Modeling heat transfer and reaction kinetics of biomass in pyrolysis feeding systems

Joseph Samaniuk
Jonathan Stickel
Tim Dunning
Daniel Carpenter
Jessie Troxler

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Acknowledgements

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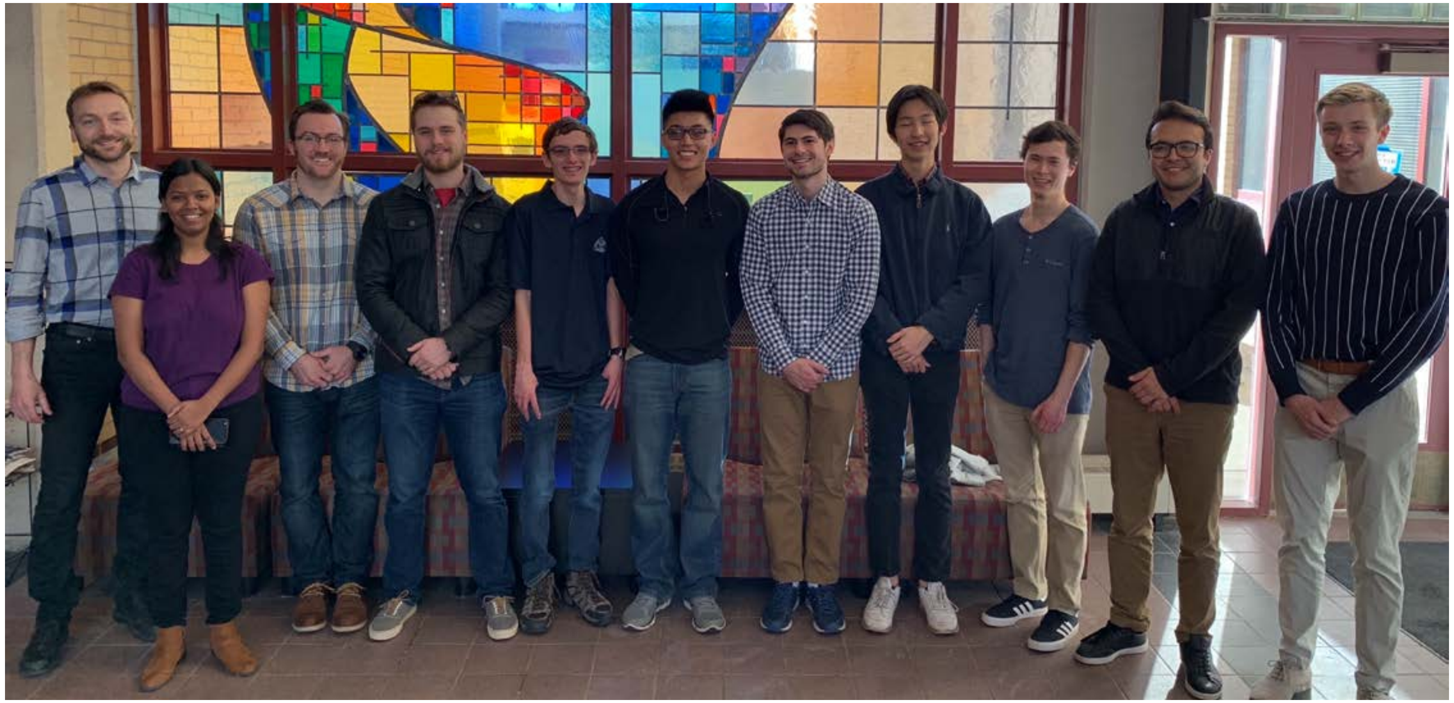
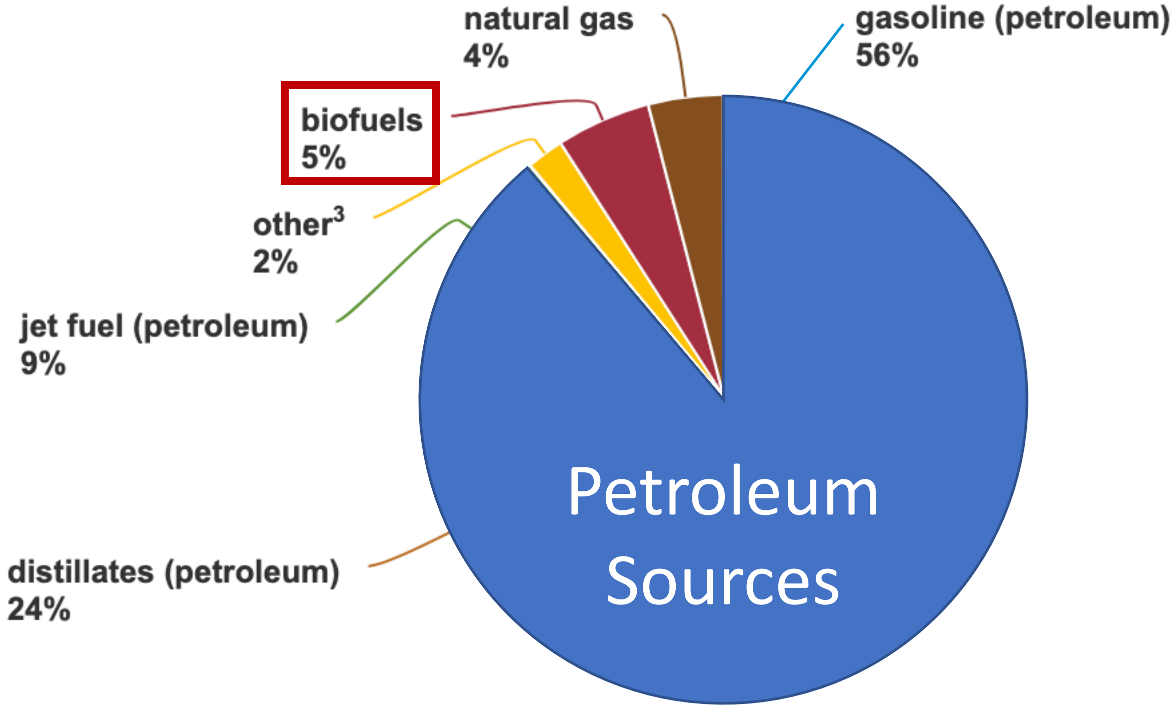
APUP



Motivation: Energy & Transportation

- Transportation accounted for 26% of energy use in the US
- Biofuels are a renewable, carbon neutral source of combustible fuel



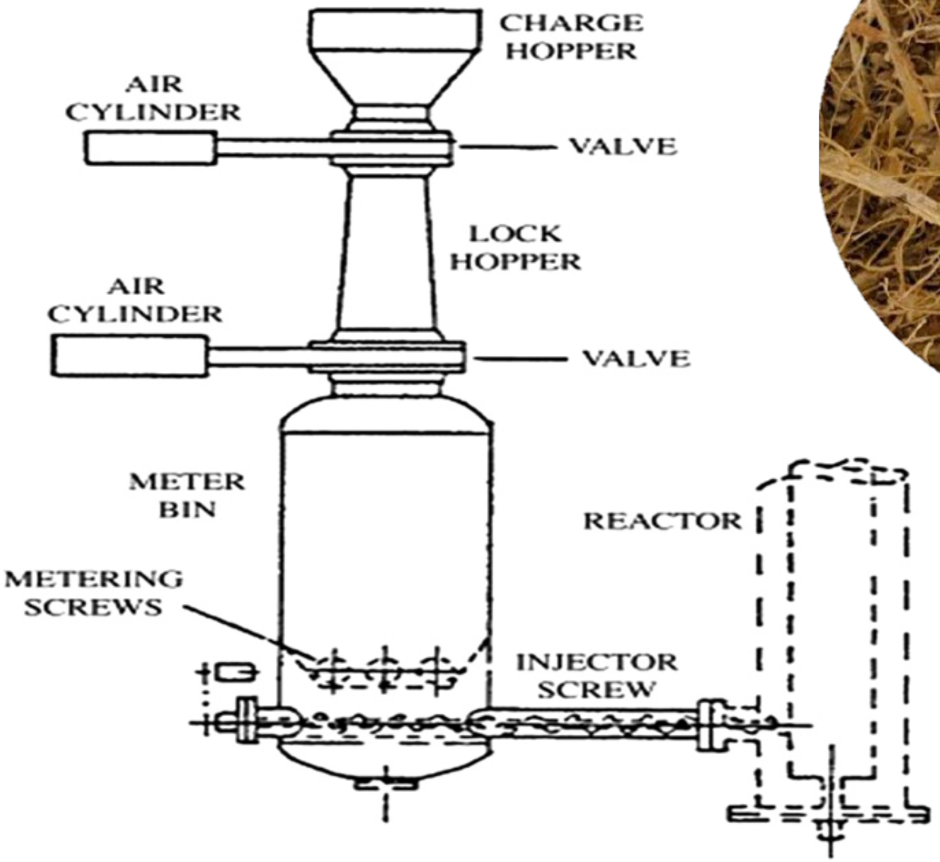
U.S. Energy Information Administration, 2021

Processing Challenges

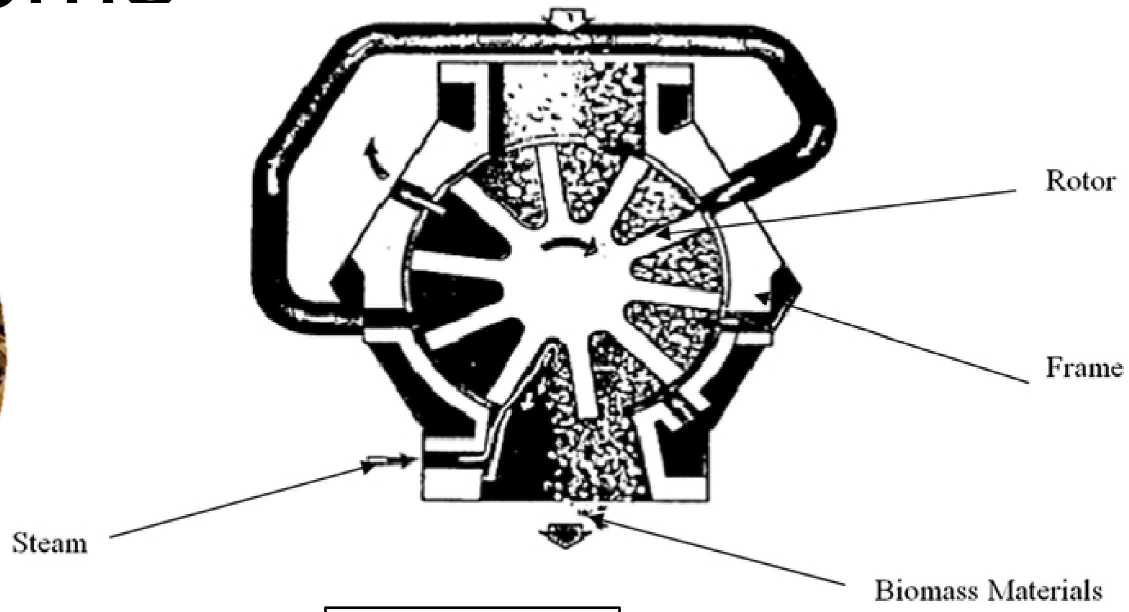
- Bio-oil immiscible with current transportation fuels
- Low output of fuel products
- Difficulty handling biomass
- Blockages in biomass feeders

Biomass Feeding Systems

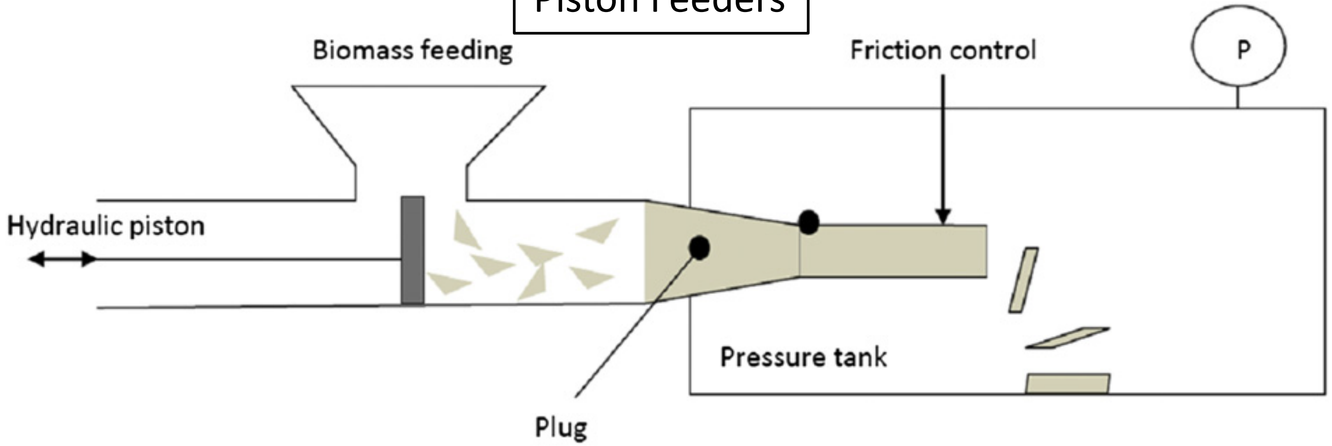
Hopper & Lock Hopper Feeders



Rotary Valve Feeders



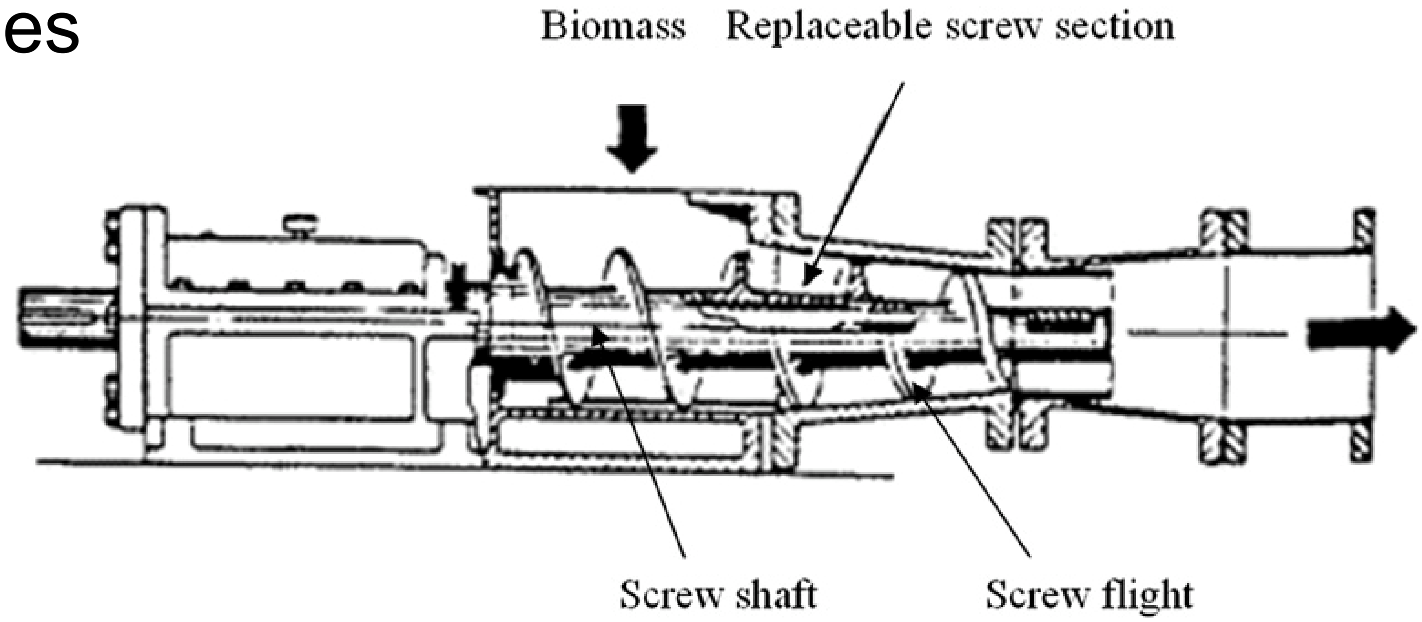
Piston Feeders



Dai, et al. Progress in Energy and Combustion Science, 38: 716-736 (2012)
Xia, et al. ACS Sustainable Chemistry & Engineering, 8: 6142-6156 (2020)

