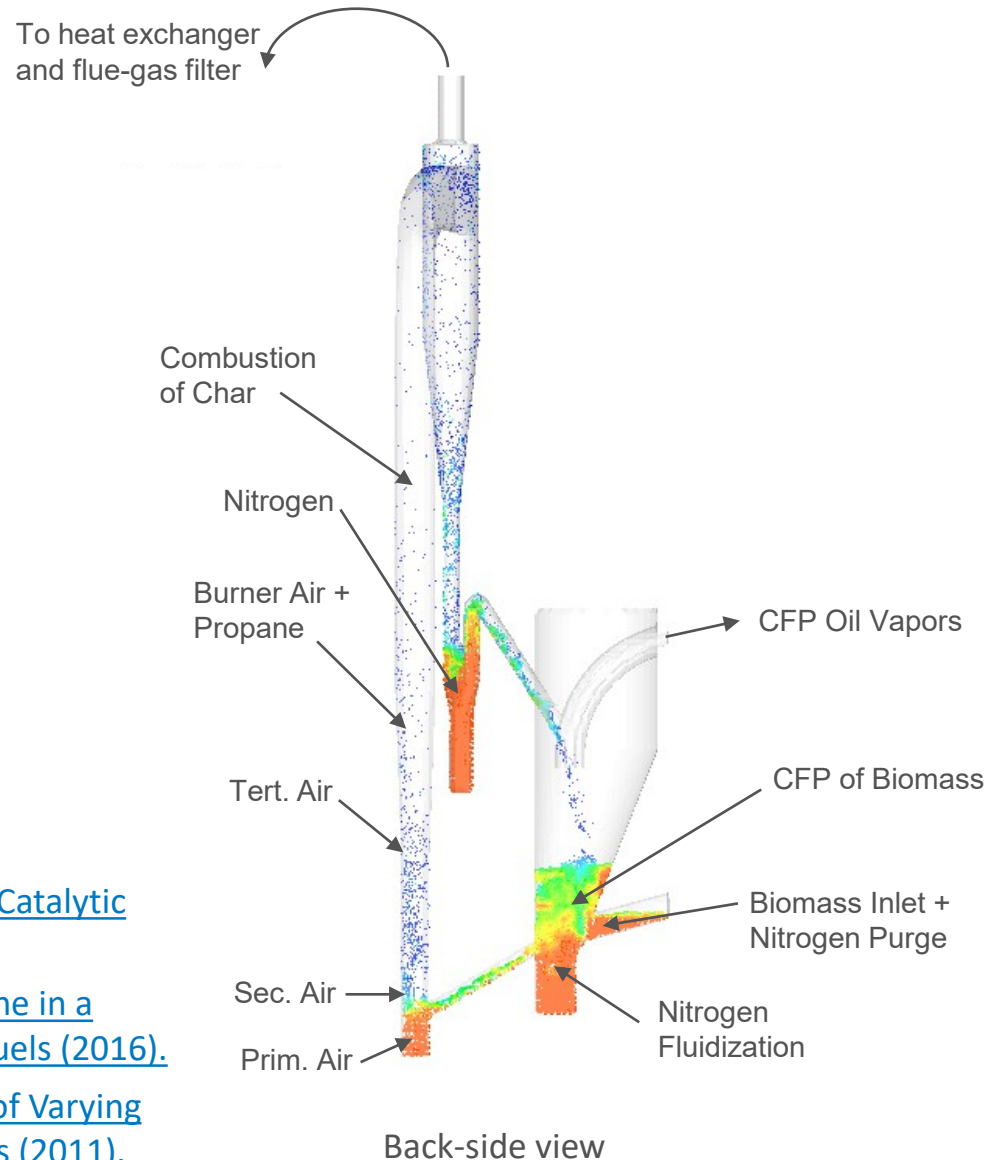
Reconfiguration to Pyrolyzer

- Lower temperature (550 C instead of 850 C)
- Nitrogen instead of steam for fluidization.
- Bed material with higher surface area and mild acidity.
- Extraction tube, reduced freeboard, and lower bed height to achieve vapor residence time of 1s.
- Modified downstream equipment (scrubbers, filters, ...)

[D. Dayton et al., "Design and Operation of a Pilot-scale Catalytic Biomass Pyrolysis Unit," Green Chemistry \(2015\).](#)

[K. Iisa et al., "In Situ and ex Situ Catalytic Pyrolysis of Pine in a Bench-Scale Fluidized Bed Reactor System," Energy & Fuels \(2016\).](#)

[K. R. Gaston et al., "Biomass Pyrolysis and Gasification of Varying Particle Sizes in a Fluidized-Bed Reactor," Energy & Fuels \(2011\).](#)



Multiphase Particle-in-Cell Method (MP-PIC) Using Barracuda Virtual Reactor[®] by CPFD, LLC

- Fluid Phase (Eulerian)
 - Mass, momentum, and energy equations are solved using finite volume approach
 - Laminar fluid viscosity terms generally neglected for gases: balance between inertia, pressure, body force, and interphase interaction force
 - LES turbulence model used – Smagorinsky sub-grid scale model with viscosity coefficient of 0.01.
- Particle Phase (Hybrid Lagrangian/Eulerian)

- Described by a PDF

$\phi(\vec{x}, \vec{u}_p, \rho_p, \omega_p, t)$ Probability of finding a particle at position x , velocity u_p , density ρ_p , volume ω_p , and time t .

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \phi \vec{u}_p + \nabla \vec{u}_p \cdot \phi \vec{A} = 0$$

Equation describing how the particle PDF changes in time. \vec{A} includes interphase drag and inter-particle stress model.

Local properties are determined from integrating the particle PDF:

$$\theta_p = \iiint \phi \omega_p d\omega_p d\rho_p d\vec{u}_p \quad \text{Particle volume fraction}$$

Drag Model: Wen Yu

$$\vec{u}_p = \frac{1}{\theta_p \rho_p} \iiint \phi \omega_p \rho_p \vec{u}_p d\omega_p d\rho_p d\vec{u}_p \quad \text{Mean particle velocity}$$

