SEPARATION PROCESS - II

PYROLYSIS OF WOOD

Estimating Optimized parameters

Gaurav Budhwani | 22110085
Kaushik | 22110113

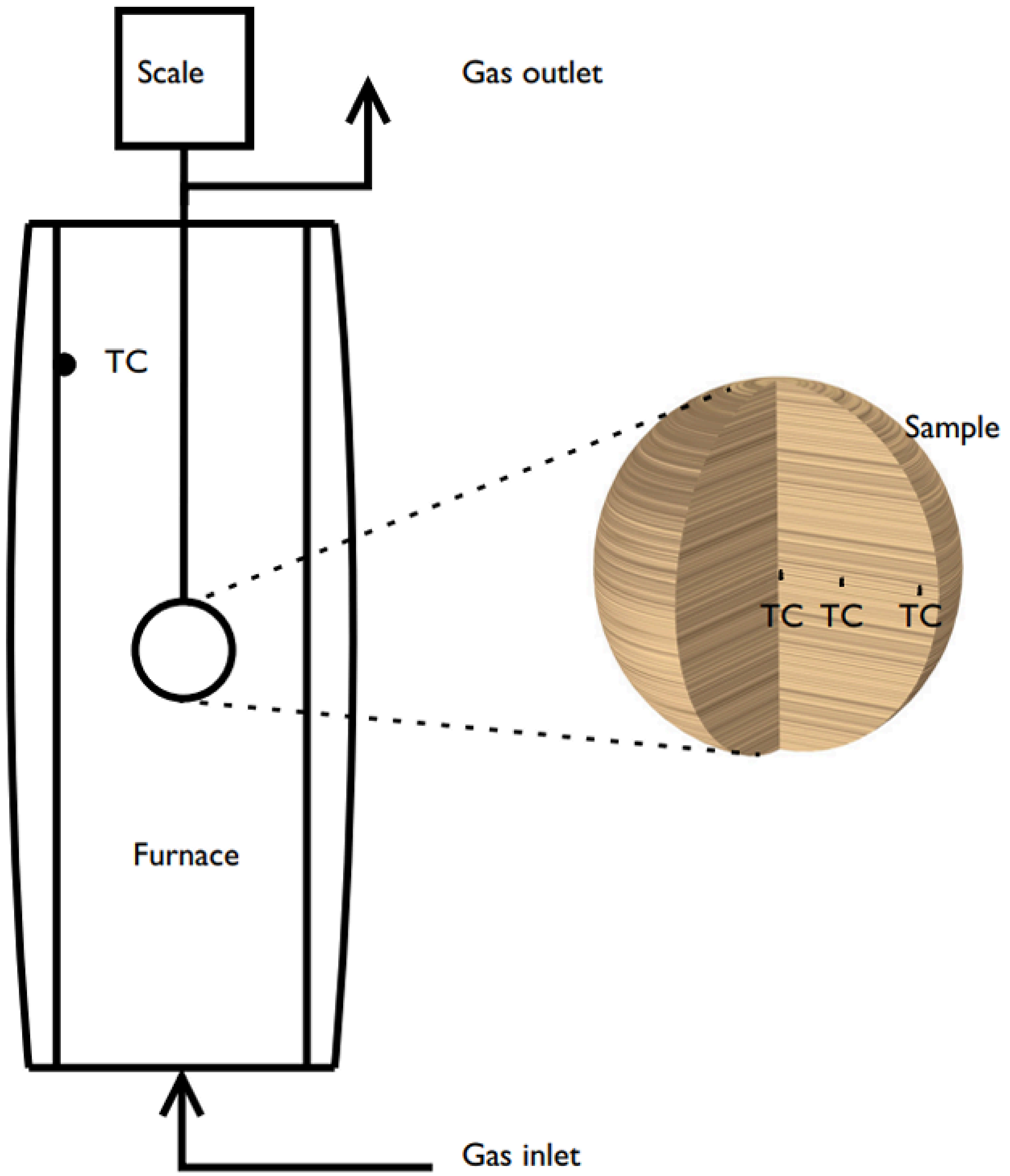
Under the guidance
Prof. Karthik Subramaniam Pushpavanam

WHAT IS PYROLYSIS?

Pyrolysis is the chemical process where a material decomposes by heat in the absence of oxygen, breaking down into simpler substances like gases, liquids (tar/bio-oil), and solid char.

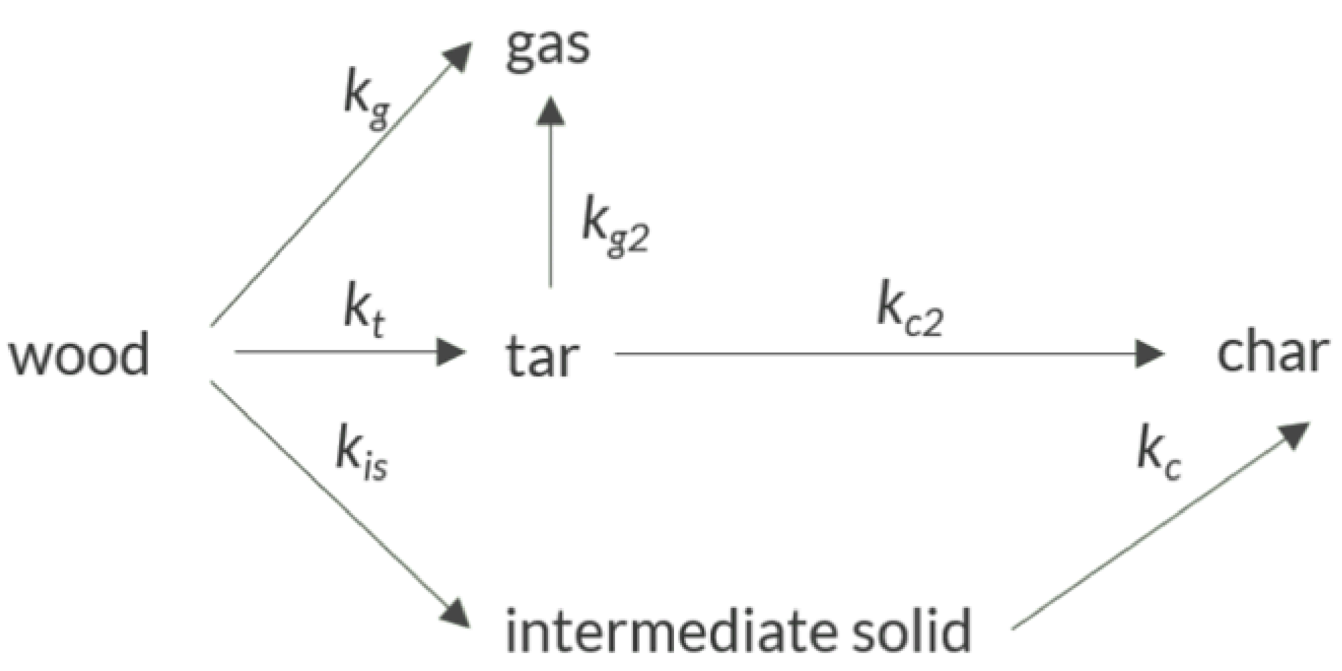
Importance of Pyrolysis

- Energy generation (biofuels, syngas).
- Waste reduction (plastic and biomass waste).
- Environmental protection (carbon capture, reduced emissions compared to open burning).