Auger Feeders

- Most common in industry
- Used with other feeder types
- Wide range of feed rates

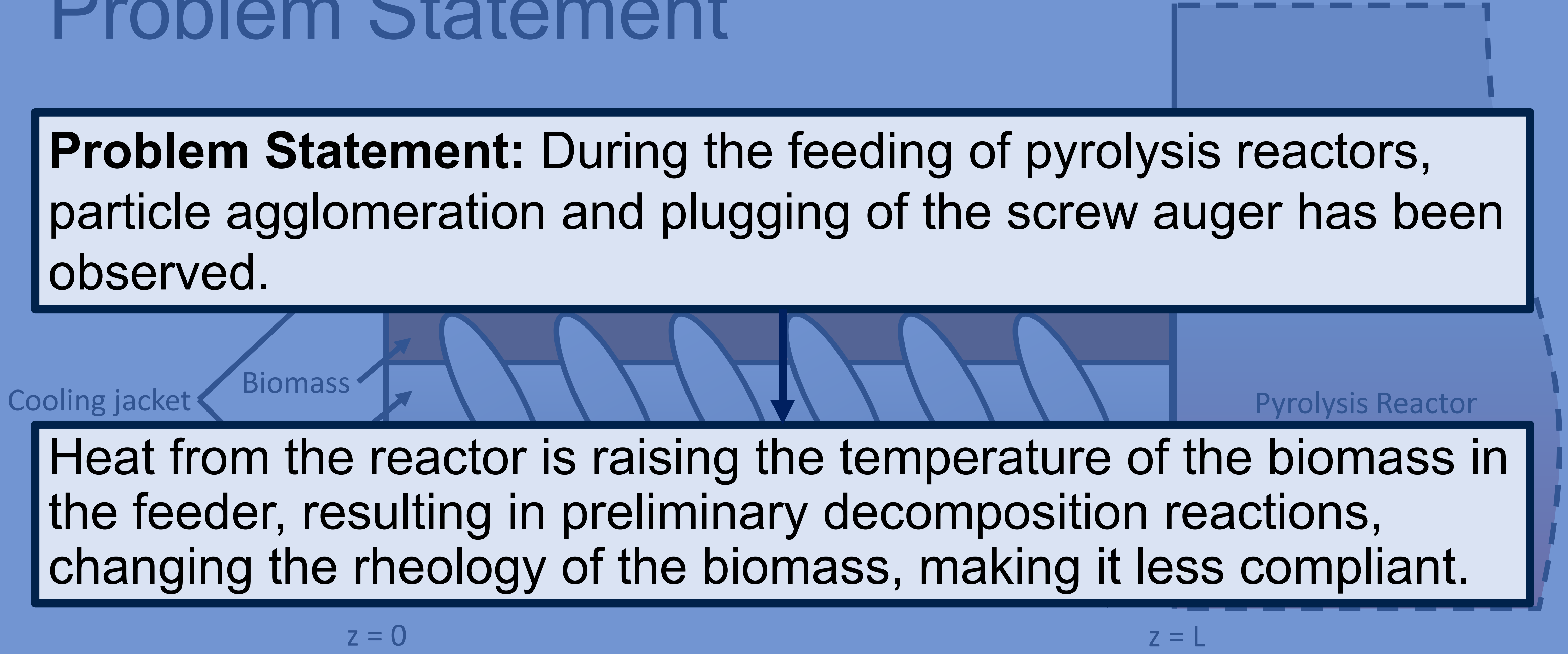


Dai, et al. Progress in Energy and Combustion Science, 38: 716-736 (2012)

Problem Statement

Problem Statement: During the feeding of pyrolysis reactors, particle agglomeration and plugging of the screw auger has been observed.

Heat from the reactor is raising the temperature of the biomass in the feeder, resulting in preliminary decomposition reactions, changing the rheology of the biomass, making it less compliant.



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Modeling Methods

Heat Transfer

- Runge-Kutta
- Bulk scale

$$\frac{\partial \rho C_p T}{\partial t} = -\nabla \cdot (\rho C_p T v) - (\nabla \cdot q) + (-\Delta H)\left(\frac{\partial \rho}{\partial t}\right)$$

Kinetics

- Multiscale problem
- Debiagi, et al. 2018
  - Speciated
  - Multistage

Primary decomposition | Secondary cracking | Re-polymerization

Perkins, et al. Renewable and Sustainable Energy Review, 90: 292-325 (2018)

1D Heat Transfer Equations

System of equations

Screw rod:

$$0 = \alpha_r \frac{d^2T_r}{dz^2} + \gamma_{rb}\tilde{A}_r(T_b - T_r)$$

Biomass:

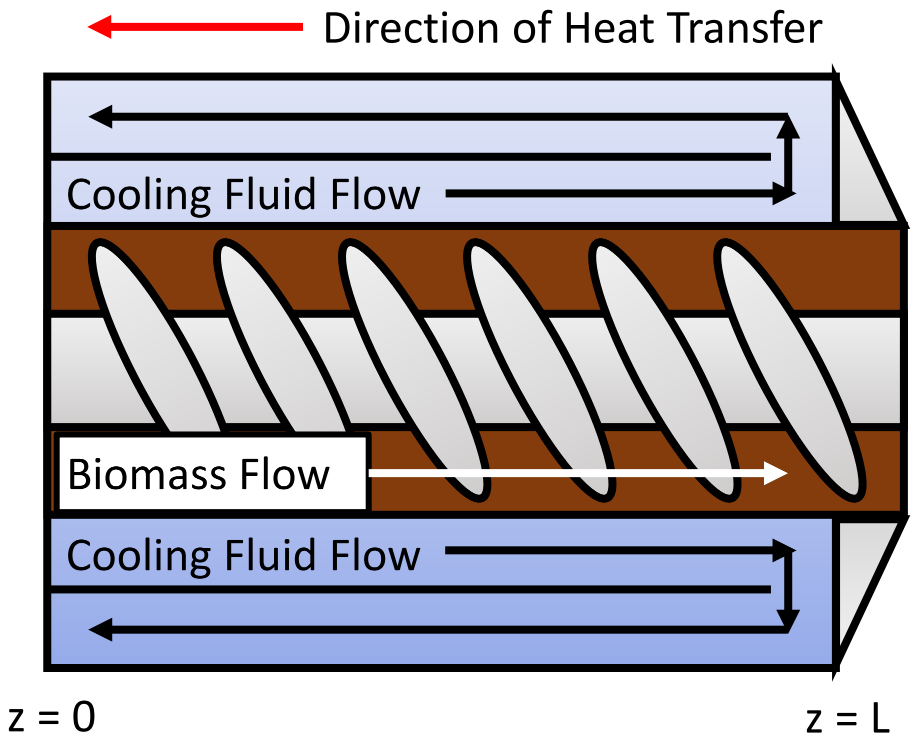
$$0 = \alpha_b \frac{d^2T_b}{dz^2} + v_b \frac{dT_b}{dz} + \gamma_{br}\tilde{A}_{br}(T_r - T_b) + \gamma_{bc}\tilde{A}_b(T_c - T_b)$$

Inner cooling loop:

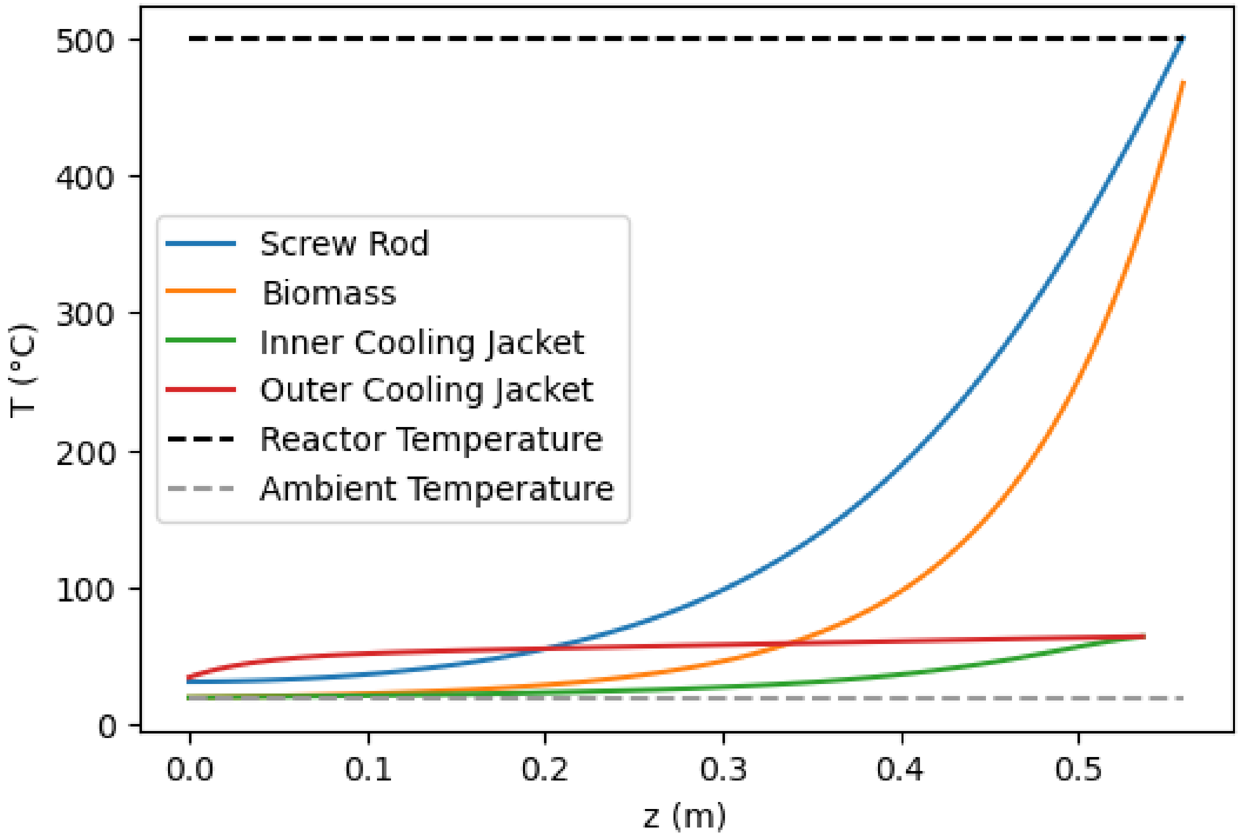
$$0 = \alpha_c \frac{d^2T_c}{dz^2} + v_c \frac{dT_c}{dz} + \gamma_{cb}\tilde{A}_{cb}(T_b - T_c) + \gamma_{cd}\tilde{A}_c(T_d - T_c)$$

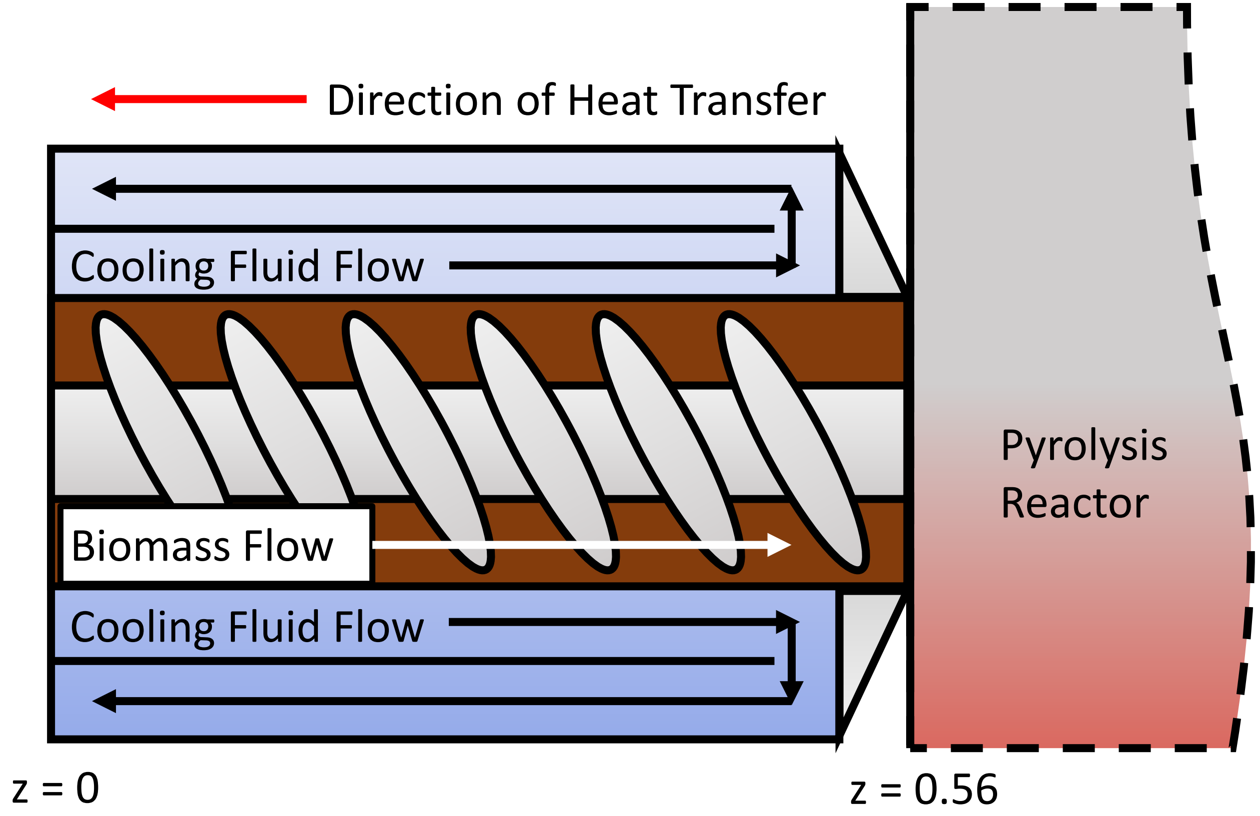
Outer cooling loop:

$$0 = \alpha_d \frac{d^2T_d}{dz^2} + v_d \frac{dT_d}{dz} + \gamma_d\tilde{A}_{dc}(T_c - T_d) + \gamma_{da}\tilde{A}_d(T_0 - T_d)$$