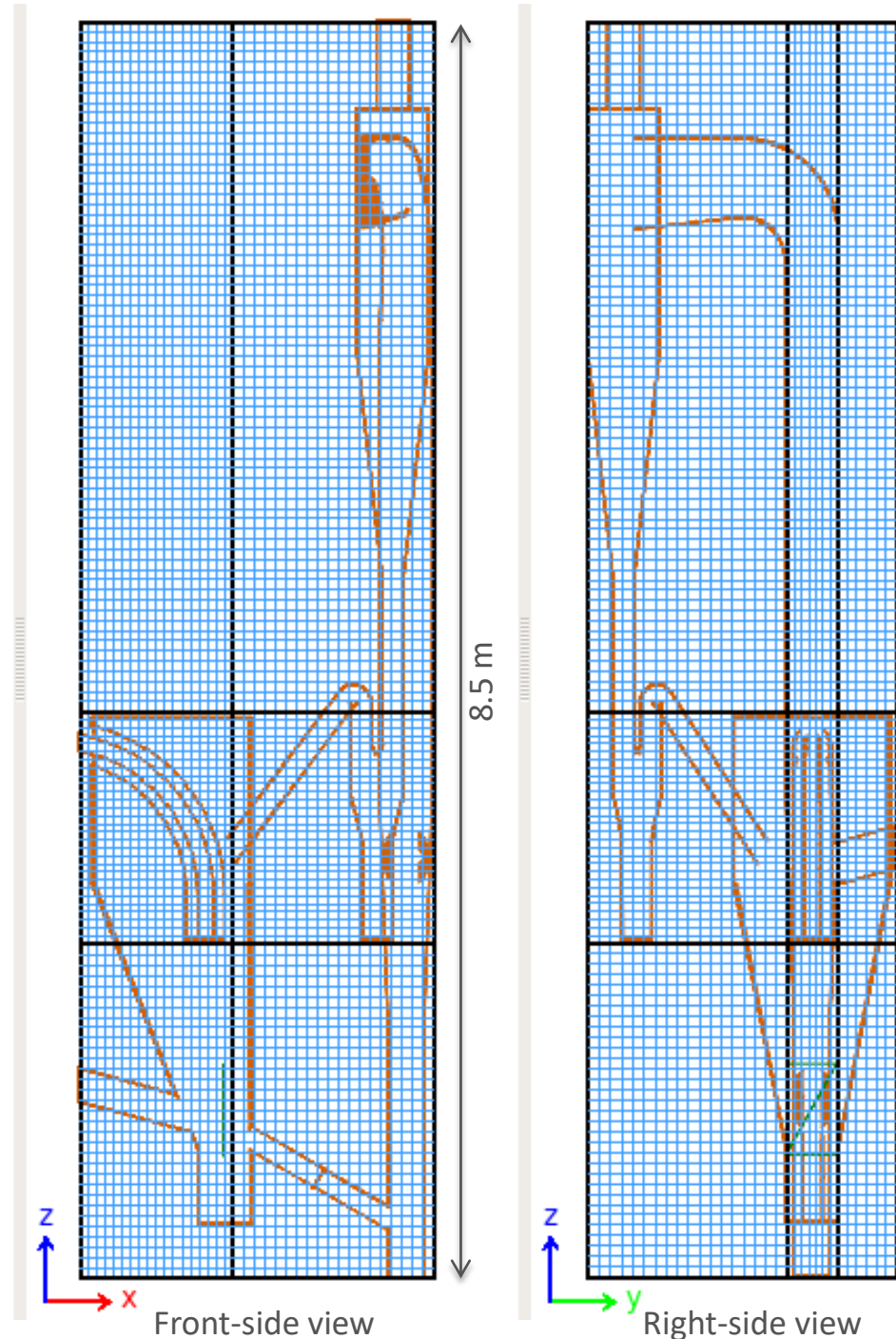
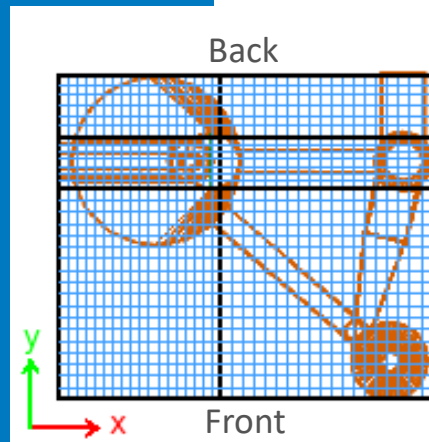
[M.J. Andrews and P.J. O'Rourke, "The multiphase particle-in-cell \(MP-PIC\) method for dense particulate flows," International Journal of Multiphase Flow \(1996\).](#)

[D.M. Snider, "An Incompressible Three-Dimensional Multiphase Particle-in-Cell Model for Dense Particle Flows," Journal of Computational Physics \(2001\).](#)

Grid: Orthogonal with variable cell width.

To resolve small features, the grid can be made finer in certain sections.

To model large particles, the grid has to be larger than the size of the particles.

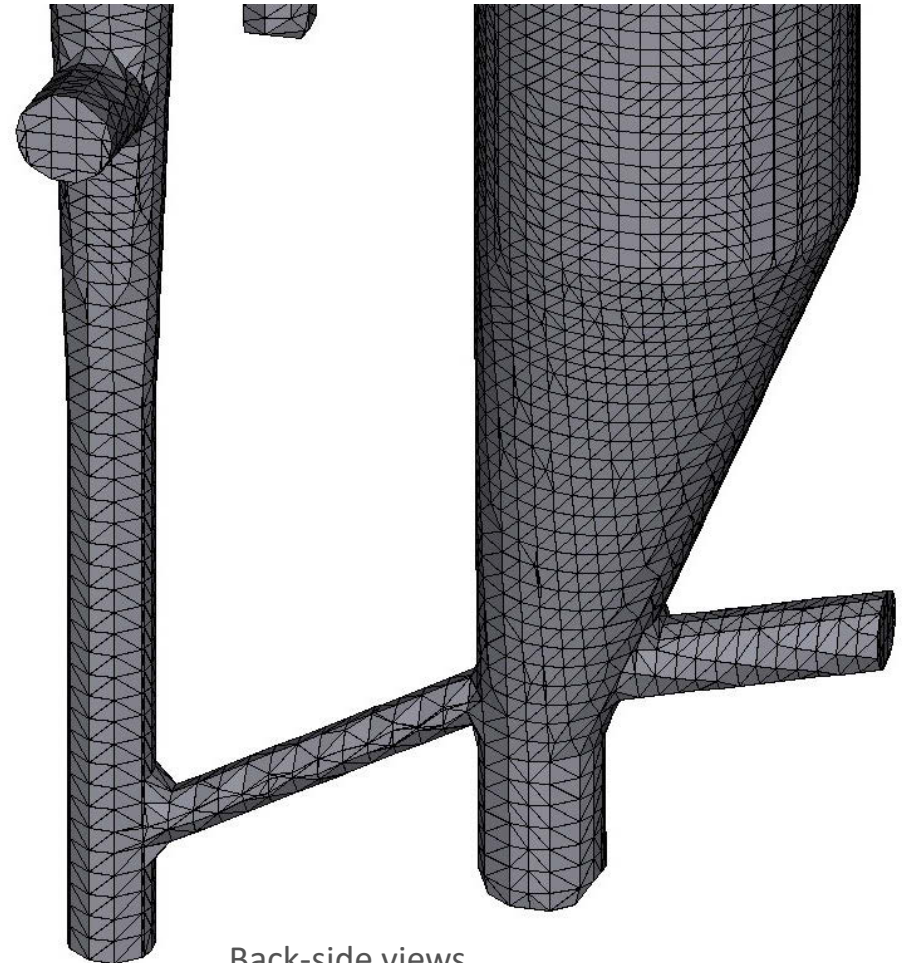
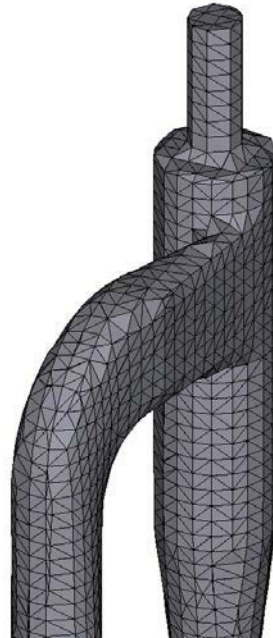