OBJECTIVE

- **Arrhenius pre-exponential factor** : The rate constant that describes the reaction rate for the pyrolysis of wood.
- **Heat of reaction for wood → tar :** The enthalpy change associated with the conversion of wood into tar during pyrolysis.
- **Heat of reaction for intermediate solid → char**: The enthalpy change for the conversion of intermediate solid phases into char.
- **External convective heat-transfer coefficient, h_{conv}**: The heat transfer rate due to convection in the system during pyrolysis.



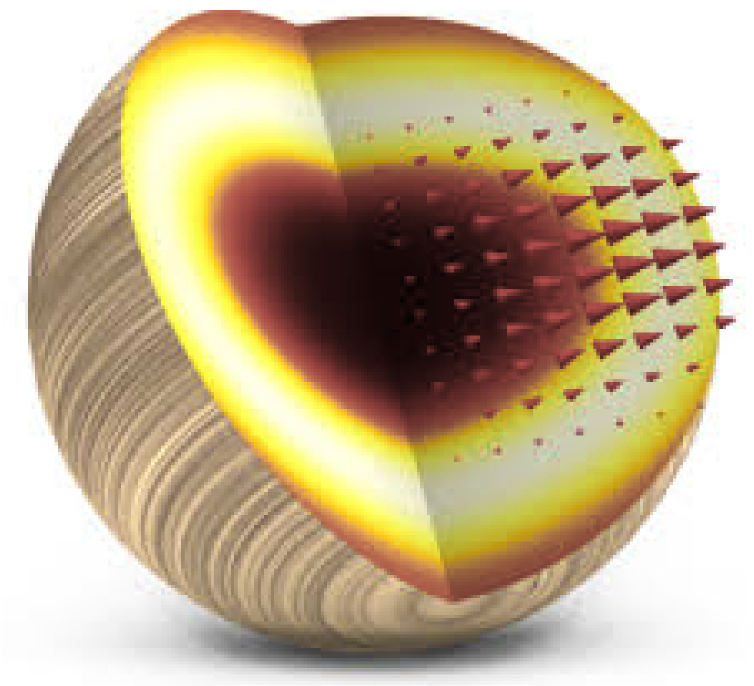
PHYSICS INTERFACES

Transport of Concentrated Species in Porous Media (tcs)
→ Models the movement of chemical species (volatiles, gases, tar) through the wood's porous structure.

Darcy's Law (dl)
→ Governs fluid flow (gas flow) through the porous wood matrix, driven by pressure gradients.

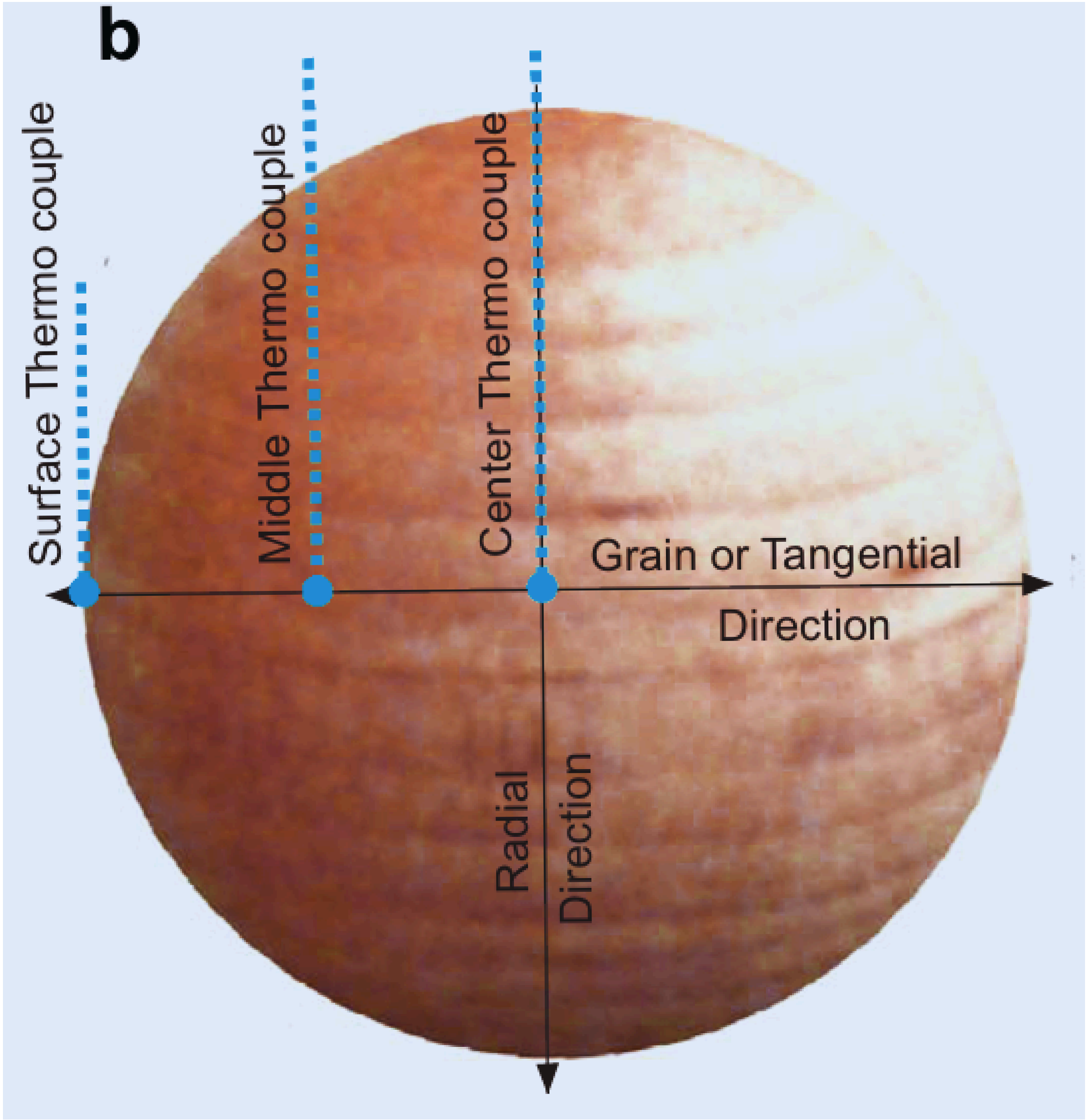
Heat Transfer in Porous Media (ht)
→ Simulates how heat moves through the wood, accounting for conduction, convection (via gas flow), and possibly reaction-generated heat.

Domain ODEs and DAEs (dode)
→ Handles the chemical reaction kinetics inside the solid wood matrix (such as pyrolysis reactions) using user-defined ordinary differential equations (ODEs).