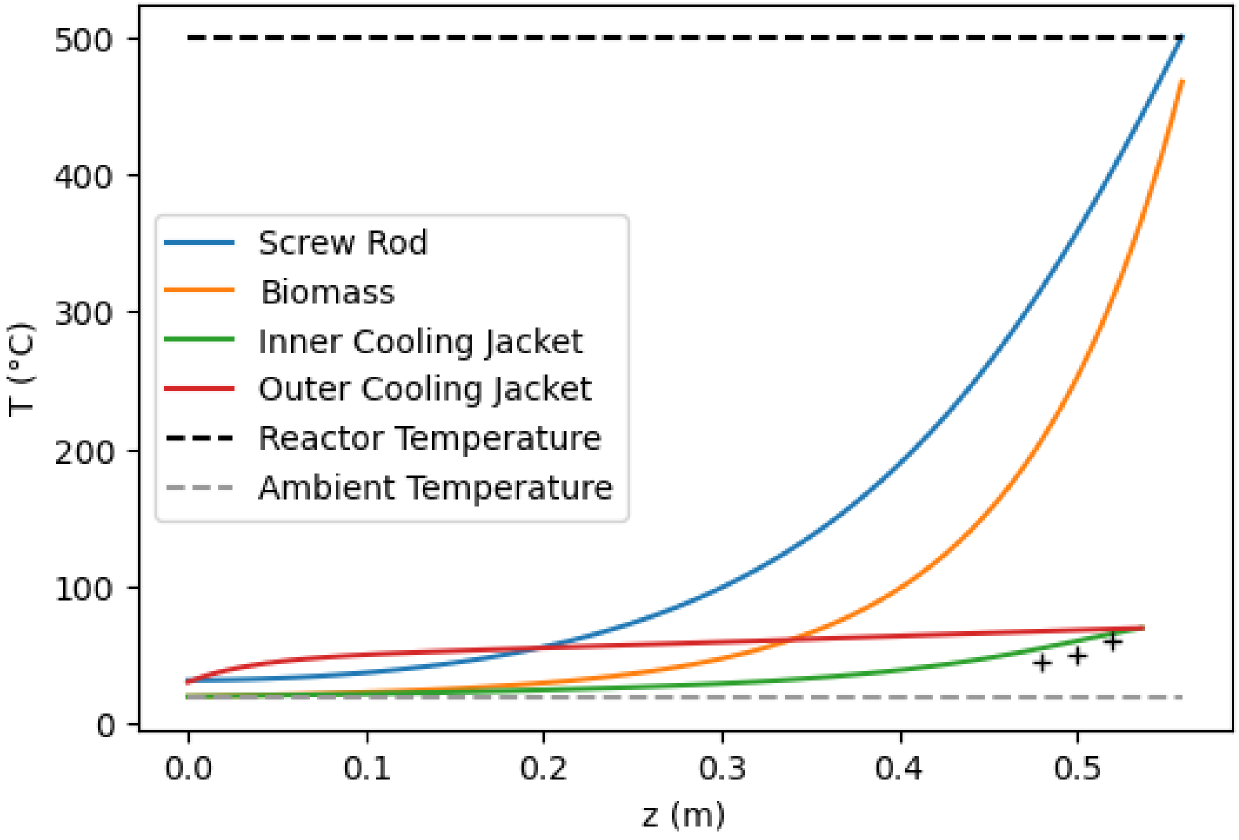


1D Temperature Profiles

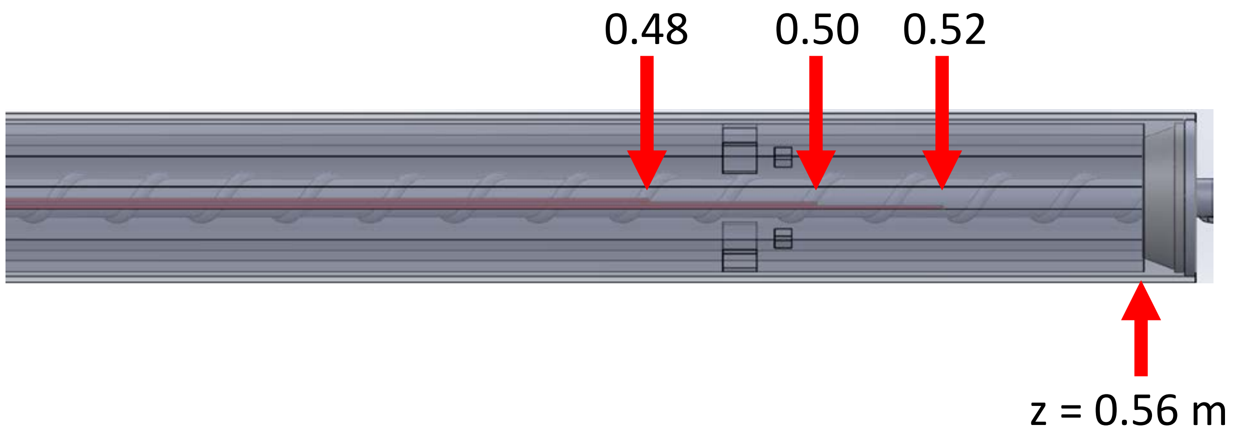




Comparison with Experimental



Position (m)	Temperature (°C)
0.48	~ 40-45
0.50	~ 45-50
0.52	~ 60



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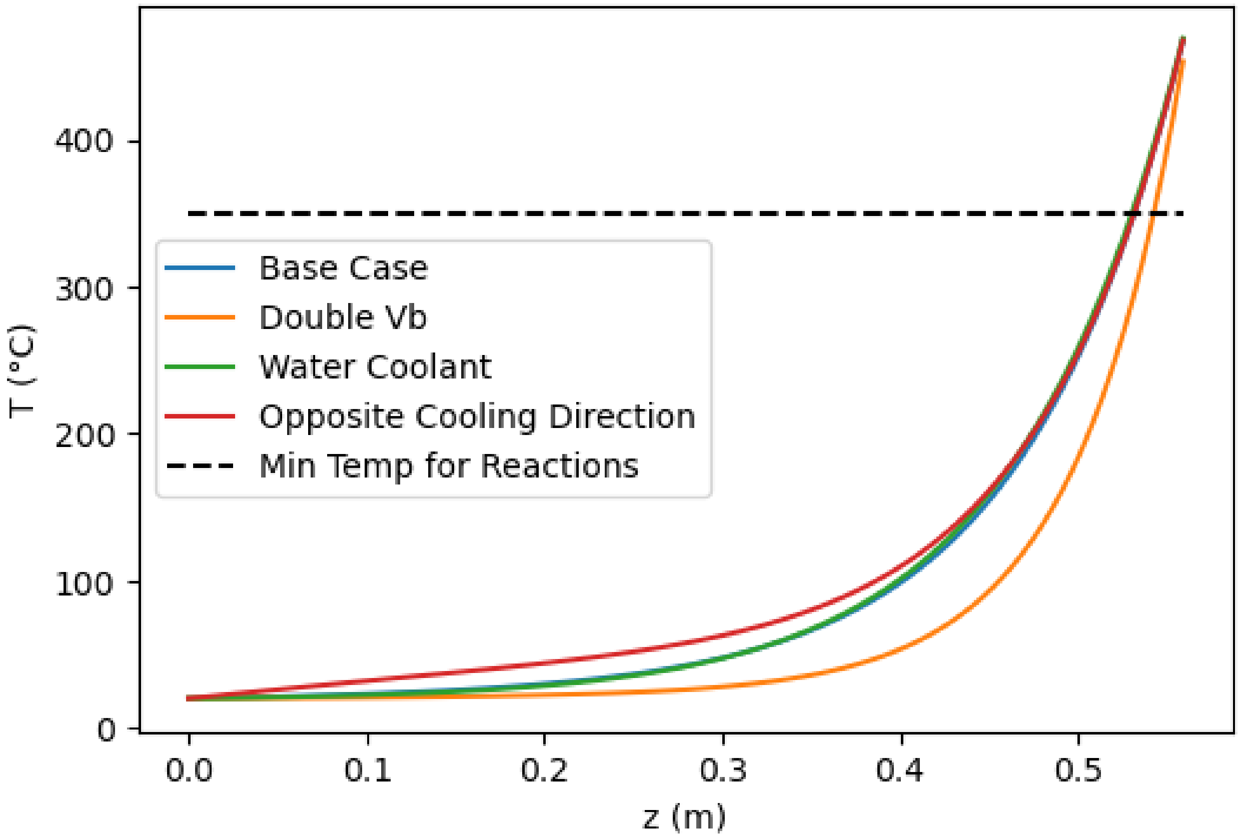
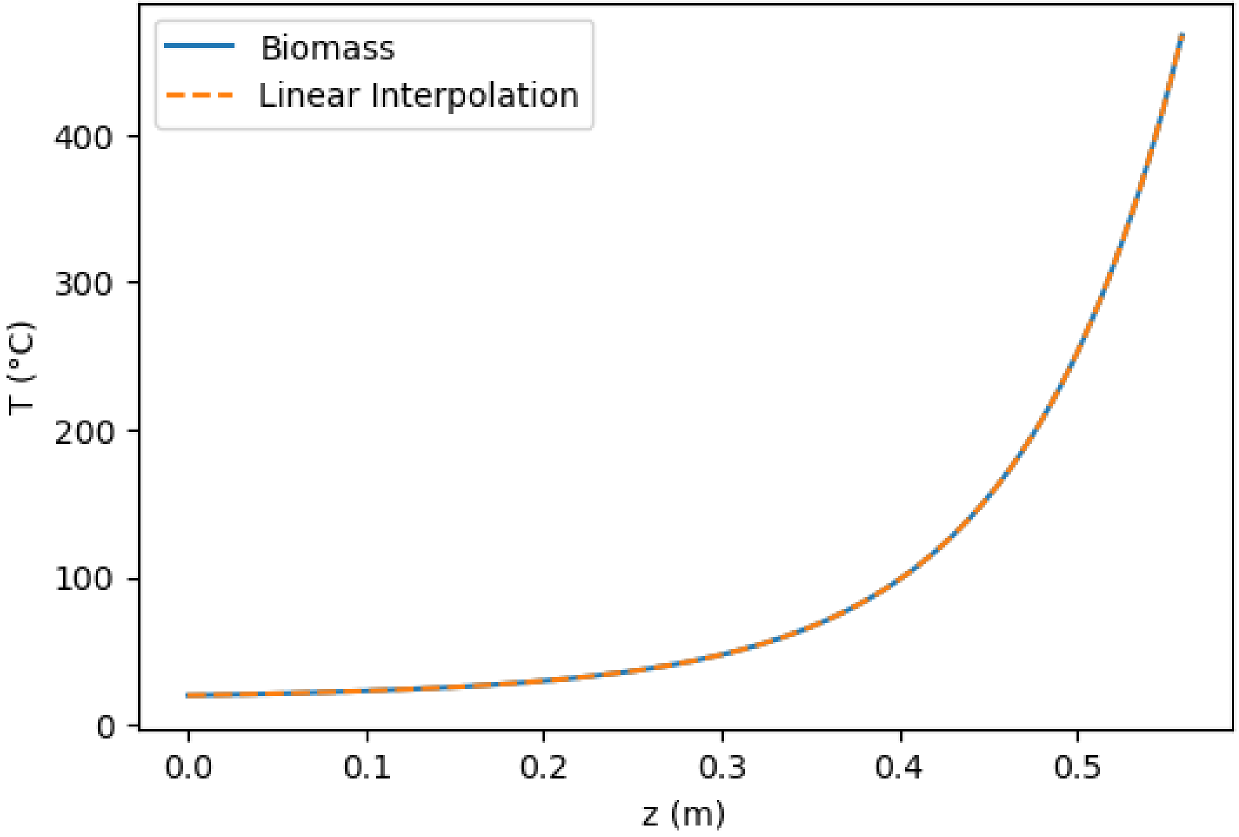
Changing Operating Parameters



- **Base Case**—normal operating parameters
- **Double Vb**—doubled biomass velocity
- **Water coolant**—water instead of air in the cooling loop
- **Opposite cooling direction**—switching the entrance from the inner to the outer layer