Generated Grid

- Cyclone inlet and pyrolyzer cone are well resolved



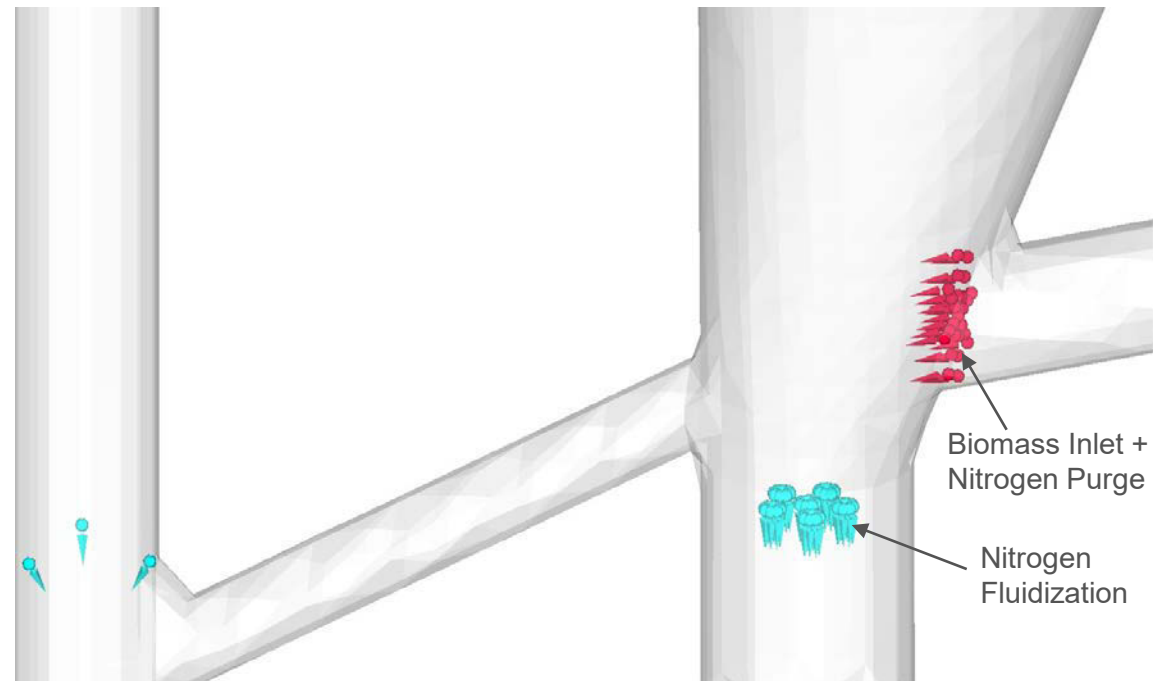
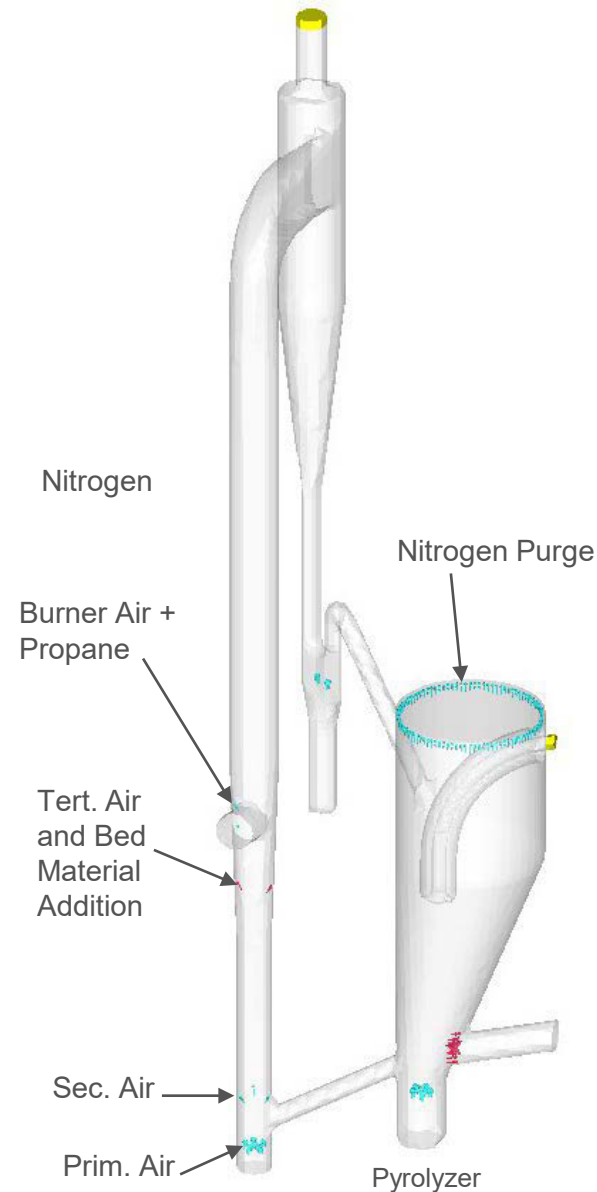
Pyrolyzer



Back-side views

Boundary Conditions

- Pressure boundaries: yellow
 - Injection boundaries for gases: light blue
 - Injection boundaries for solids: dark red
- (Triangles point toward flow direction)



Chemical Reactions Used in Modeling

Heterogeneous reactions	Reaction rate expression
Biomass drying Moisture in Biomass _(s) → H ₂ O _(g) (R1)	$r_1 = 5.13 \times 10^{10} \exp\left(\frac{-10585}{T_p}\right) m_{Biomass}$
Biomass pyrolysis Biomass _(s) → Nonpolar Biooil _(g) + Polar Biooil _(g) + Biochar _(s) + CO, CO ₂ , H ₂ , C ₃ H ₆ , H ₂ O _(g) (R2)	$r_2 = 1 \times 10^4 \exp\left(\frac{-3000}{T_p}\right) m_{Biomass}$
Char combustion Biochar + n ₁ O ₂ → n ₂ CO ₂ + n ₃ H ₂ O (R3)	$r_3 = 1.5 \times T \times \exp\left(\frac{-5000}{T_p}\right) A_{Biochar}[O_2]$
Homogeneous reactions	Reaction rate expression
Biooil cracking Nonpolar Biooil _(g) + 0.6CO ₂ + 5.8H ₂ → 3.3CO + 3.9C ₃ H ₆ (R4)	$r_4 = 0.3 \exp\left(\frac{-1340}{T_g}\right)[Nonpolar\ Biooil]$
CO oxidation CO + 0.5O ₂ → CO ₂ (R5)	$r_5 = 1.28 \times 10^{17} \exp\left(\frac{-34761}{T_g}\right)[CO][O_2]^{0.25}[H_2O]^{0.5}$
H ₂ oxidation H ₂ + 0.5O ₂ → H ₂ O (R6)	$r_6 = 1.0 \times 10^{14} \exp\left(\frac{-5052}{T_g}\right)[H_2][O_2]$
C ₃ H ₈ oxidation C ₃ H ₈ + 5O ₂ → 3CO ₂ + 4H ₂ O (R7)	$r_7 = 8.6 \times 10^{11} \exp\left(\frac{-15000}{T_g}\right)[C_3H_8]^{0.1}[O_2]^{1.65}$
Water gas shift reaction CO + H ₂ O → CO ₂ + H ₂ (R8)	$r_8 = 2.75 \exp\left(\frac{-10079}{T_g}\right) v_{Al_2O_3}[CO][H_2O]$