MODEL SETUP

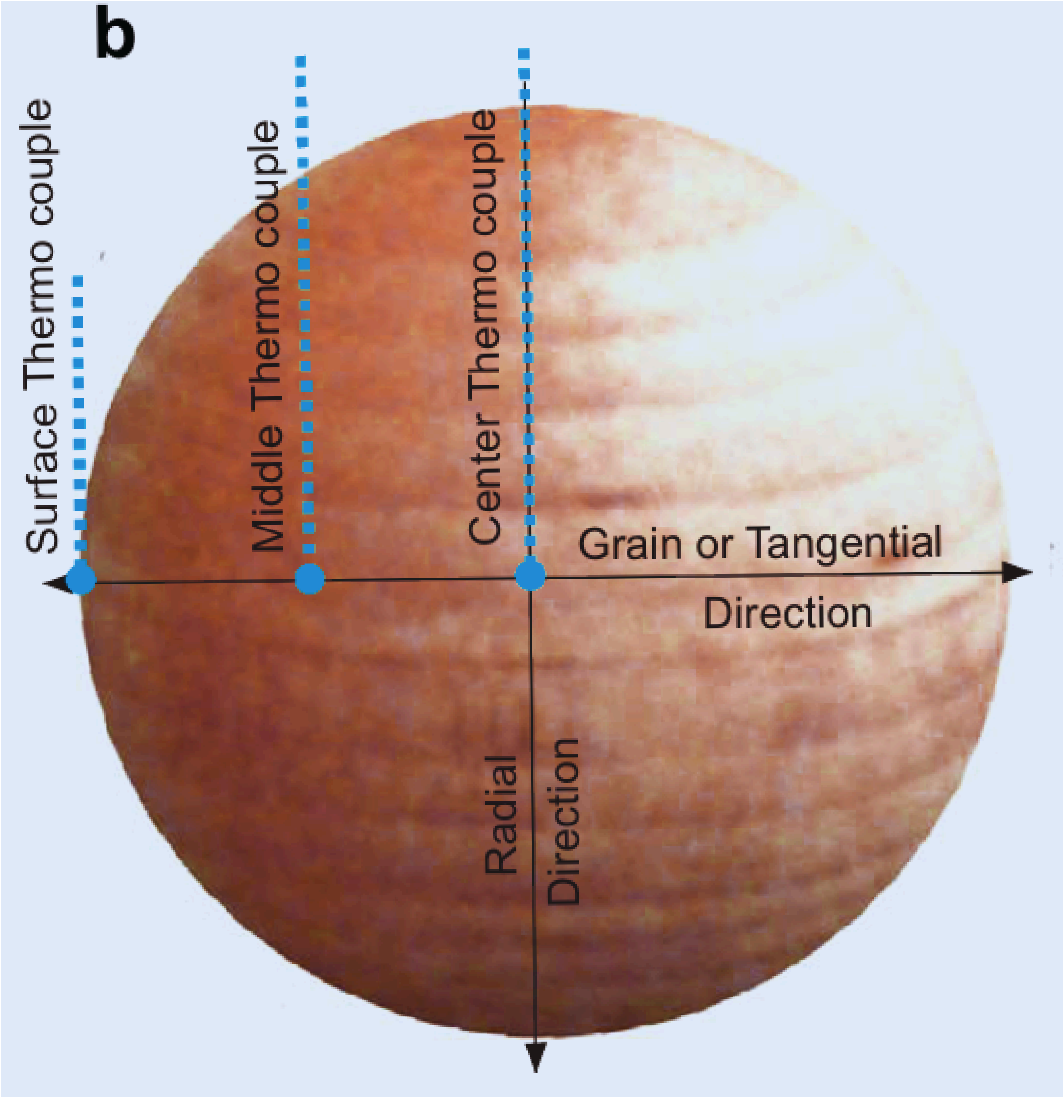
A spherical wood sample is inserted into hot furnace with an inert atmosphere.
The sample temperature is measured with **thermocouples (TC)** at
three positions
(surface, middle, and center).



MODEL SETUP

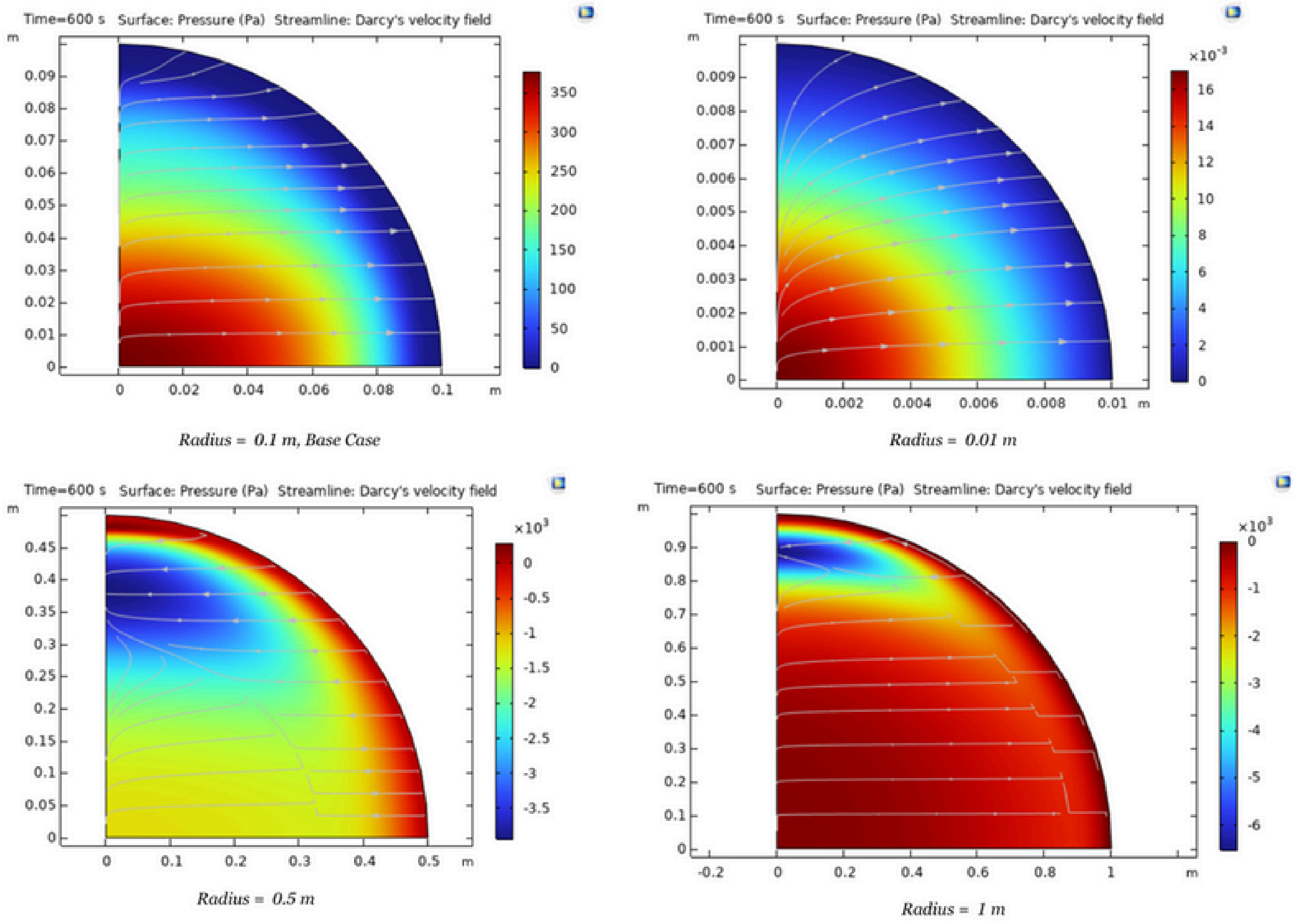
Why Sphere is Preferable to any other shape for Pyrolysis Modeling?

- **Simplified Modeling:** A sphere reduces complex 3D heat and mass transfer to a simpler 2D radial problem.
- **Uniform Heating:** Spheres heat evenly from all sides, unlike cubes, which heat faster at edges and corners.
- **No Geometric Artifacts:** Spheres avoid issues like corner overheating and stress concentrations seen in cubes.
- **Experimental Consistency:** Spheres are easier to make, instrumented with thermocouples, and are the standard shape in experiments.