Biomass Temperatures and Kinetics

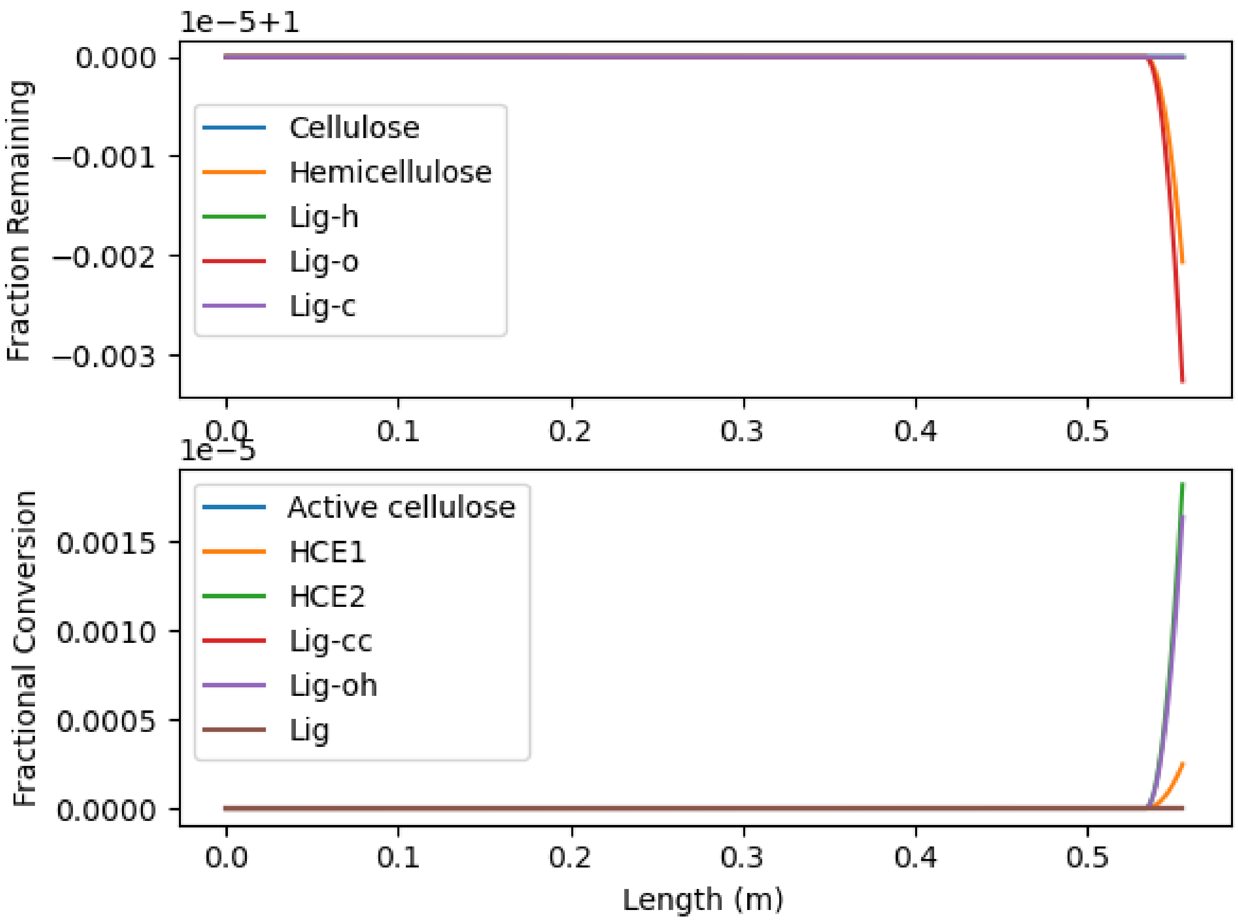


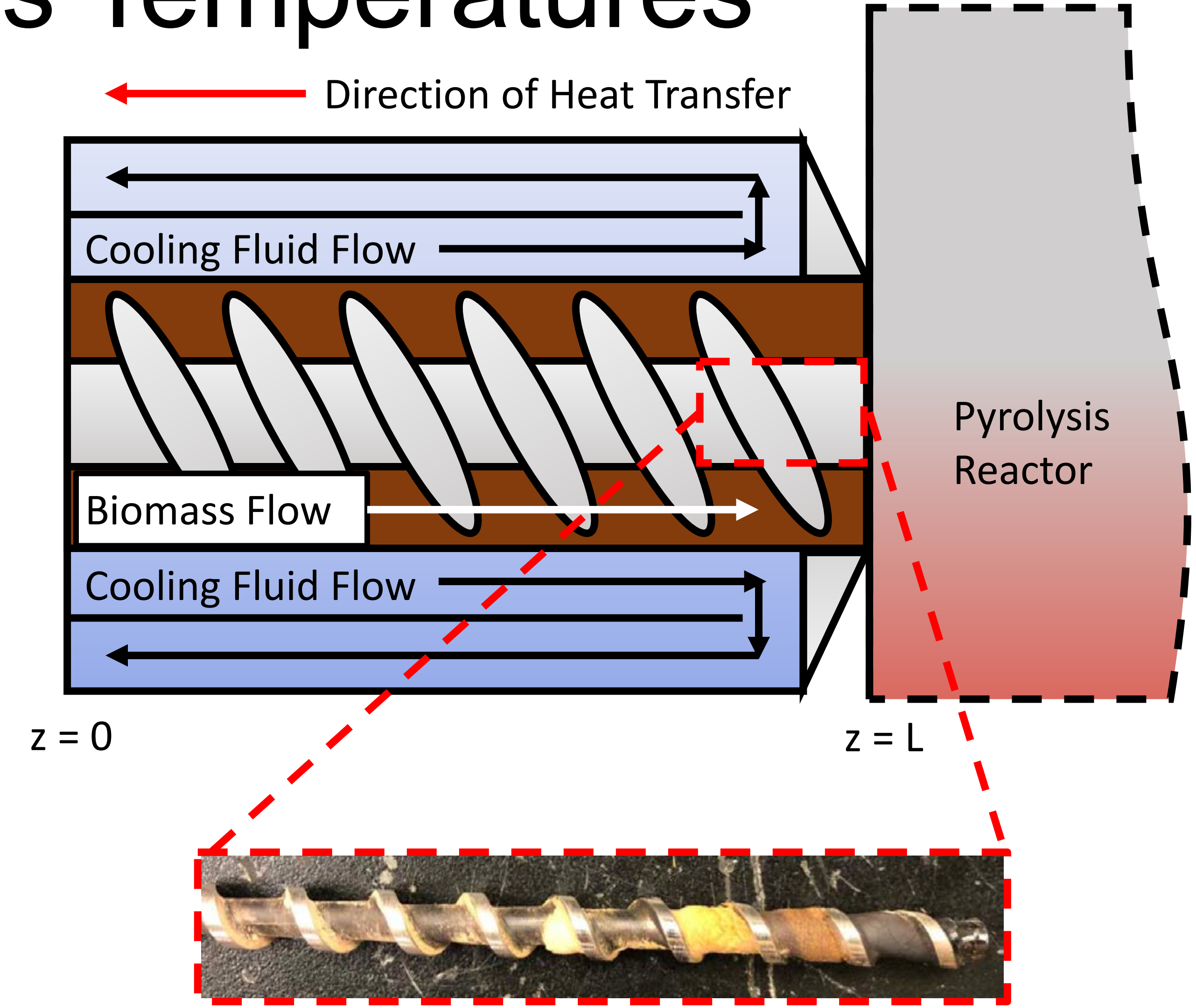
Temperature profile model, T = f(z)

Rate constant, k = f(T)

Rate constant, k = f(T(z))

Kinetics with Biomass Temperatures





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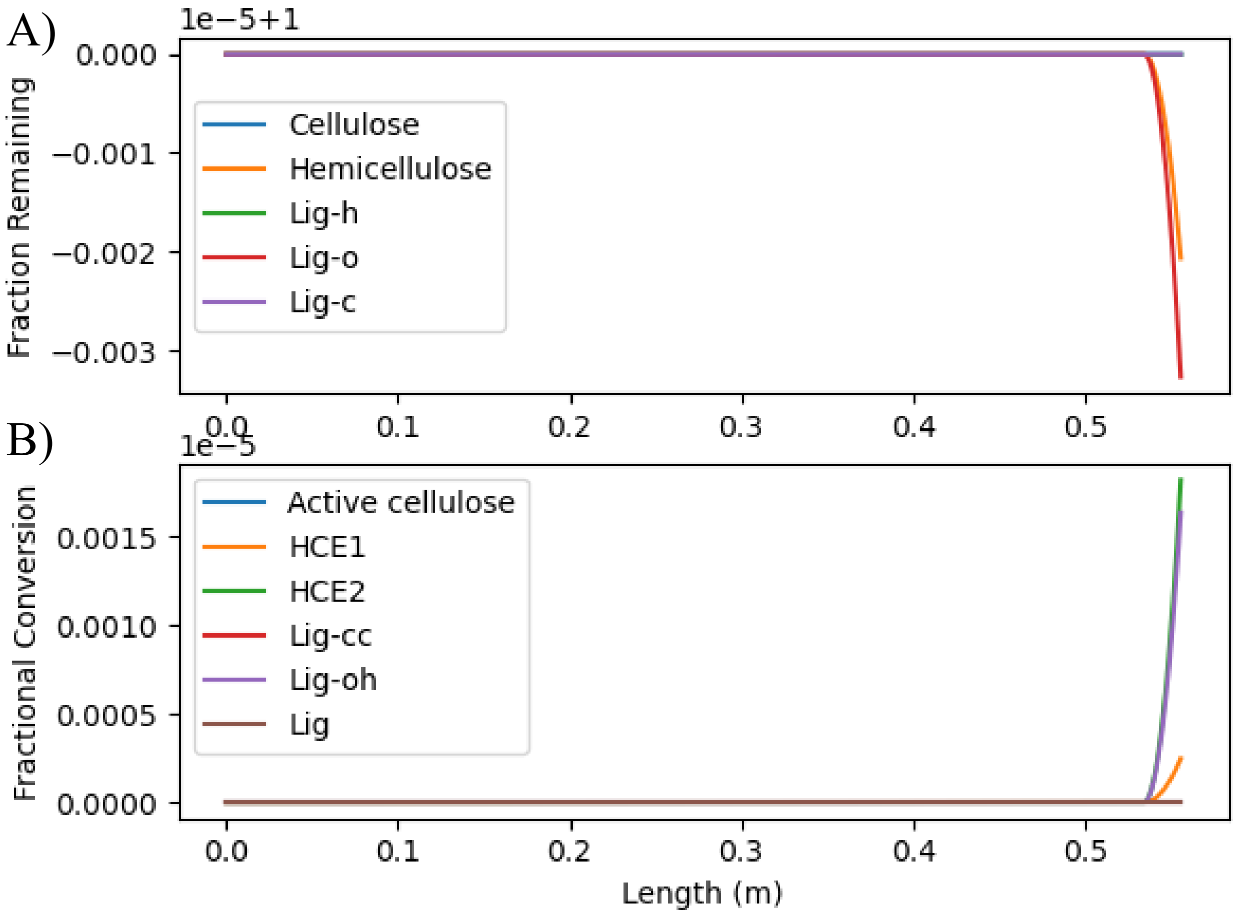
A)

B)



C)

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Conclusions

- Developed 1D temperature profiles
- Changing operating parameters has little effect
- Reactions occurring in the auger feeder

Next Steps

- 2D temperature profiles
- Experimental validation
- Rheology and tribology

Thank you!

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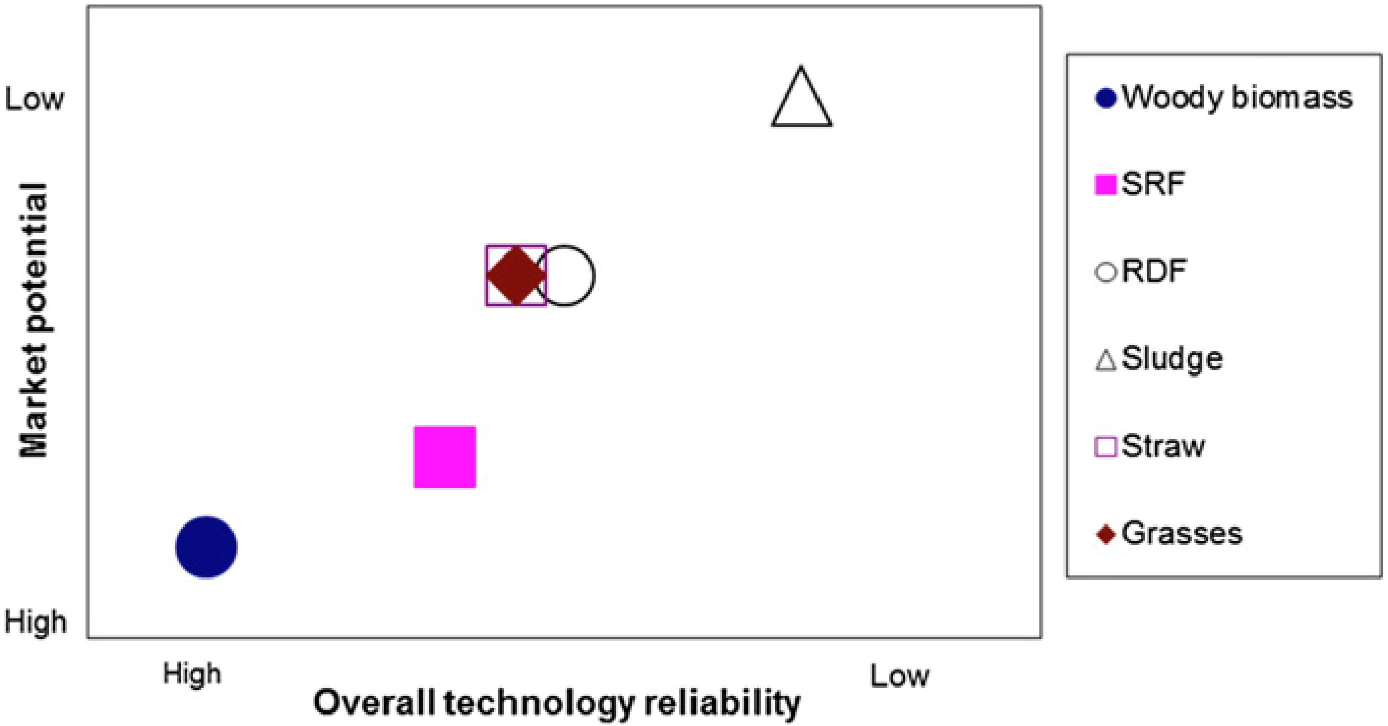
Biomass Feedstocks

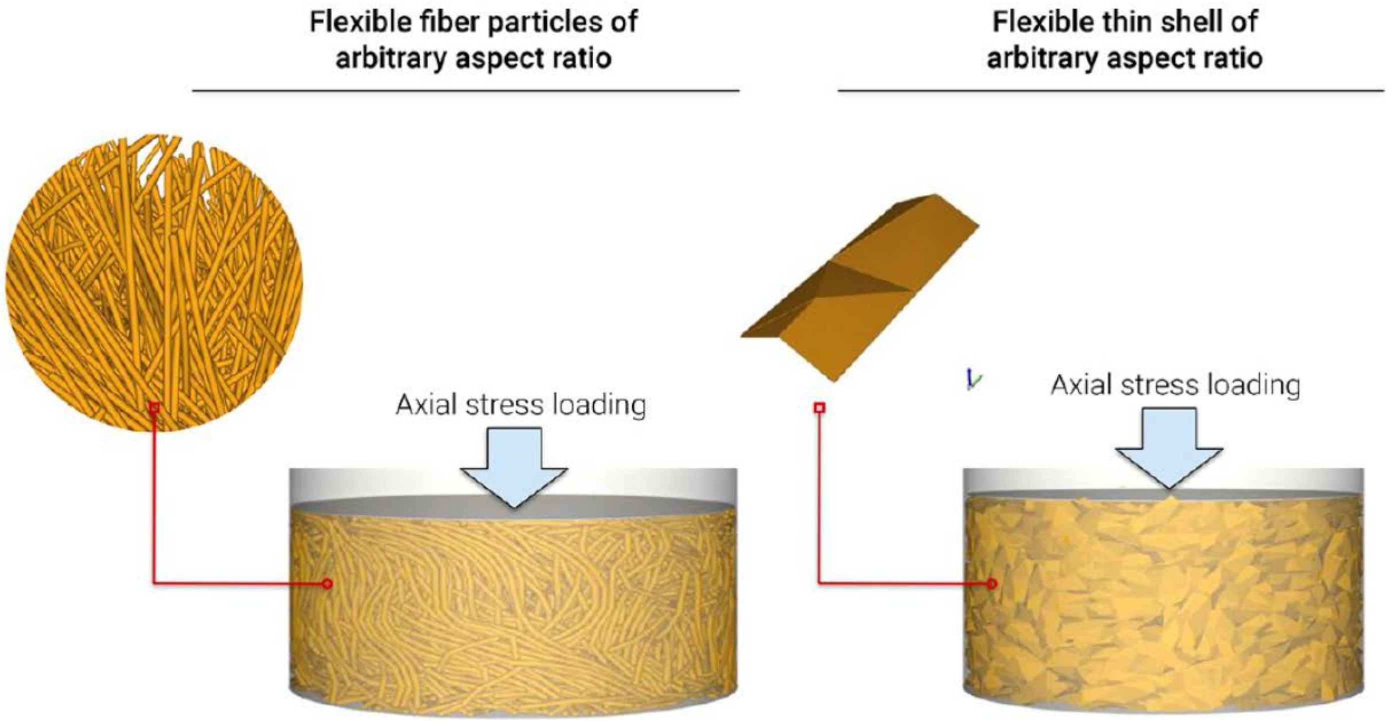


- Woody biomass
  - Even size distribution
  - Regular particle shape
- Sludge
  - High moisture content
  - High contaminant concentration

Dai, 2012

Biomass Rheology

- Shear thinning, viscoelastic solid
- Difficult to model
- DEM, FEM, MPM



Xia, et al. ACS Sustainable Chemistry & Engineering, 8: 6142-6156 (2020)

Heat Transfer Models

- Modeling
  - Runge-Kutta
  - Matrix methods
  - Finite difference

- Particle scale

$$\frac{\partial \rho C_p T}{\partial t} = -(\nabla \cdot q) + (-\Delta H)\left(\frac{\partial \rho}{\partial t}\right) \quad (1)$$