Reaction rates:

r₁ from J. Xu and L. Qiao, Energy & Fuels 2012 26 (9), 5759-5768, <https://doi.org/10.1021/ef3008745>.

r₂, r₃, r₄ adjusted to match mass balances measured at RTI International using Al₂O₃ bed material¹.

r₅ and r₆ from H. Liu et al., International Journal of Hydrogen Energy, Volume 41, Issue 28, 2016,

<https://doi.org/10.1016/j.ijhydene.2016.04.205>.

r₇ from C. Westbrook and F. Dryer, Combustion Science and Technology, 27:1-2, 31-43, 1981,

<https://doi.org/10.1080/00102208108946970>.

r₈ adjusted from X. Lu and T. Wang, Fuel, Volume 108, 2013,

<https://doi.org/10.1016/j.fuel.2013.02.023>.

T_p...particle temperature

T_G...gas temperature

m_{Biomass}...mass of biomass

A_{Biochar}...surface area of biomass

v_{Al2O3}...volume fraction of bed material

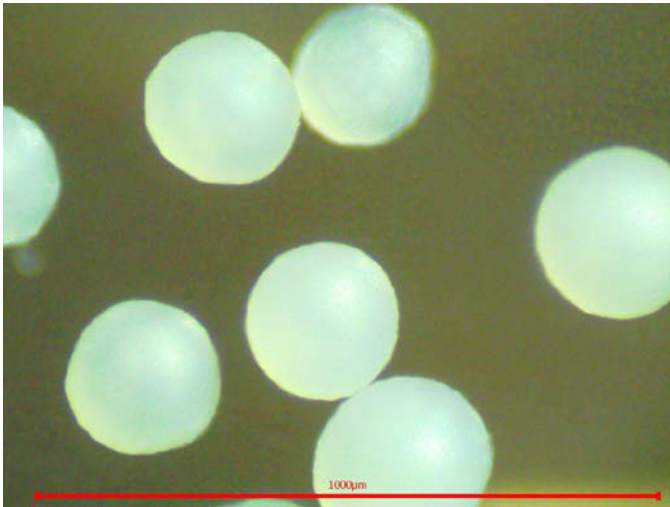
R1-R3 defined on a mass basis per kg of reactant consumed, using mass balance from experiment at RTI International¹.

In the model, particles shrink as solids are converted to gases.

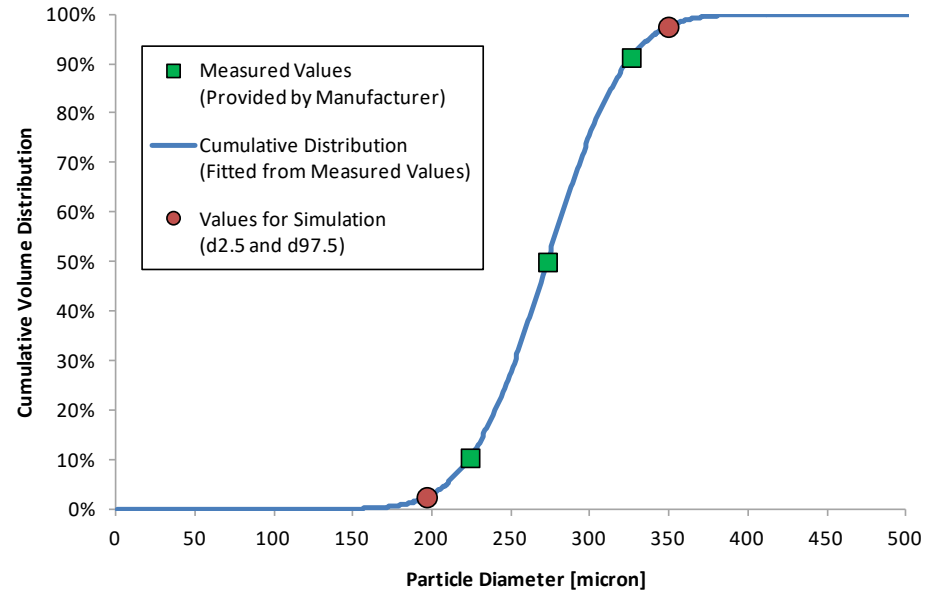
¹O. Mante et al., "Pilot-scale catalytic fast pyrolysis of loblolly pine over γ-Al₂O₃ catalyst," Fuel (2018).

Bed Material

Microscope Images of Sasol Puralox
300/130 (10x Magnification)



Particle Size Distribution



Properties

Particle Density: 1680 kg/m³

Bulk Density: 941 kg/m³

Close-pack Particle Volume Fraction: 0.56

Total weight: 241 kg

Total particle volume: 0.143 m³

Total bulk volume: 0.256 m³

D₁₀: 224 micron (10% of volume smaller than D₁₀)