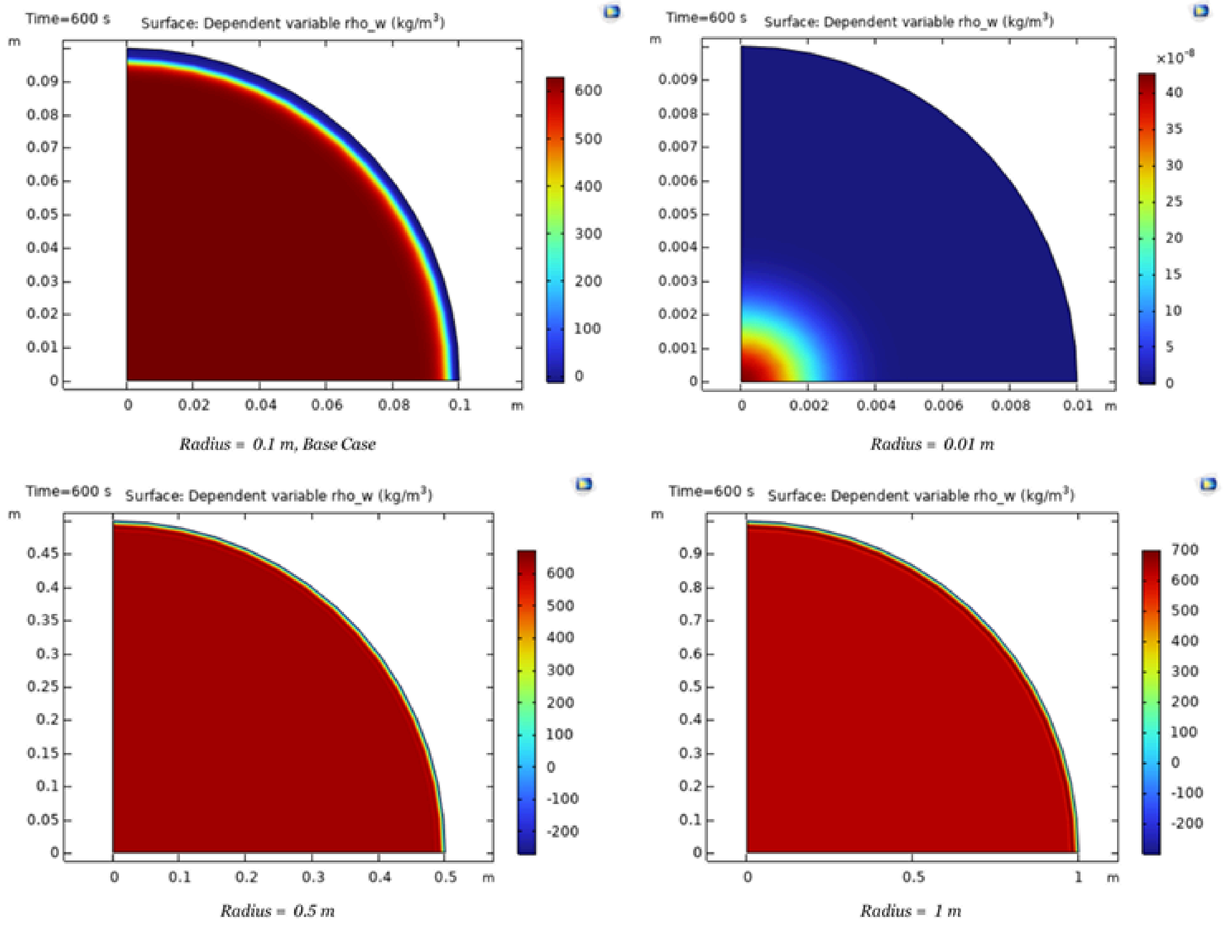


VARYING RADIUS OF WOOD PARTICLE

R = 0.01m, 0.1m, 0.5m, 1m



Surface Pressure



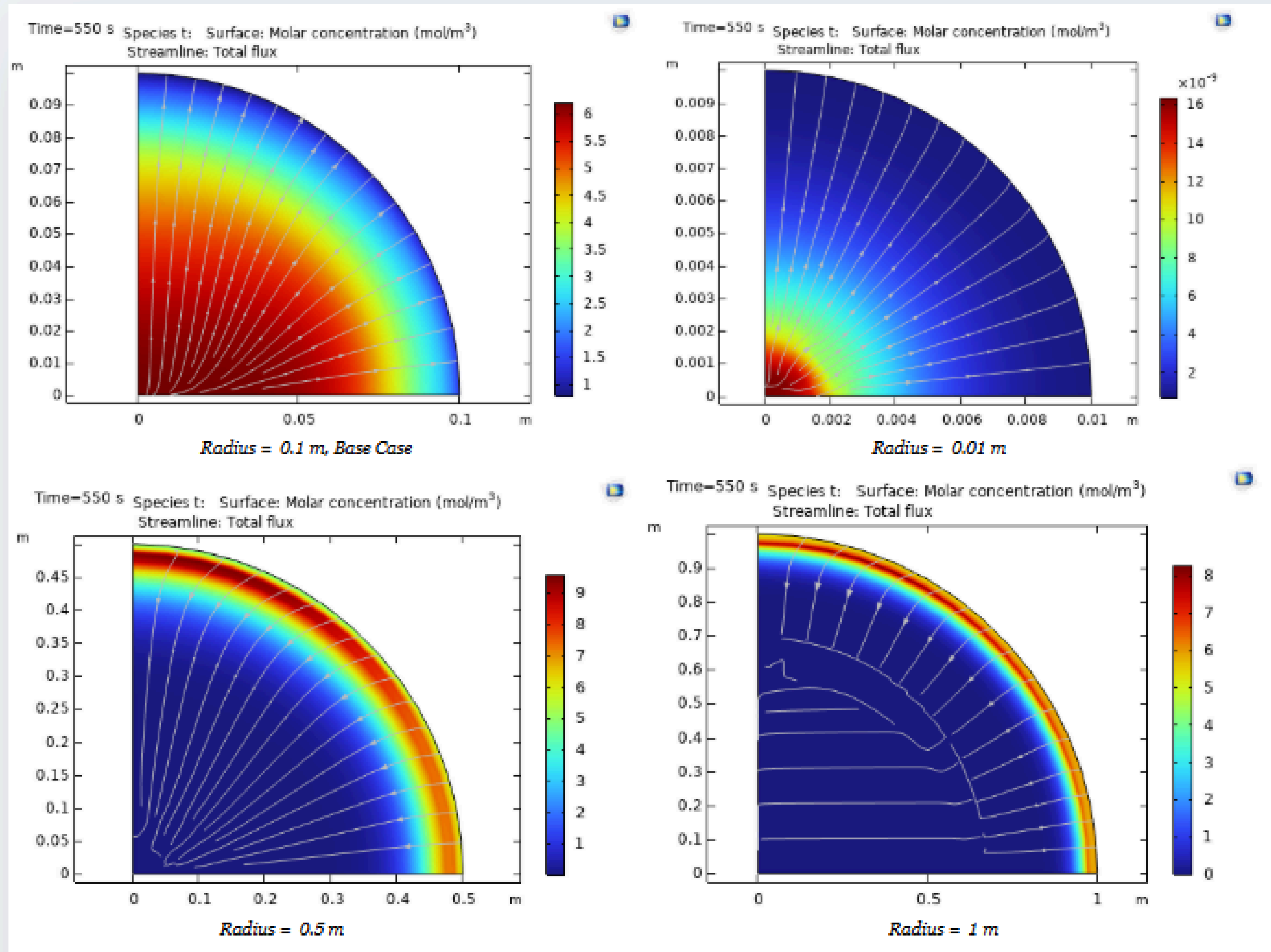
Density of wood

Larger particles trap volatiles longer, creating stronger out ward pressure gradients and delayed gas release compared to small particles.