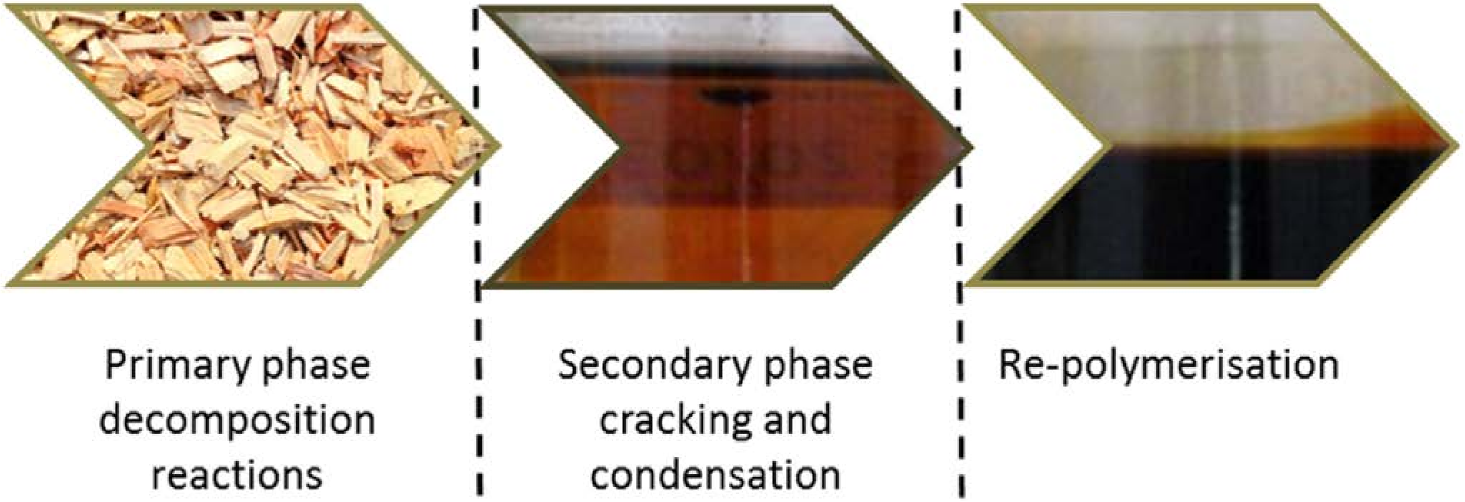
- Bulk scale

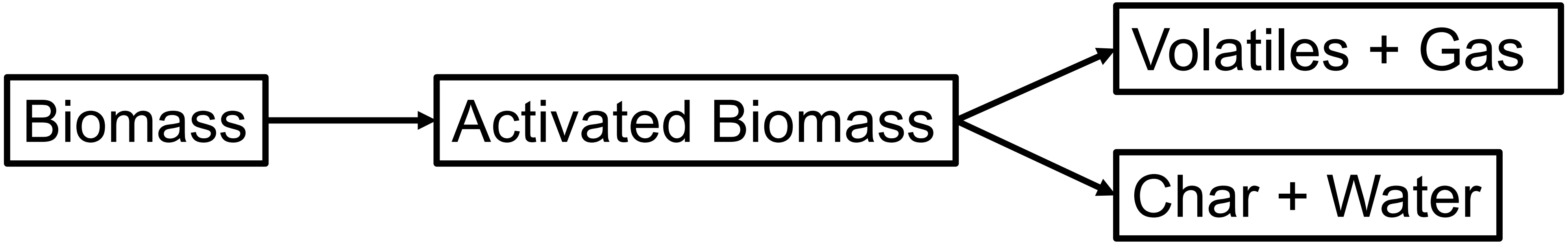
$$\frac{\partial \rho C_p T}{\partial t} = -\nabla \cdot (\rho C_p T v) - (\nabla \cdot q) + (-\Delta H)\left(\frac{\partial \rho}{\partial t}\right) \quad (2)$$

1. Babu. Biofuels, Bioproducts and Biorefining, 2: 393-414 (2008)
2. Koufopanos, et al. The Canadian Journal of Engineering, 67: 75-83 (1989)

Pyrolysis Kinetics

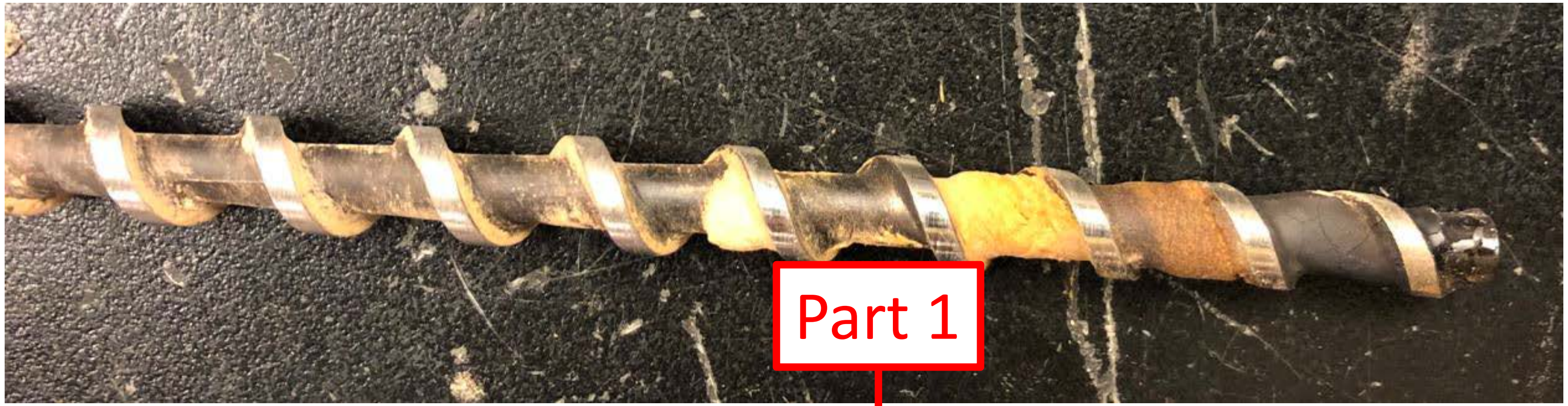
- Multiscale problem
- Models
  - Global or speciated
  - Single or multistage
  - Phase changes
- Debiagi Model





Perkins, et al. Renewable and Sustainable Energy Review, 90: 292-325 (2018)

Working Hypothesis



Heat from the reactor is raising the temperature of the biomass in the feeder, resulting in preliminary decomposition reactions, changing the rheology of the biomass, making it less compliant.

Part 3

Part 2

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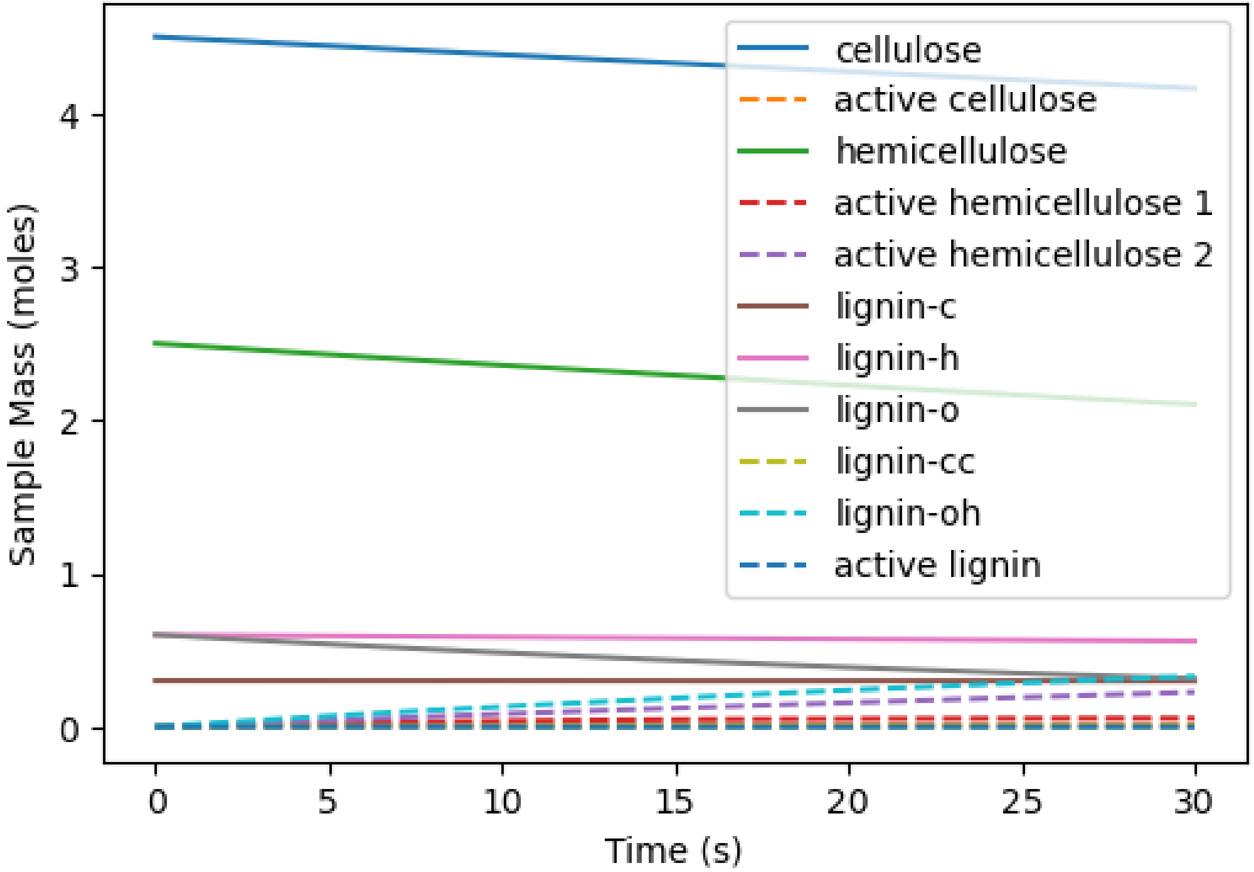
Accomplishments to Date

Kinetic Modeling

- Model developed by Debiagi, et al, 2018
- Medium pyrolysis
- Tested at constant temperature

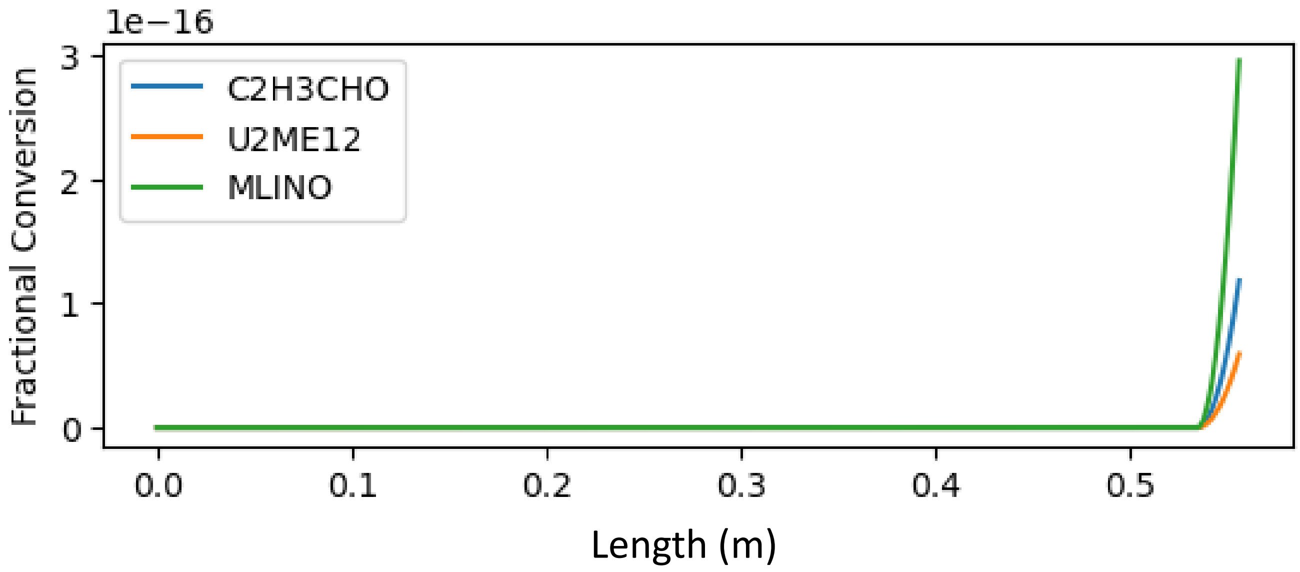


Debiagi, et al. Journal of Analytical and Applied Pyrolysis, 134: 326-335 (2018)

Species of Interest

Diterpenoid Resin Acid (1)
Abietic Acid
Neoabietic Acid
Palustric Acid
Pimaric Acid
Dehydroabietic Acid
Levopimaric Acid
Isopimaric Acid