D₅₀: 273 micron

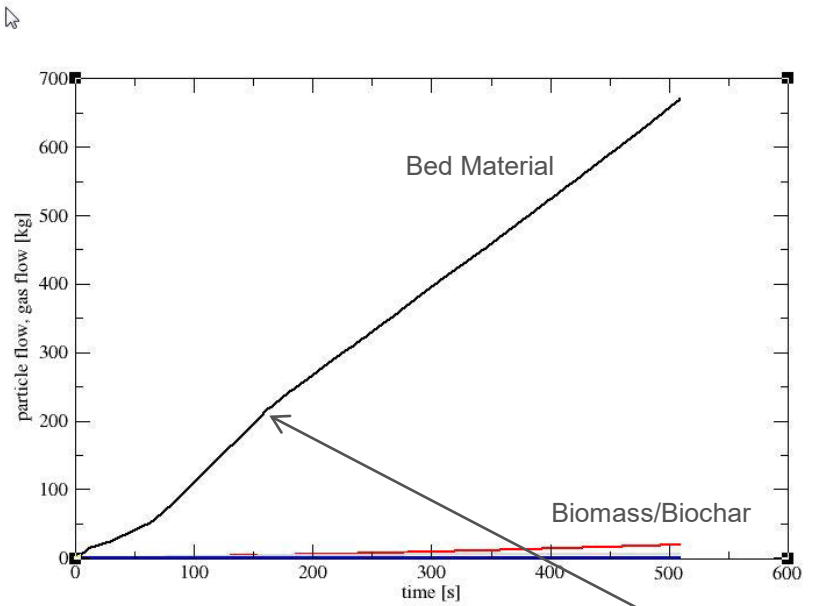
D₉₀: 326 micron

Total number of particles: 1.54e10

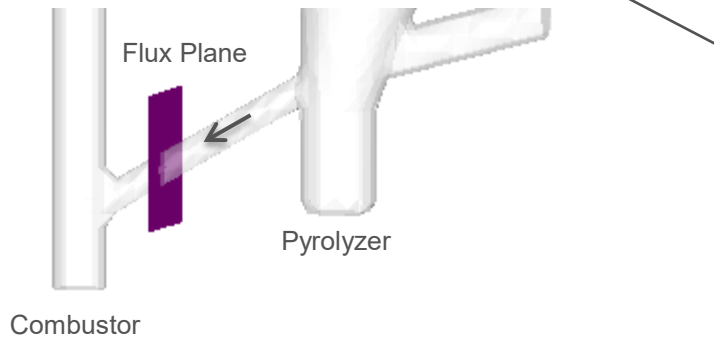
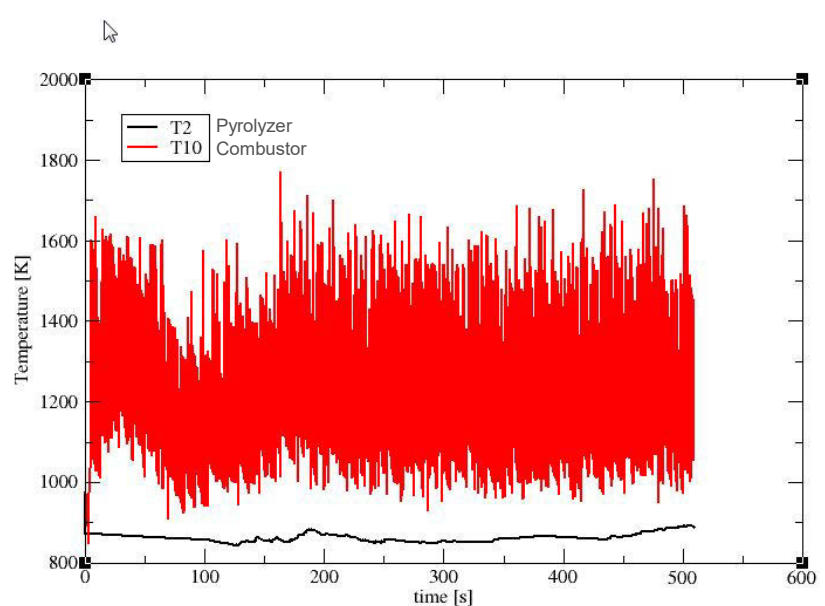
Number of computational particles: 4.63e5

Circulation Rate, Temperatures for CFP in Bubbling Bed

Cumulative Mass Flow across Bottom Chute



Temperatures in Pyrolyzer and Combustor



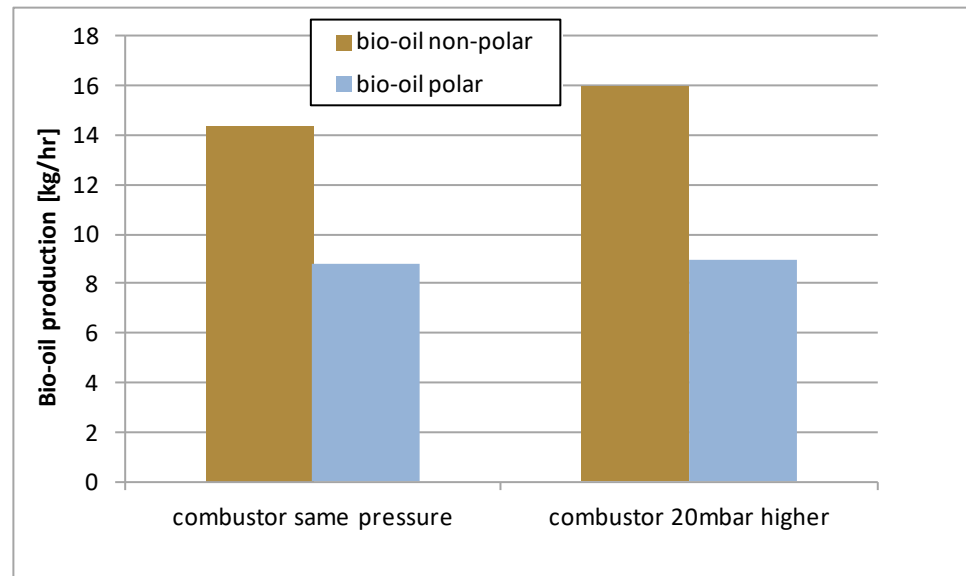
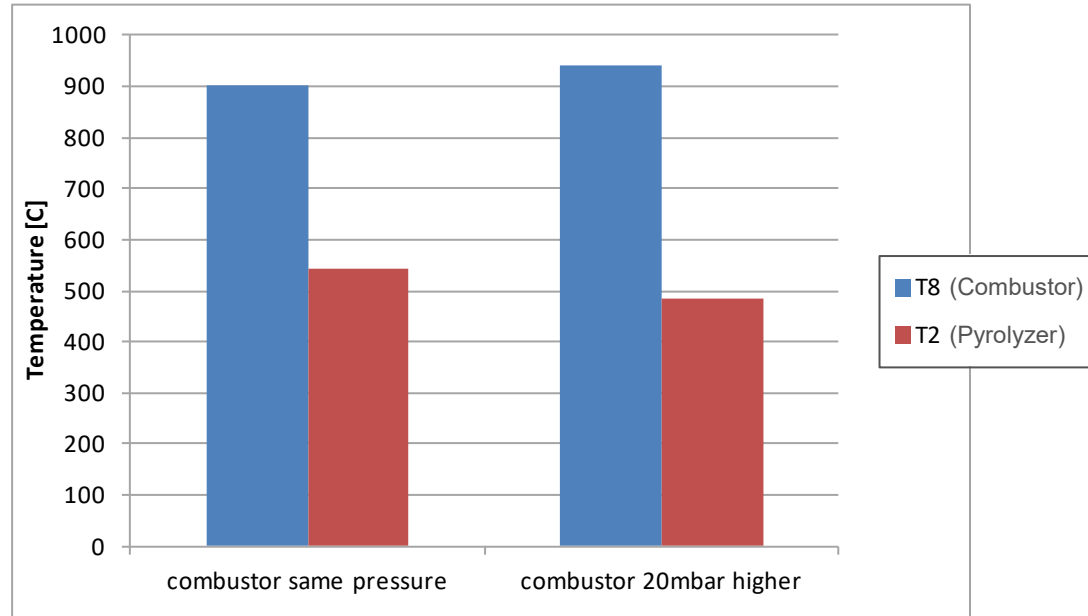
At 160s, the pyrolyzer pressure was decreased by 10 mbar in order to slow down the circulation rate.