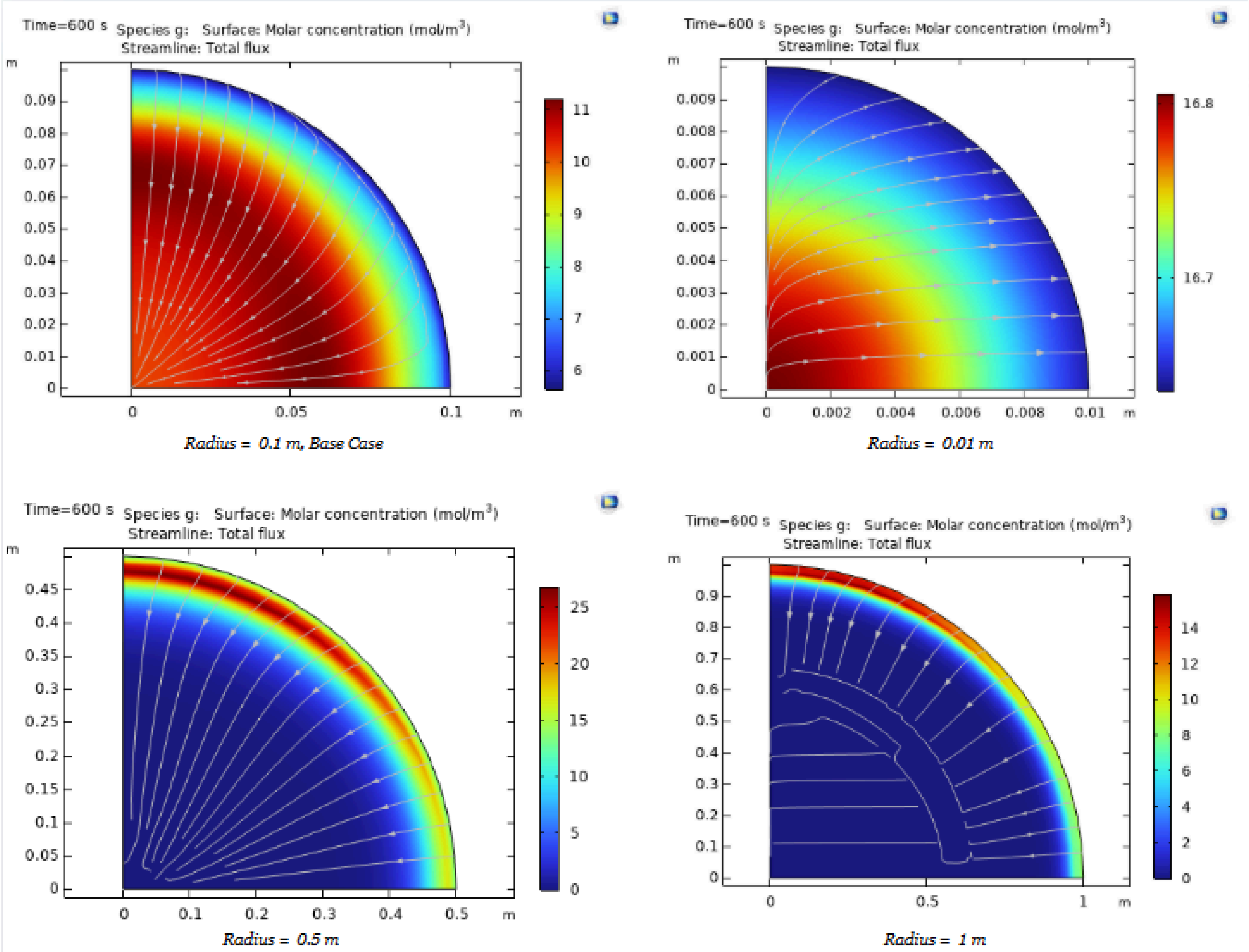
Small particles decompose uniformly due to fast heat penetration, while large particles exhibit "shrinking-core" behavior where only surface layers pyrolyze initially.

VARYING RADIUS OF WOOD PARTICLE

R = 0.01m, 0.1m, 0.5m, 1m



Surface Molar Concentration and Flux of Tar Species



Surface Molar Concentration and Flux of Gas Species

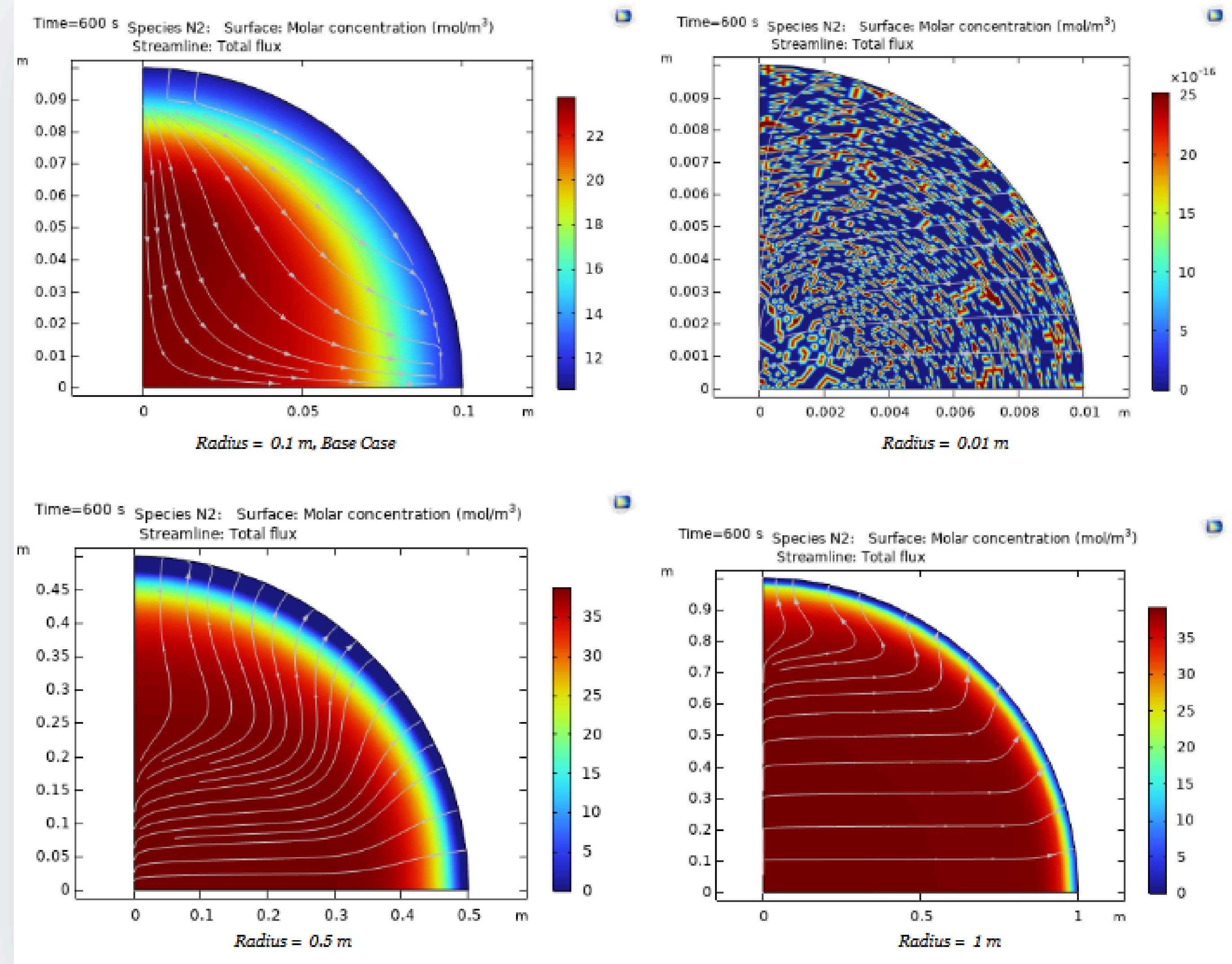
Smaller wood particles enable faster tar release, while larger particles show tar buildup due to slower diffusion and delayed pyrolysis.