Extractives	(2)
TGL →	C_2H_3CHO+0.5U2ME12+2.5MLINO

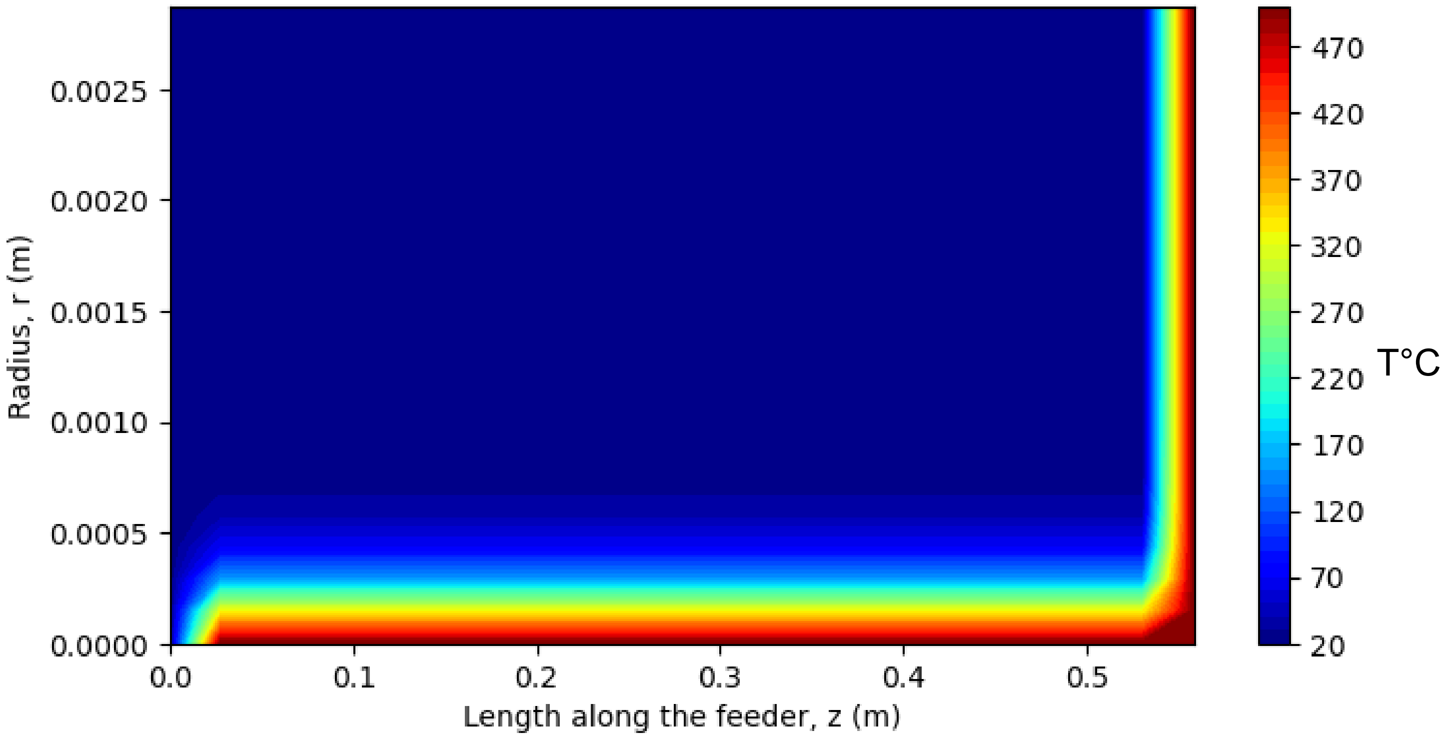


1. Harman-Ware, et al. Journal of Analytical and Applied Pyrolysis, 124: 343-348 (2017)

2. Debiagi, et al. Journal of Analytical and Applied Pyrolysis, 134: 326-335 (2018)

Proposed Research

2D Temperature Profiles



- Screw auger
- Finite difference method
- In agreement with 1D

2D Kinetic Models

- 2D isothermal model
- Use the 2D temperature profile

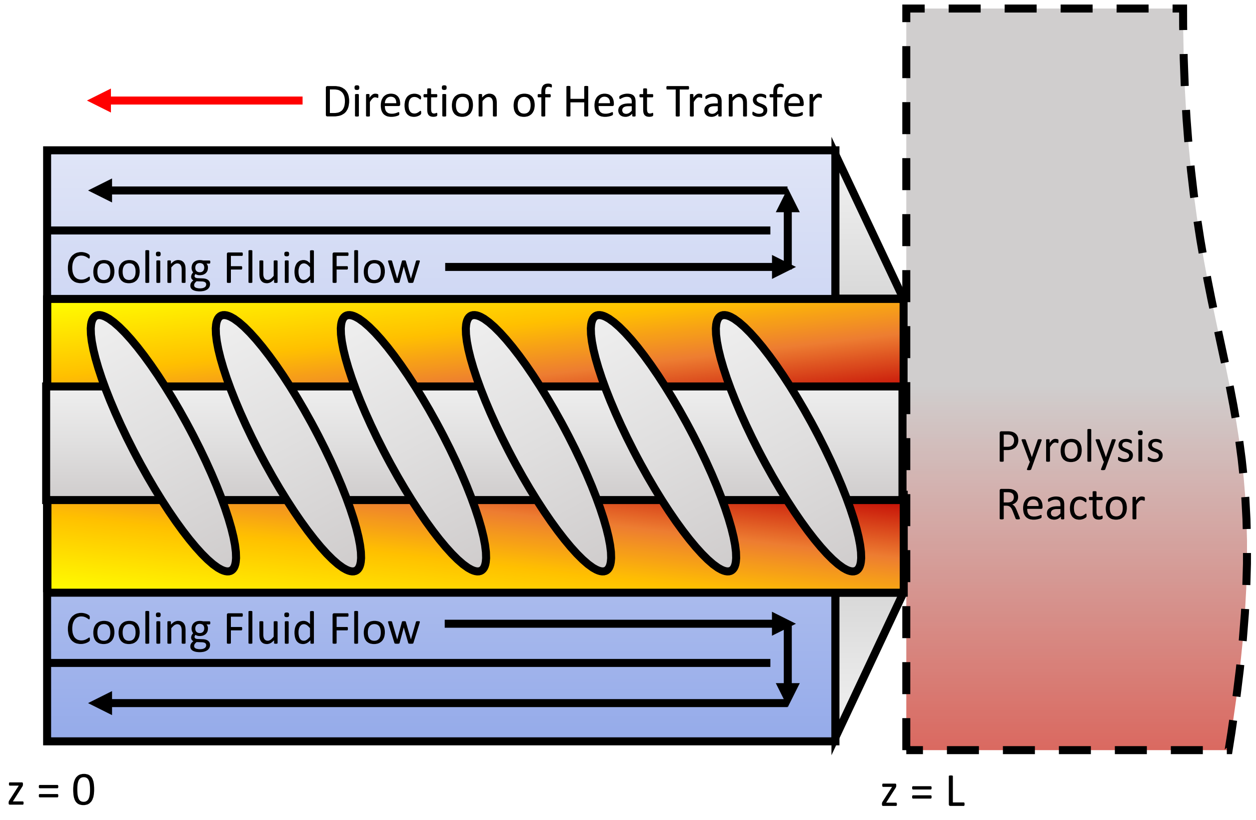
Temperature profile model, T = f(r,z)

↓

Temperature profile model, T = f(t) | Rate constant, k = f(T)

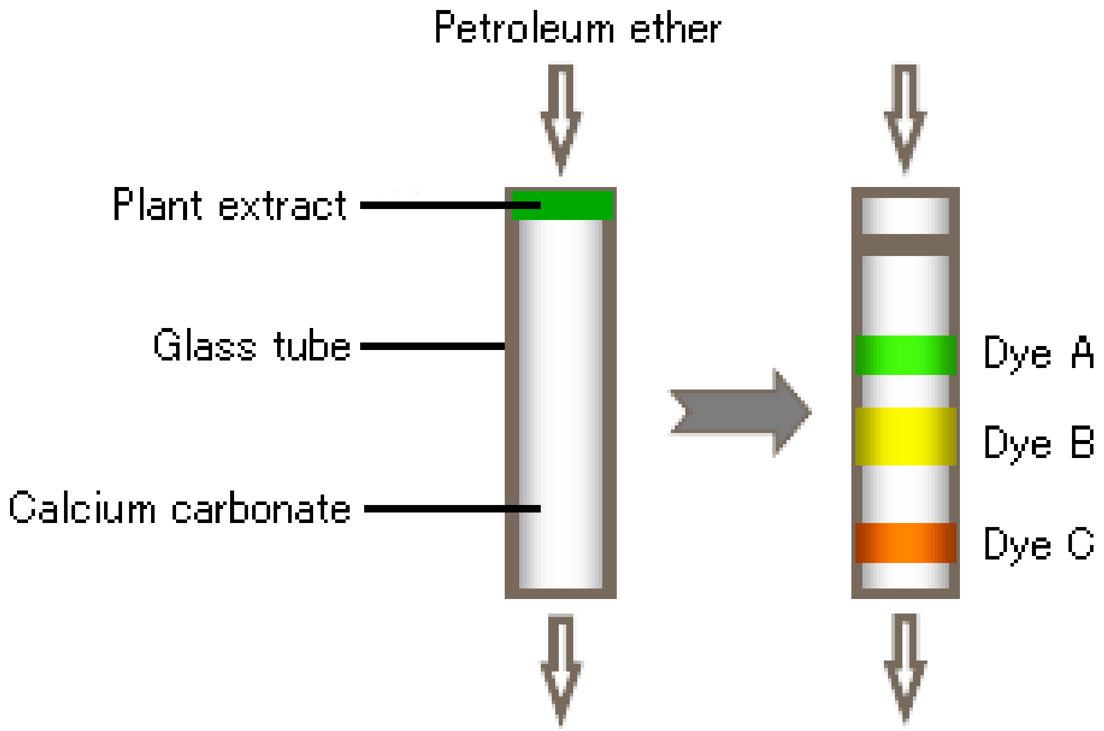
↓

Rate constant, k = f(T(t))



Biomass Compositional Analysis

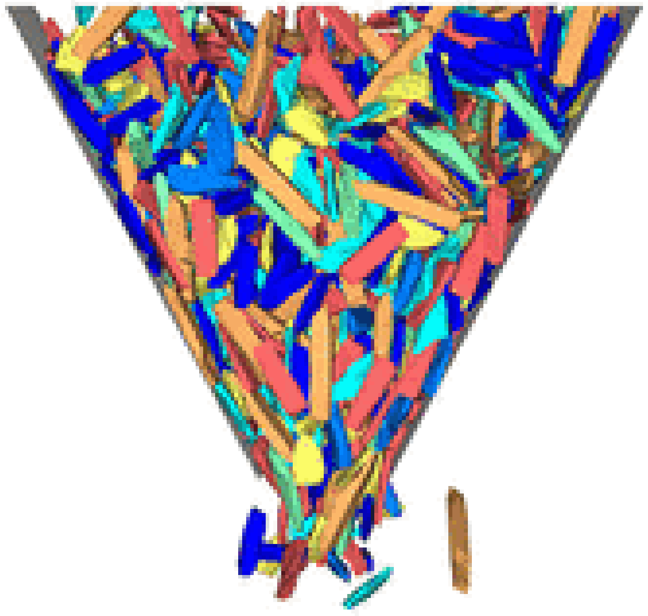
- High-Performance Liquid Chromatography (HPLC)
- Species of interest
- Verify kinetic models
- Verify temperature profile models



Hitachi High-Tech Corporation. 2001, 2021.

Rheology Models

- DEM
- Four scenarios:
    1. Control
    2. Temperature only
    3. Temperature and Kinetics
    4. Kinetics only

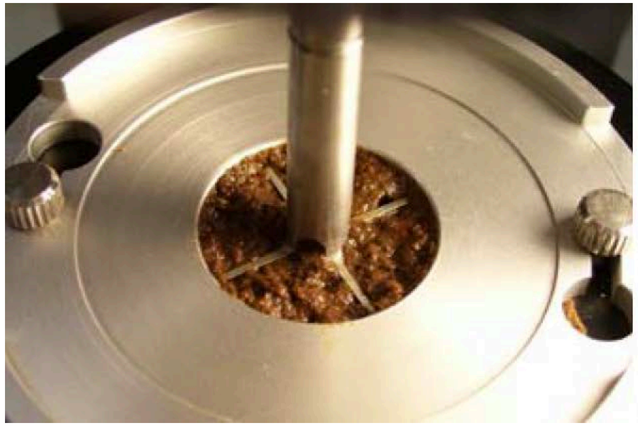


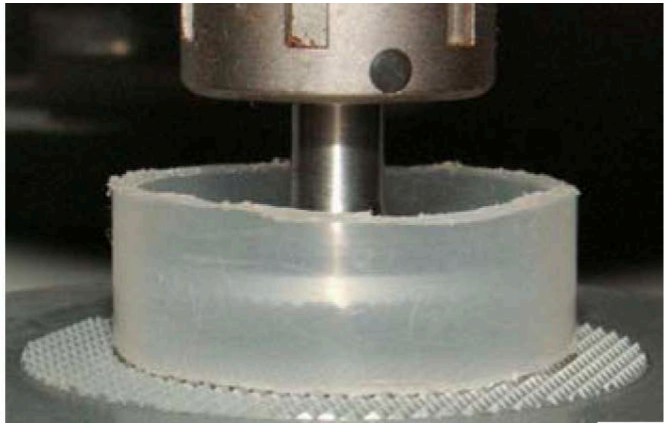
A v-shape hopper discharge simulation

Xia, et al. ACS Sustainable Chemistry & Engineering, 8: 6142-6156 (2020)

Rheology Measurements

- DHR-3 rheometer
- Partially reacted biomass
- Unreacted biomass





Stickel, et al. Rheologica Acta, 48: 1005–1015 (2009)

Expected Outcomes

Aim 1: Heat Transfer Modeling

Aim 2: Pyrolysis Kinetics

Aim 3: Biomass Rheology

Reactions within the auger feeder

Connecting kinetics to rheology

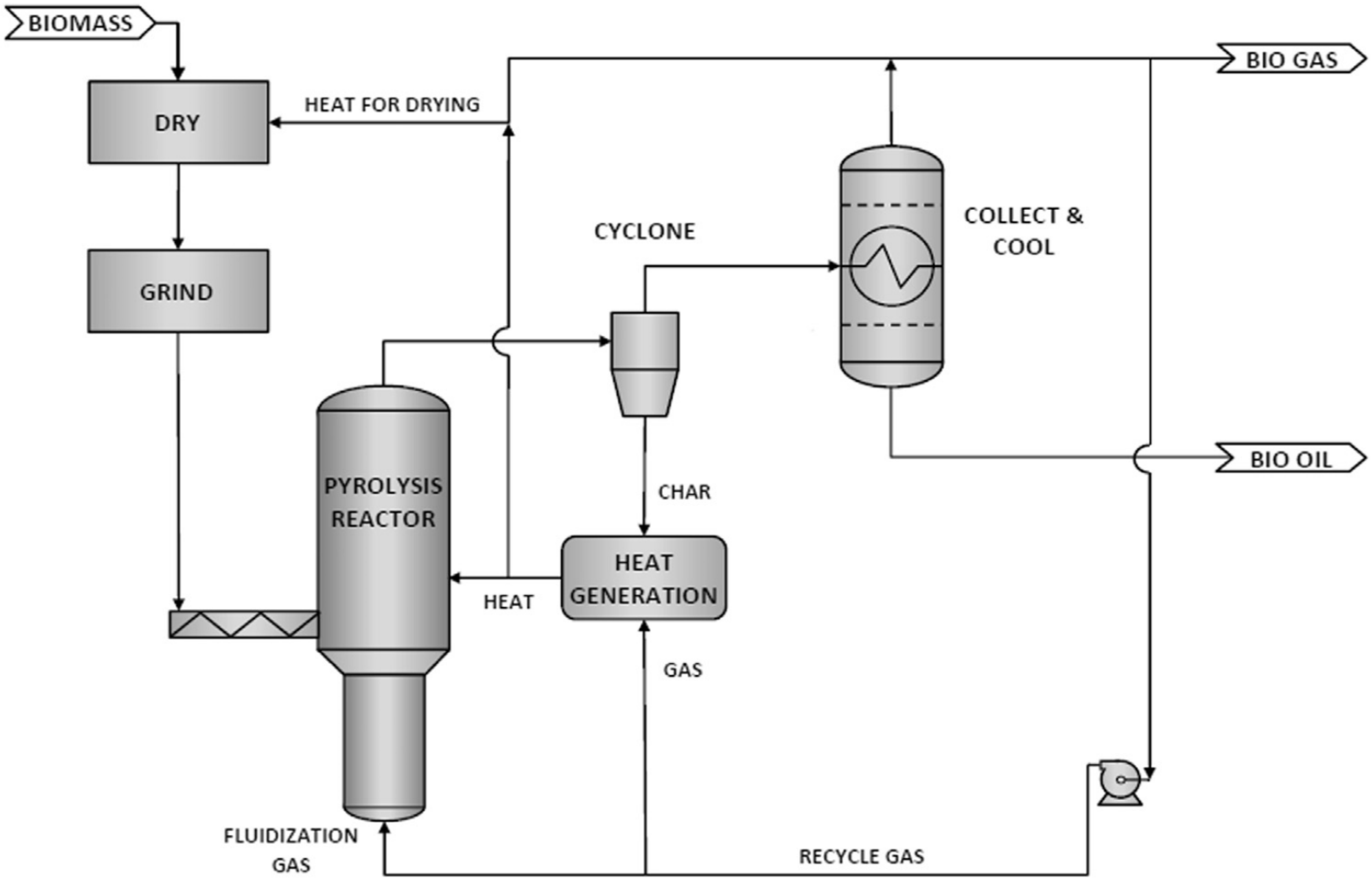
Timeline

	Task	2021	2022				2023				2024			
		Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Aim 1	Simple 1D Heat Transfer													
	2D Temperature Profiles			M										
Aim 2	Simple 1D Kinetic Models													
	2D Kinetics Models								M					
Aim 3	Rheology Models													
	Rheology Measurements													
	Relating Kinetics to Rheology													M

Expected Outcomes

- Understand the dominant heat transfer mechanism.
- Determine the production of intermediates and products.
- Develop a relationship between kinetics and rheology.