Higher Combustor Pressure

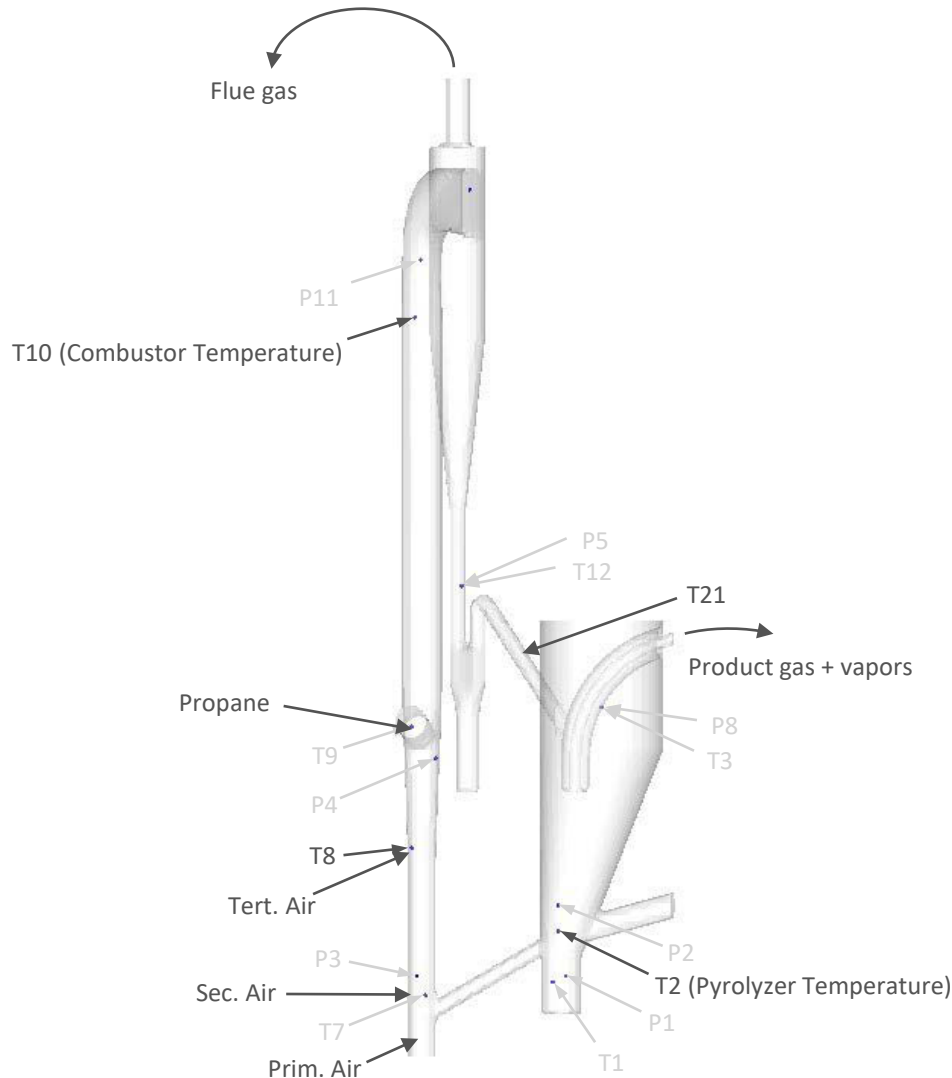
Simulation shows some success with higher combustor pressure.

- First case:
Pressure gasifier and combustor 1atm
- Second case:
Pressure gasifier: 1atm
Pressure combustor: 1atm+20mbar

Slightly higher bio-oil production with higher combustor pressure.



Measurement Locations and Process Control



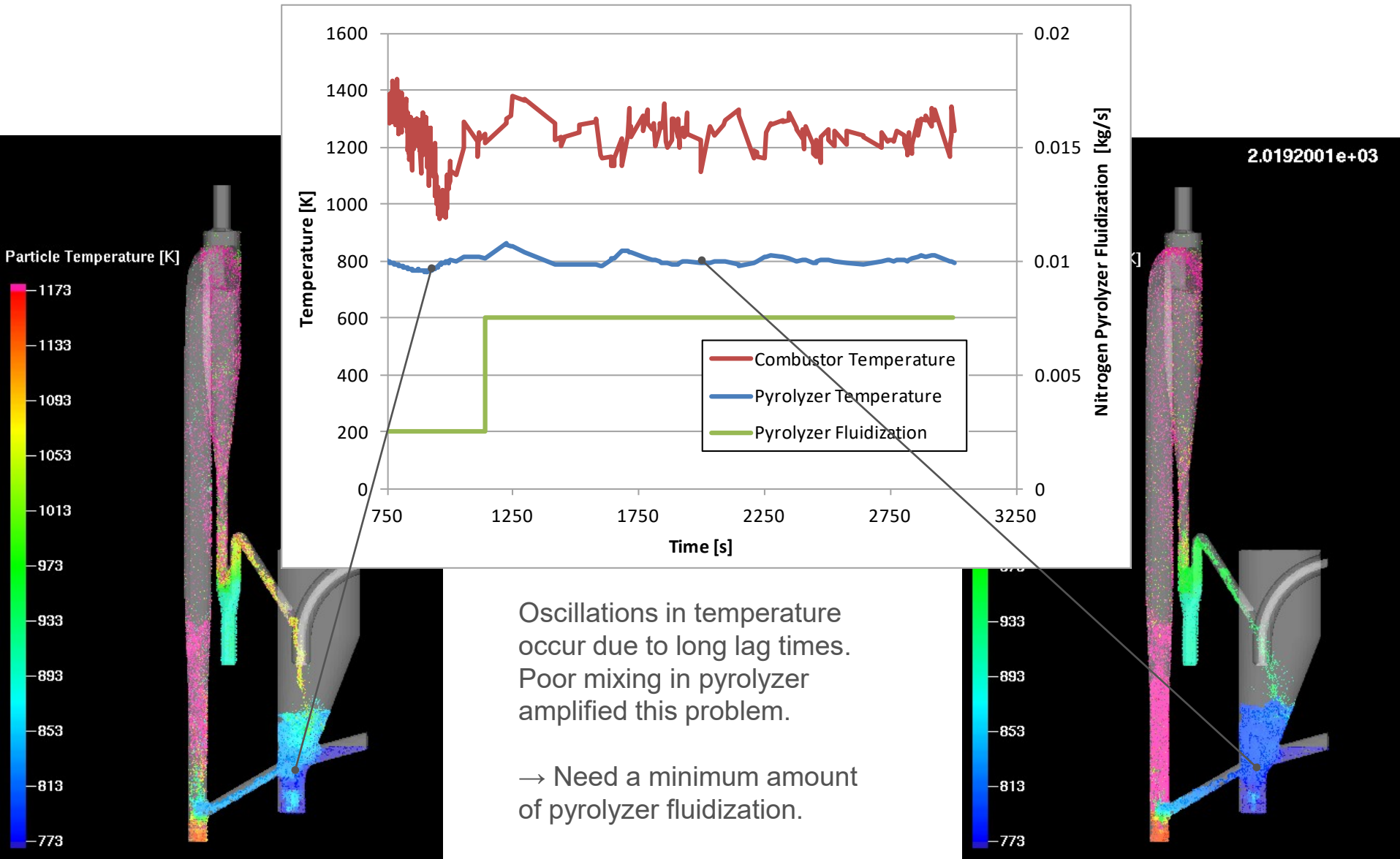
Control of Flow Rates during Simulation

- Standard File Format files (.sff) contain flow rates and wall temperatures as a function of time and can be manipulated by external software.
- Values for next time step can be calculated based on computed values from previous time steps (e.g. using a PID controller)

PID Controllers

- Combustor temperature controlled by propane addition
- Pyrolyzer temperature controlled by circulation rate (via primary and secondary air)
- Flue gas oxygen controlled by tertiary air
- Heat losses controlled by wall temperatures of six zones