Gas generation and release are faster in small particles, while large particles trap gases due to slower migration and uneven flux.

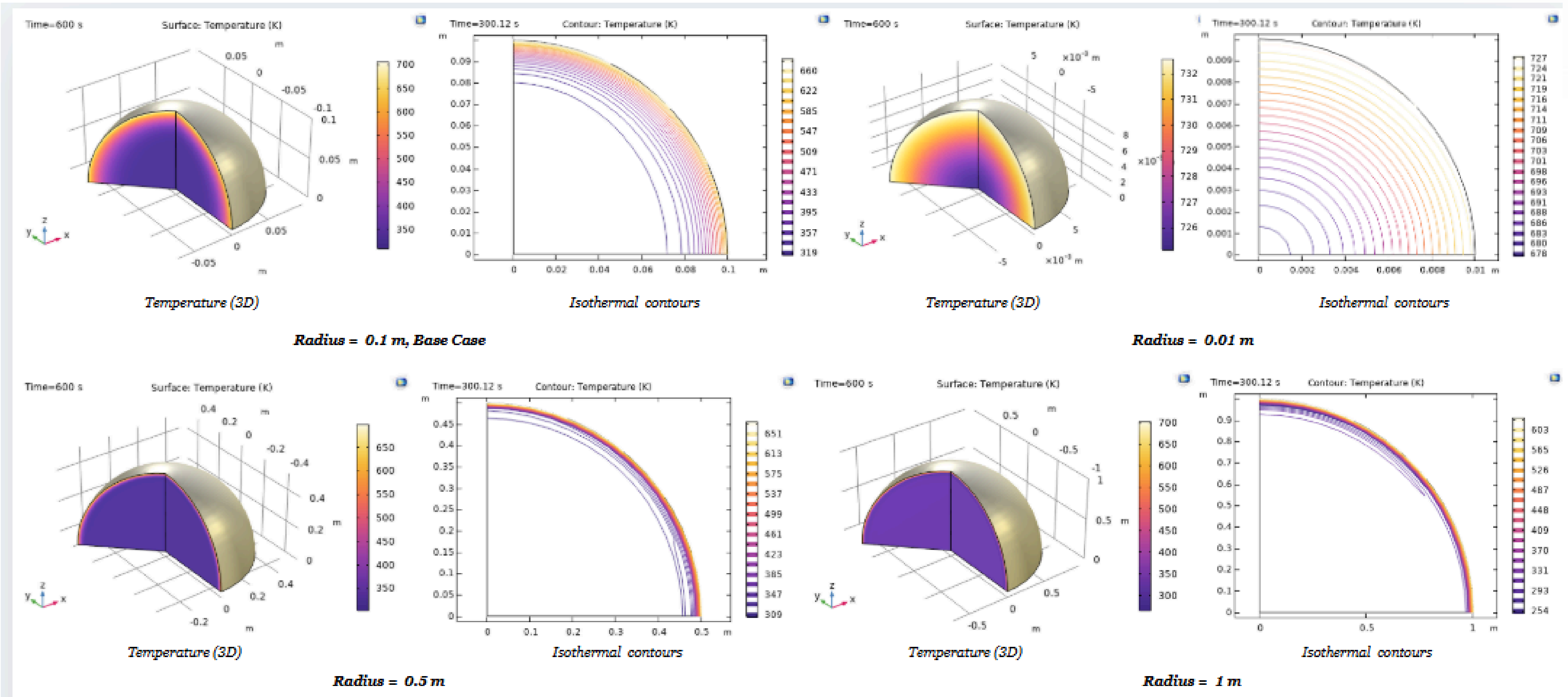
VARYING RADIUS OF WOOD PARTICLE

R = 0.01m, 0.1m, 0.5m, 1m

COMSOL



Surface Molar Concentration and Flux of Nitrogen Species



Temperature Distribution and Isothermal Contour

Nitrogen acts as a passive tracer of gas flow, showing faster flushing in small particles but no significant reaction-related changes.

Smaller particles heat uniformly and react faster, while larger particles show strong temperature gradients, slowing pyrolysis due to delayed core heating.

VARYING POROSITY OF WOOD PARTICLES

Porosity : 0.2 , 0.4 , 0.6 , 0.8

Surface Pressure and Darcy's Velocity Field:

Higher porosity improves gas flow inside wood, with densest streamlines at porosity 0.8, but pressure buildup peaks at porosity 0.6, suggesting an optimal porosity for efficient volatile escape.

Wood Density Distribution:

Higher porosity enables deeper wood decomposition, while lower porosity slows pyrolysis by retaining higher core density.

Molar Concentration and Flux of Tar Species:

High porosity reduces tar buildup and enhances tar flux, whereas low porosity traps tar and delays decomposition.

Molar Concentration and Flux of Gas Species:

Greater porosity speeds up gas removal, lowering core accumulation and promoting smoother gas transport.

Molar Concentration and Flux of Nitrogen Species (N_2):

Nitrogen flux improves with porosity, confirming that higher porosity enhances overall gas flow dynamics.

Temperature Distribution and Isothermal Contours:

Higher porosity leads to more uniform heating and faster pyrolysis by reducing thermal gradients across the wood particle.

VARYING REACTION KINETICS (PRE-EXPONENTIAL FACTORS AND ACTIVATION ENERGIES)

EA = 1365 J/MOL, 19567 J/MOL, 14265 J/MOL

Surface Pressure and Darcy's Velocity Field:

Higher activation energy reduces volatile generation, lowering surface pressure and weakening gas flow compared to the base case.

Wood Density Distribution:

Higher activation energies significantly delay wood decomposition, preserving core density, while the base case enables faster surface and core degradation.

Molar Concentration and Flux of Tar Species:

Increased activation energy suppresses tar production and slows tar flux, while lower activation energies promote faster and stronger tar release.

Molar Concentration and Flux of Gas Species:

Higher activation energies lead to greater gas retention in the core and weaker gas release, showing delayed pyrolysis progression.

Molar Concentration and Flux of Nitrogen Species (N_2):

Higher activation energies reduce nitrogen migration out of the particle, indicating an overall slowdown in internal gas transport.

Temperature Distribution and Isothermal Contours:

Higher activation energies slow the heating process, resulting in colder cores and less uniform temperature profiles compared to the faster heating of the base case.

EFFECT OF VARYING AMBIENT TEMPERATURE

T = 290 K, 310 K, 323 K

Surface Pressure and Darcy's Velocity Field:

Higher ambient temperatures raise internal surface pressure and gas velocities, promoting faster volatile release; lower temperatures slow down gas movement.