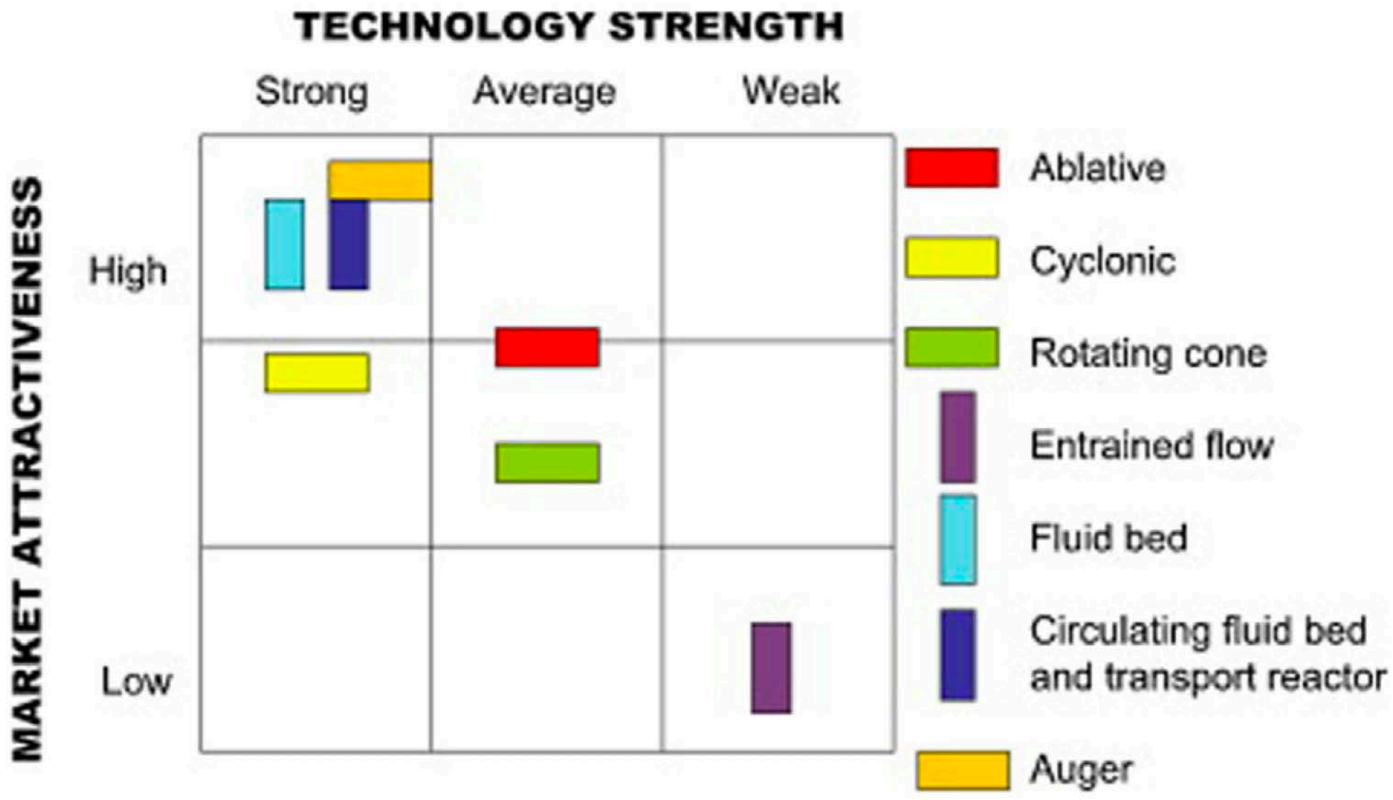
Pyrolysis



Perkins, 2018

Pyrolysis Reactors

- Retaining energy
- Feedstock considerations
- Operating conditions



Butler, 2011

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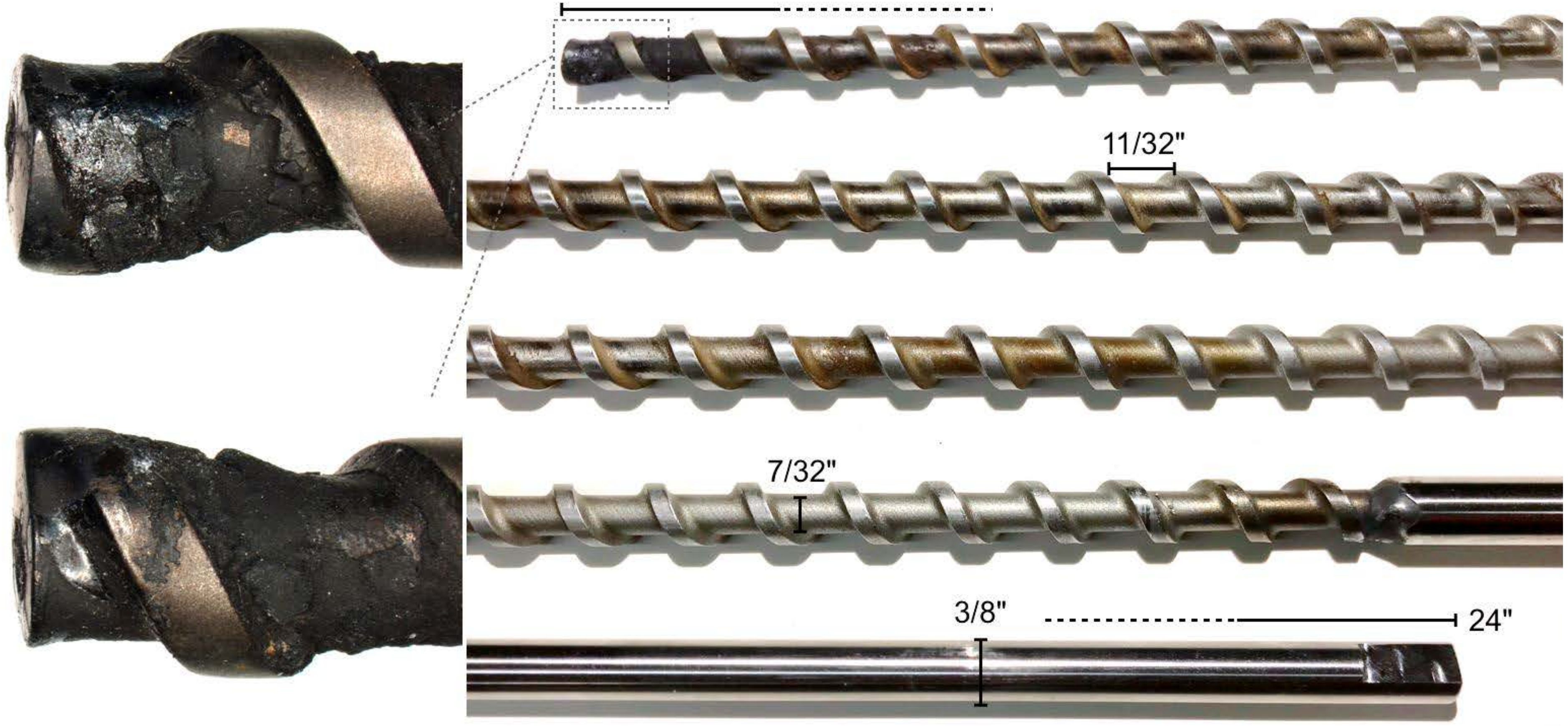
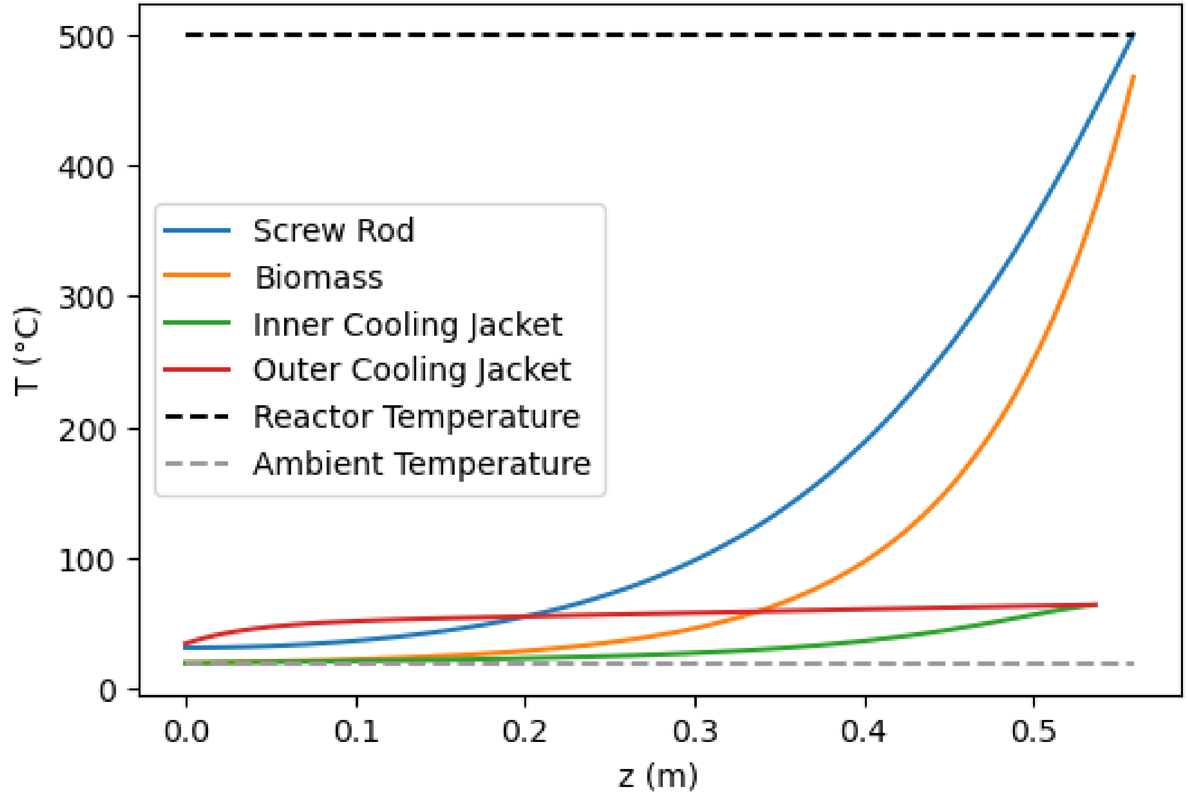
Full Length of Auger