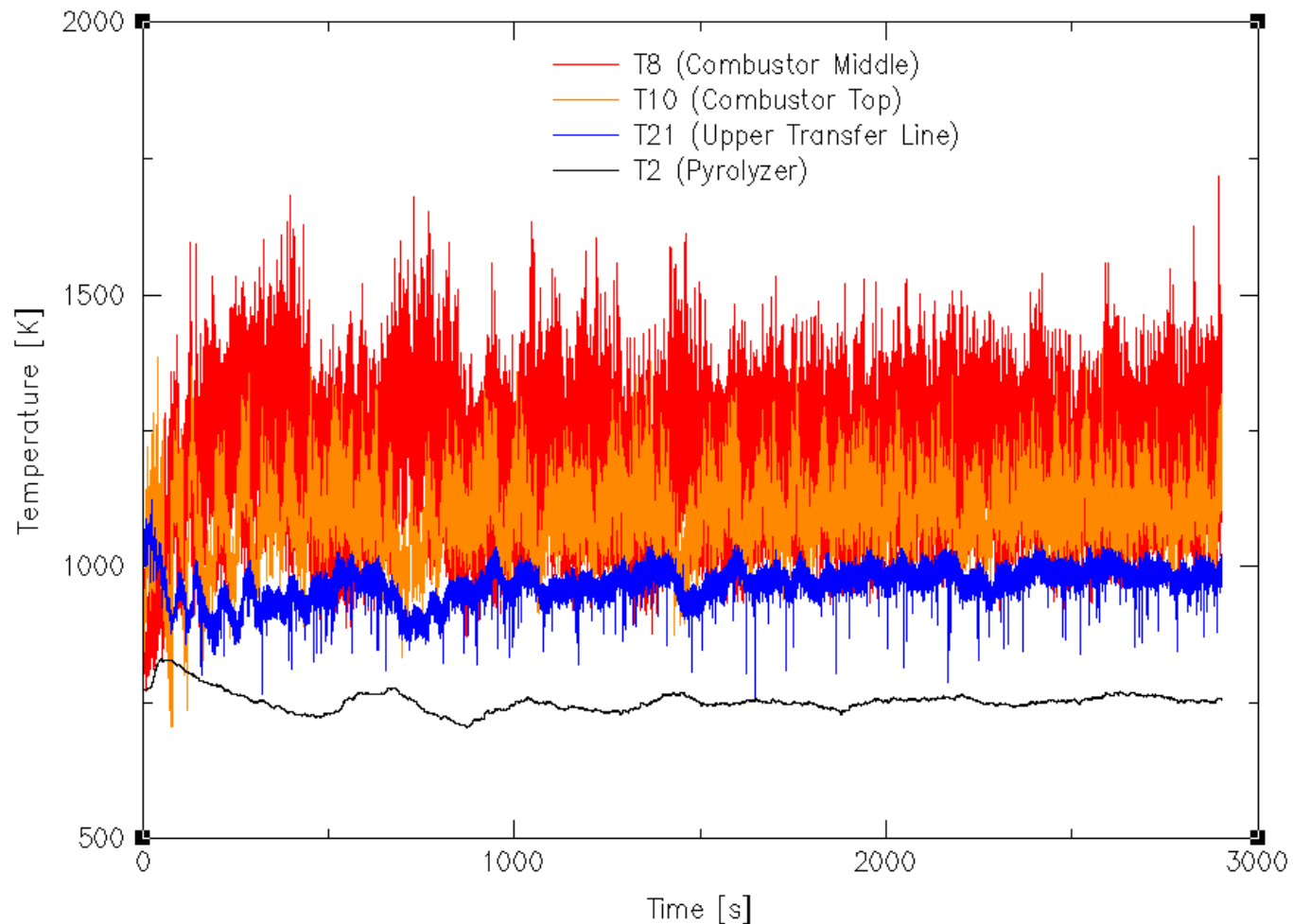
Pyrolyzer Fluidization



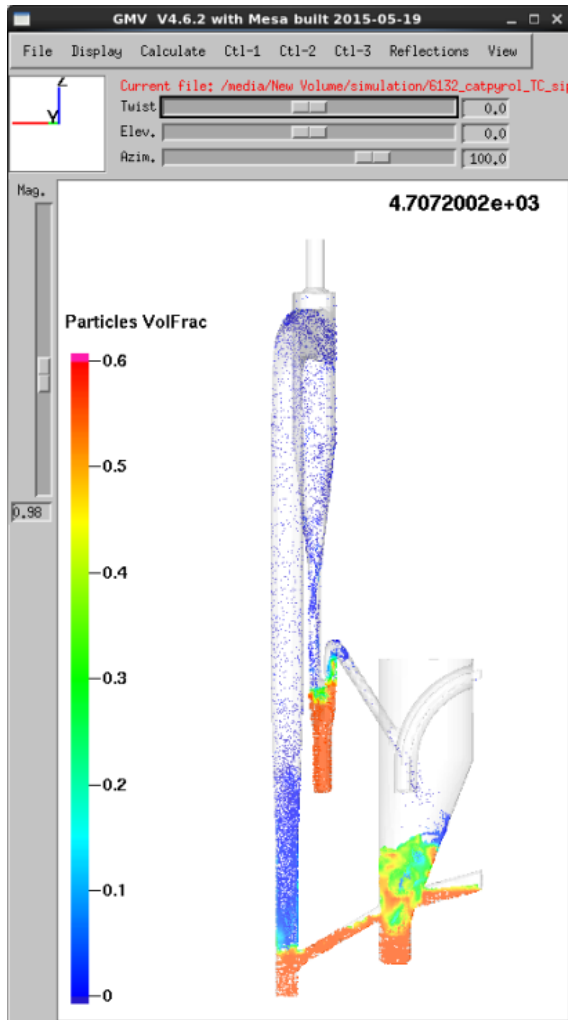
Control of Pyrolyzer Temperature

Cascade PID Control

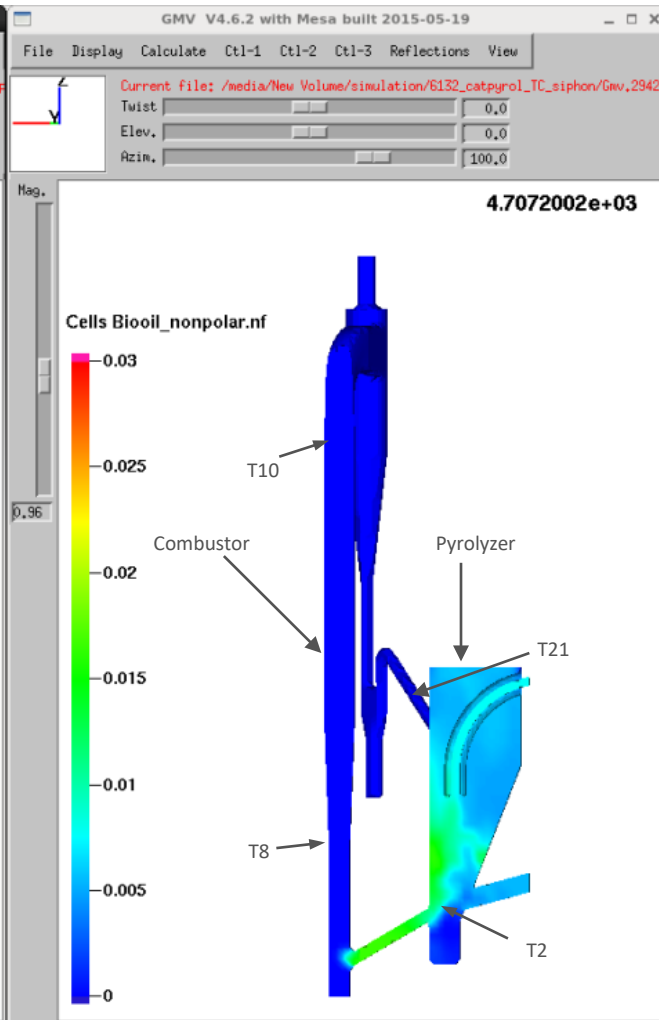
Outer control loop: Circulation rate (estimated from T_{10} - T_{21}) is controlled by pyrolyzer temperature (T_2).
Inner control loop: Secondary air and primary air are controlled by circulation rate.