Molar Concentration and Flux of Tar Species:

Higher ambient temperatures enhance tar production and migration, while cooler conditions suppress tar generation and transport.

Molar Concentration and Flux of Gas Species:

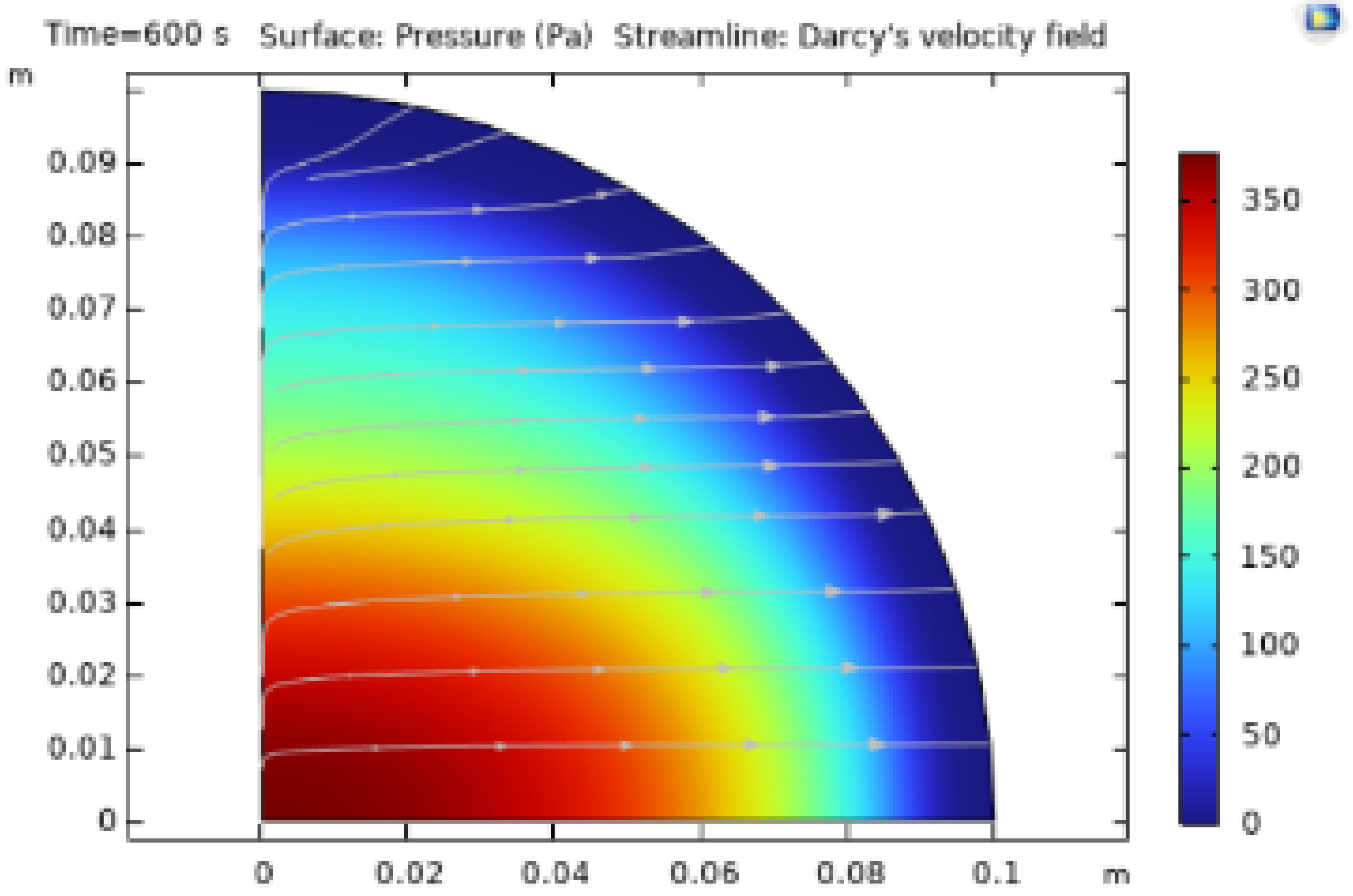
Raising the ambient temperature increases gas production and flux outward, boosting overall pyrolysis efficiency compared to cooler environments.

Molar Concentration and Flux of Nitrogen Species (N_2):

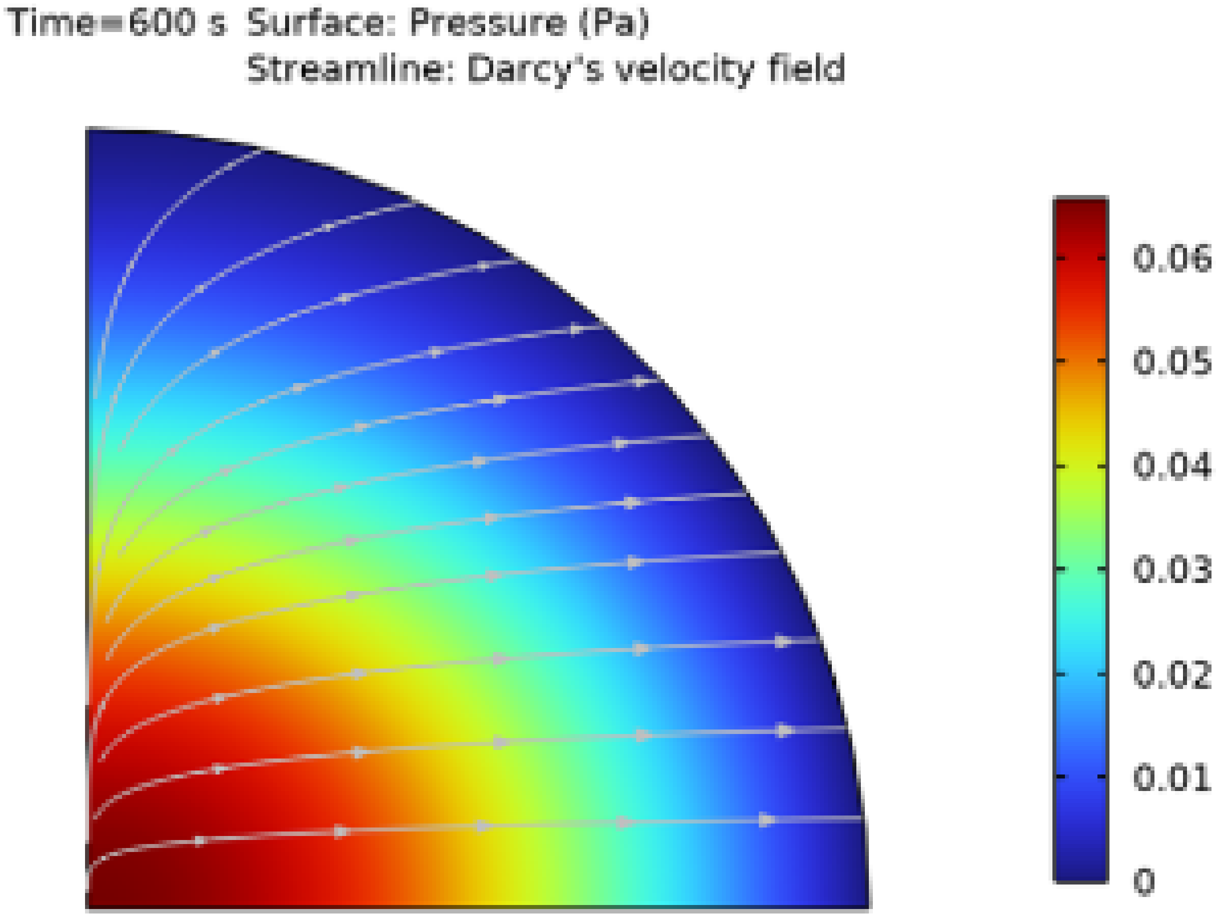
Higher temperatures accelerate nitrogen outward flow, indicating more efficient overall gas transport; lower temperatures hinder this evacuation.