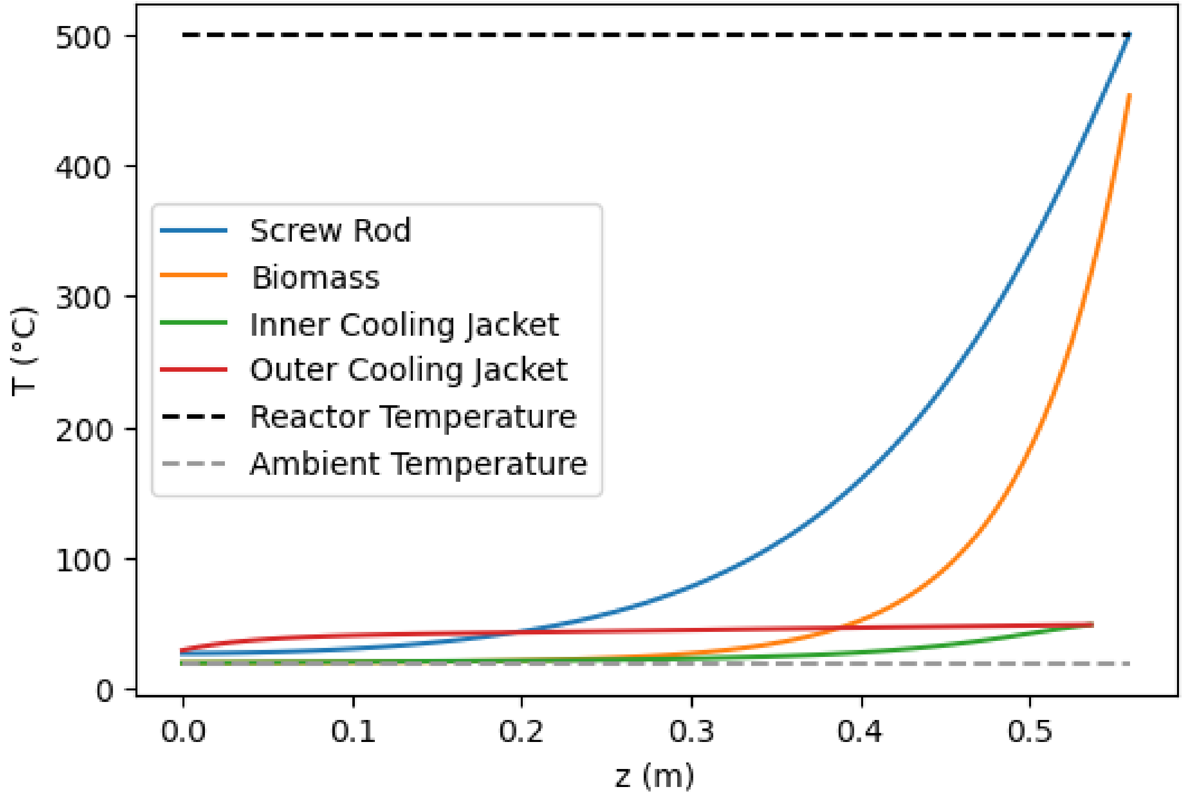


Changing Operating Parameters

Original

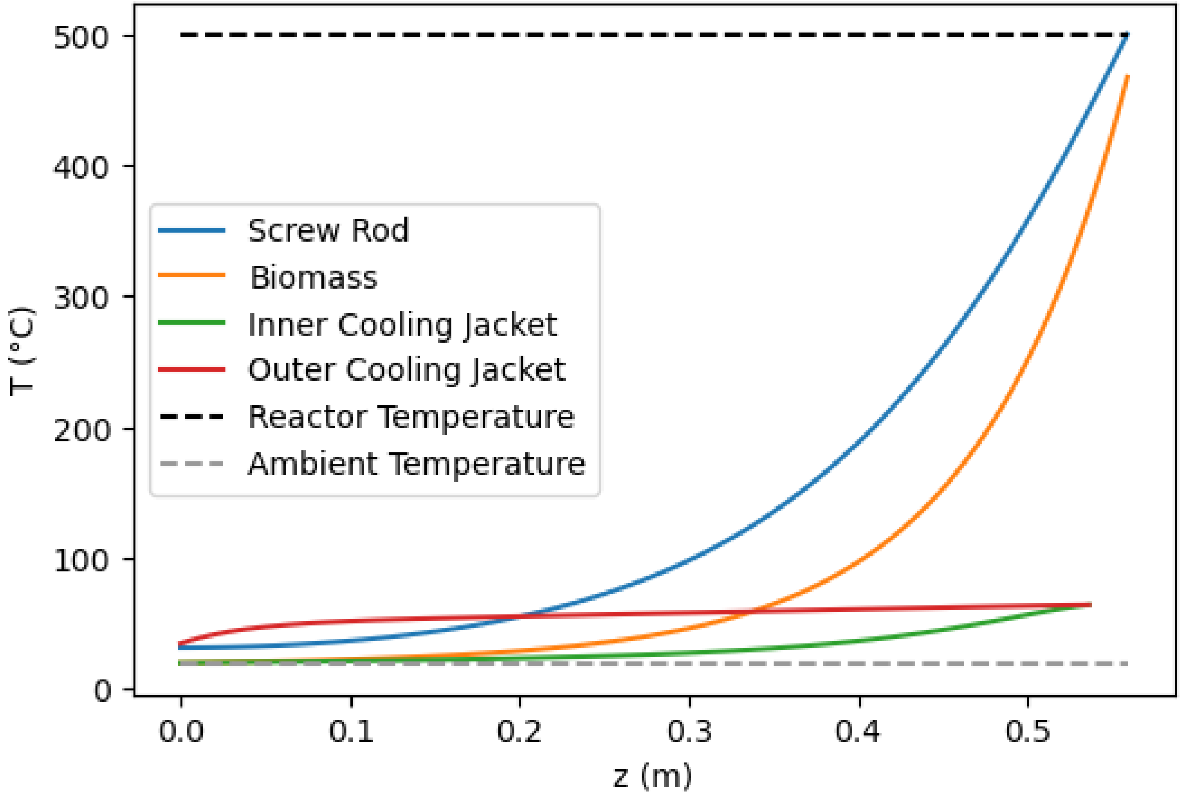


Doubled Biomass Velocity

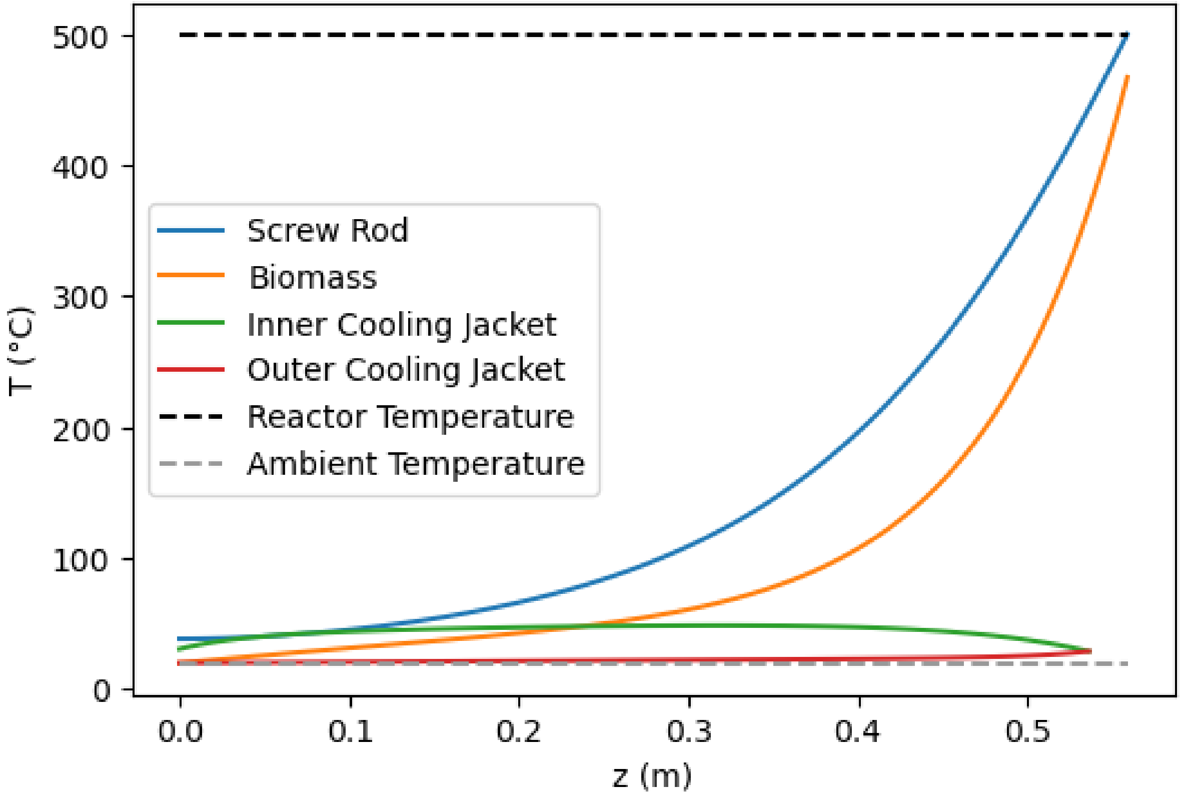


Changing Operating Parameters

Original



Cooling Flow in Opposite Direction



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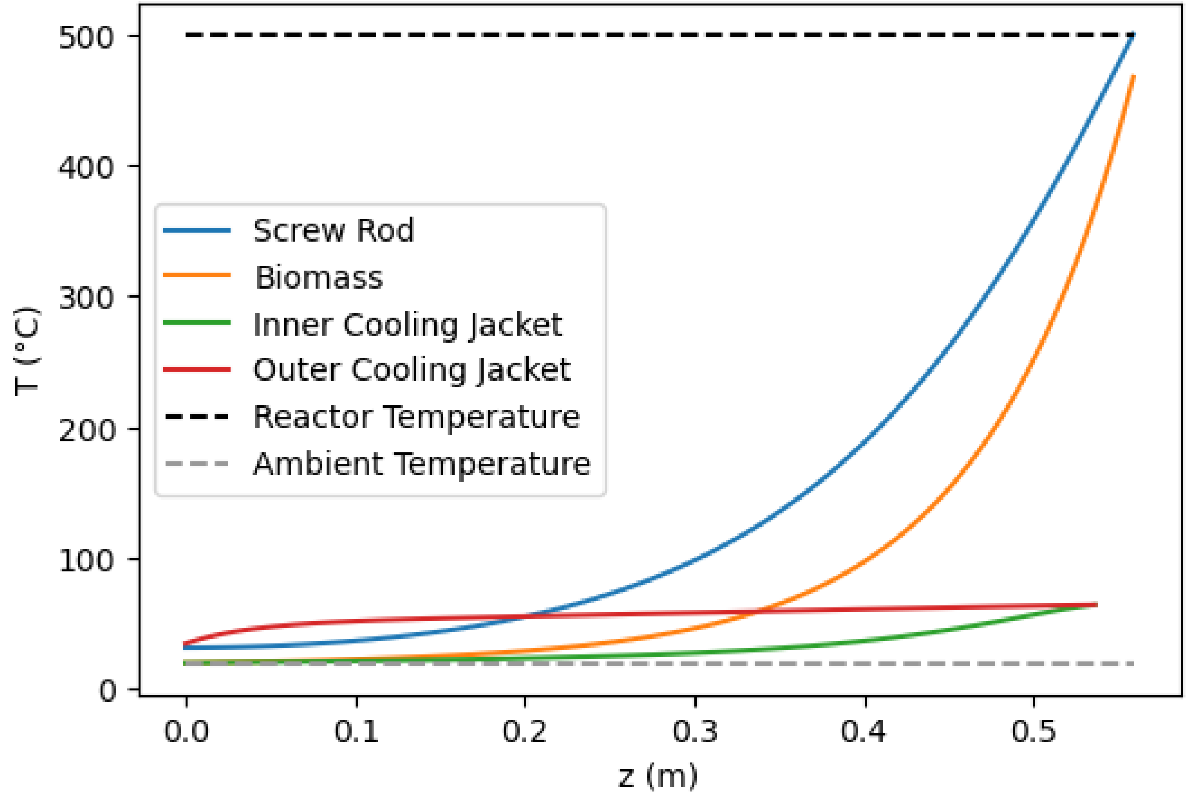
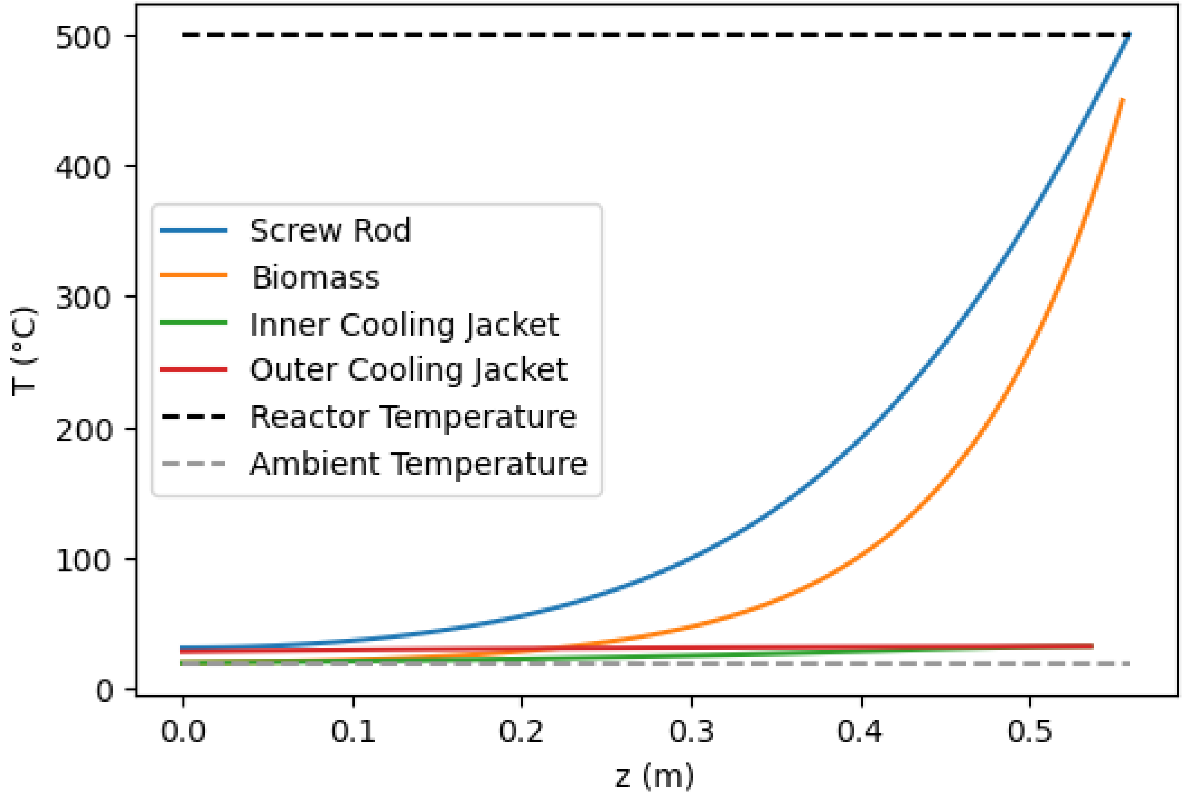
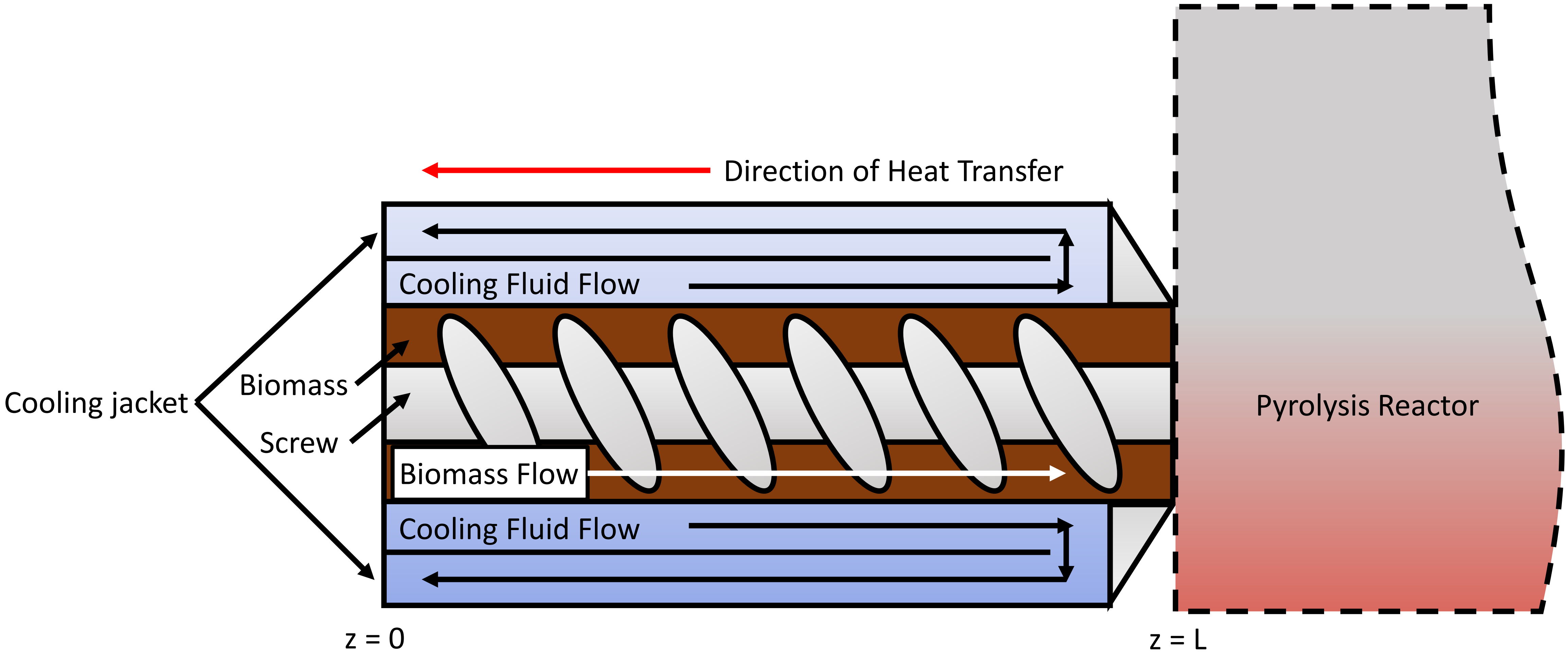
Changing Operating Parameters

Original



Water as the Coolant




Direction of Heat Transfer
Cooling Fluid Flow
Cooling jacket
Biomass
Screw
Biomass Flow
Cooling Fluid Flow
Pyrolysis Reactor
z = 0
z = L

Species Analysis

DEM Info

Table 1. List of DEM Model Parameters Pertinent to Biomass Particles[a]

DEM parameter	options and notes
particle shape	see discussion in "Particle Shapes of DEM"
particle size distribution	particle volume based; particle mass based
particle skeletal density	material density that excludes intraparticle pore volume
particle envelope density	often referred to as "particle density"
skeletal elastic modulus	material modulus
effective elastic modulus	often referred to as "particle modulus"
Poisson's ratio	
restitution coefficient	
static friction coefficient	particle–particle; particle–wall
dynamic friction coefficient	particle–particle; particle–wall
rolling friction coefficient	usually applied to mono- or composite-sphere models
damping coefficient(s)	particle–particle; particle–wall
contact cohesion	liquid bridge; viscosity; etc.
bond stiffness	bonded-sphere; multielement fiber; multielement shell

Rheology Measurement Info

Rheology vs. Tribology

- Telling viscosity from friction