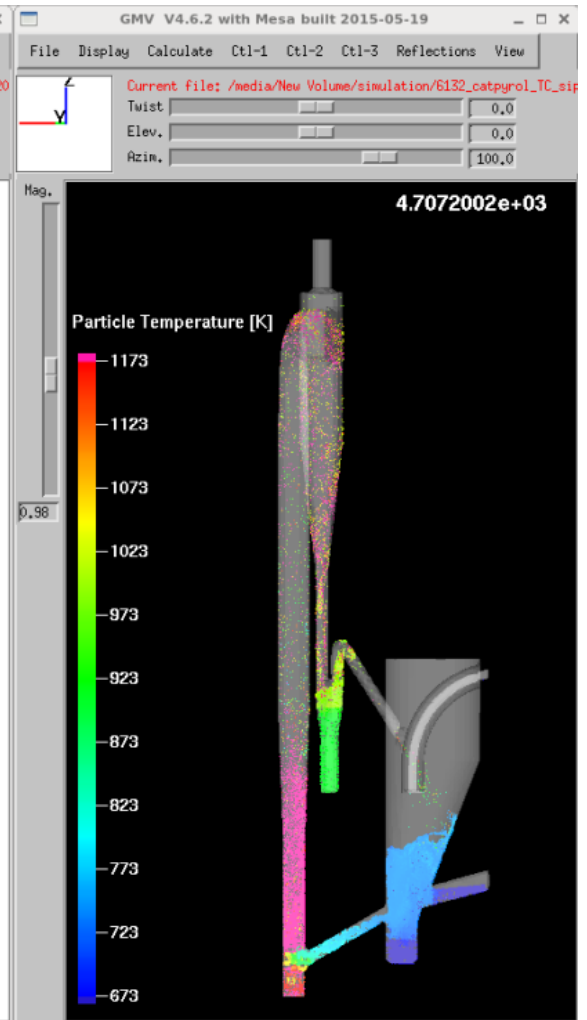
Main Results



Particle Volume Fraction

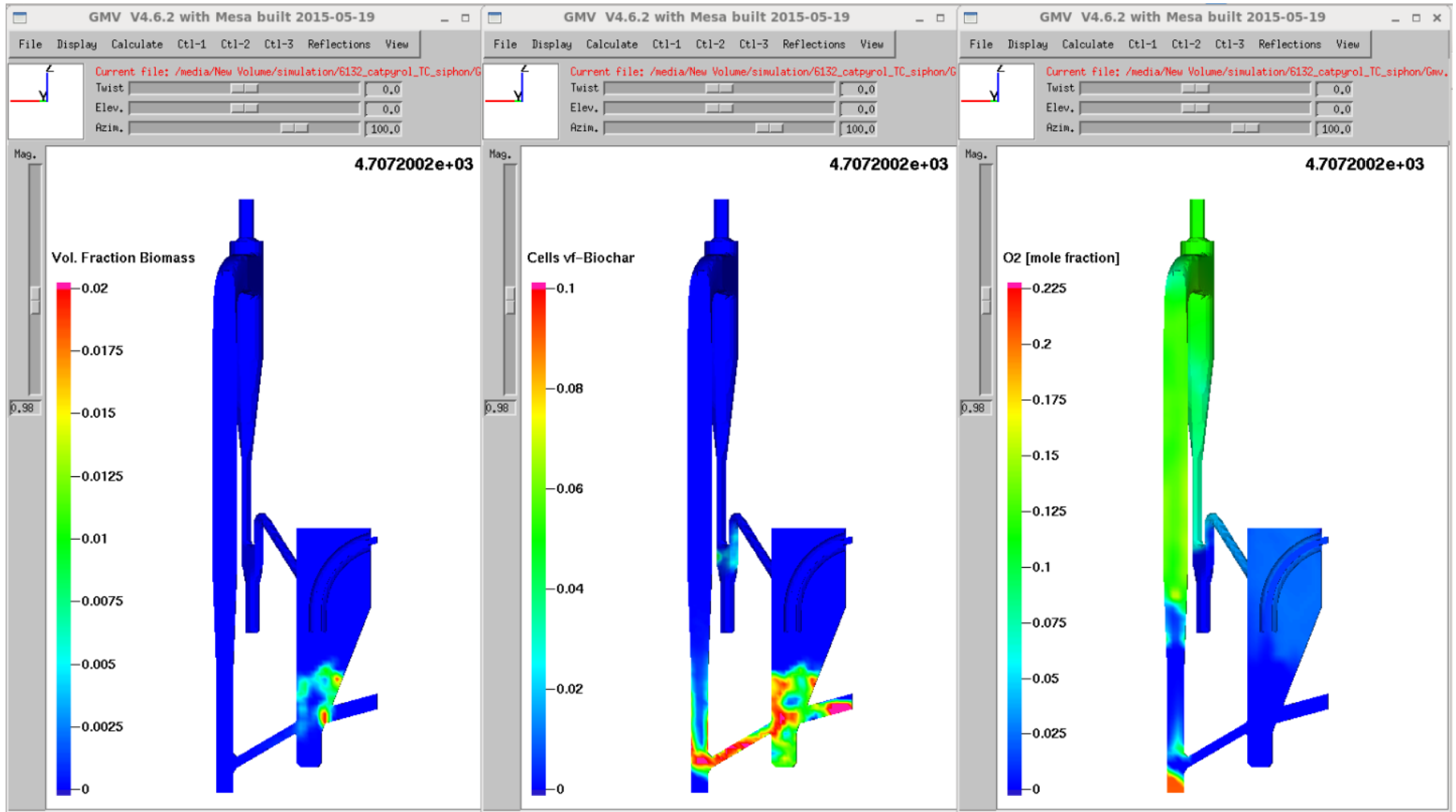


Mole fraction bio-oil



Particle Temperature [K]

Additional Results



Biomass Volume Fraction

Biochar Volume Fraction

O₂ Mole Fraction

Conclusions

- Several hardware changes are necessary to convert a pilot plant from gasification to pyrolysis.
- CFD modeling identified important parameters such as flow rates, residence times, and bed-material properties.
- Control of temperature and circulation rate is challenging in the simulation due to lack of refractory mass.
- Circulation rate is slightly higher in model than in pilot plant.
- Potential pitfalls were identified (insufficient mixing, loss of biomass to combustor).

Thank You

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