RESULTS

Pressure Profile



Base Case

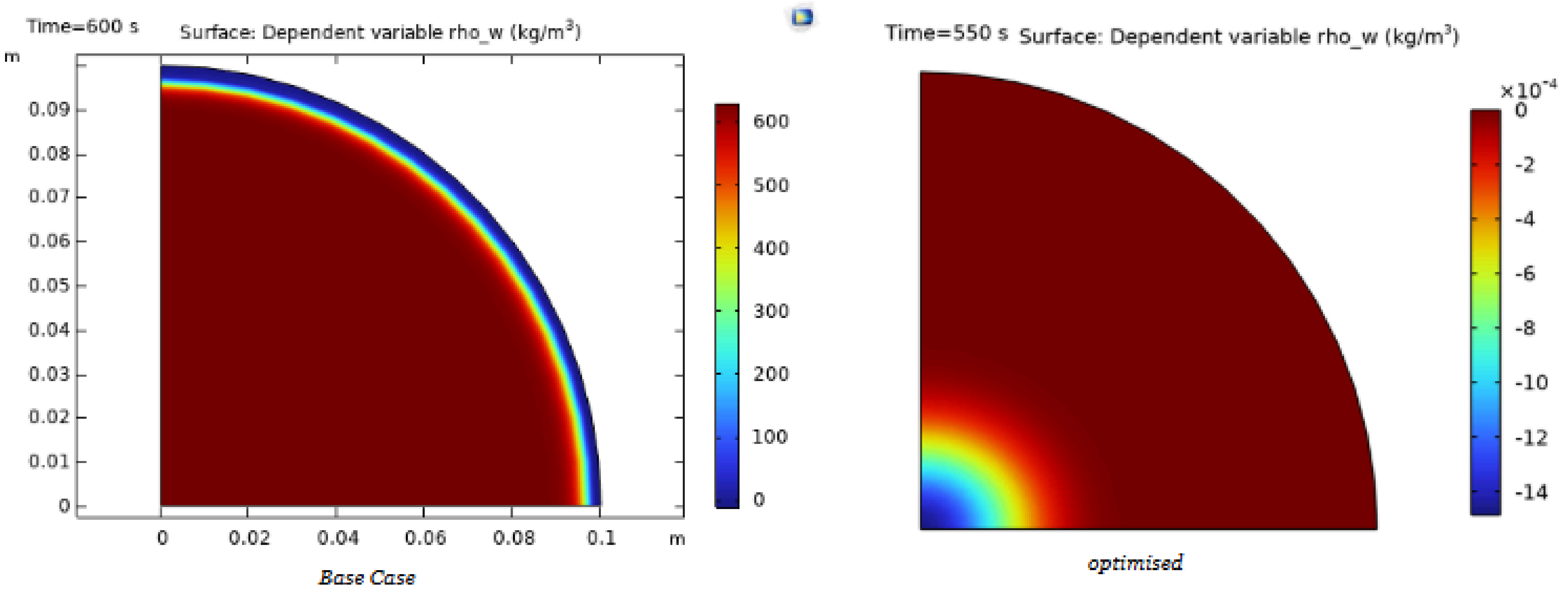


optimised

- **In the base model, high internal pressures (350 Pa) indicate restricted volatile escape, suggesting slow pyrolysis and possible internal structural stress.**
- **In the optimized model, the pressure is drastically reduced (close to at mospheric levels), implying efficient volatile release.**

RESULTS

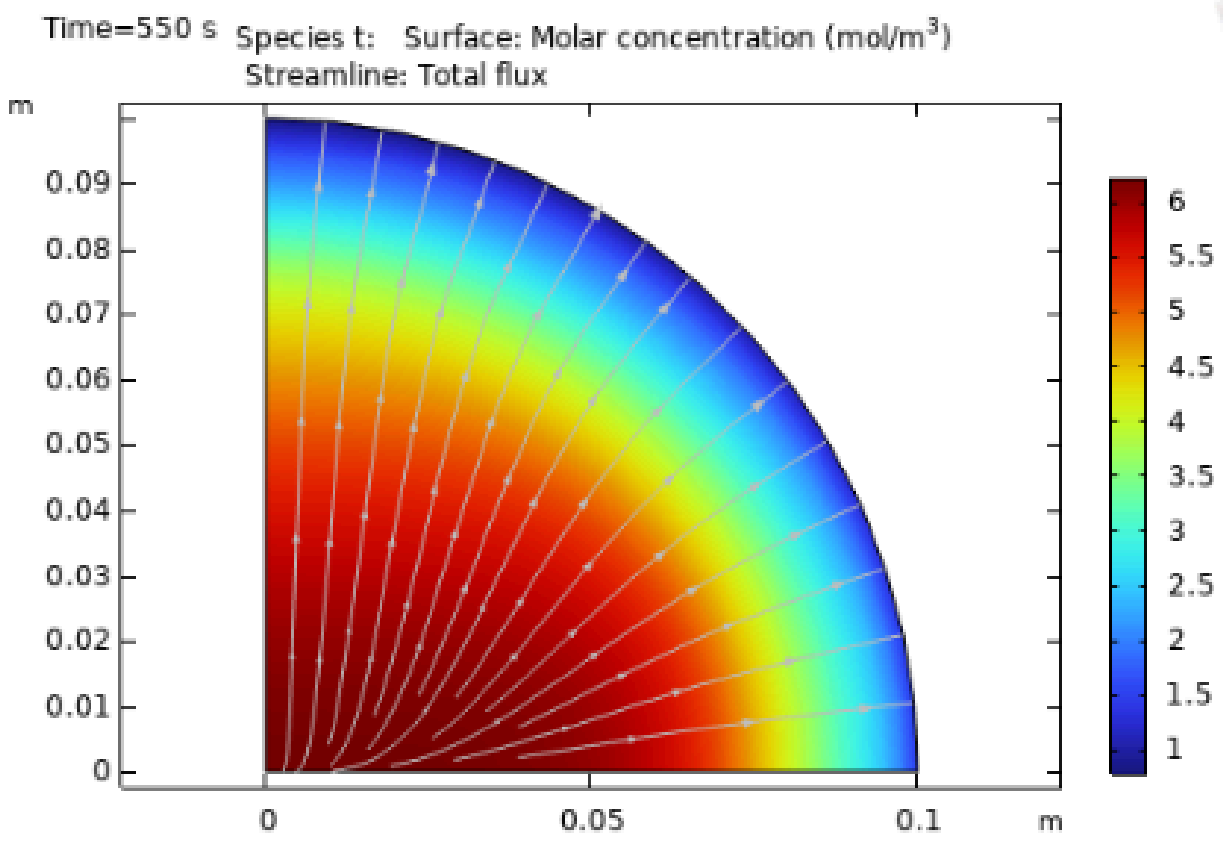
Wood Density Profile



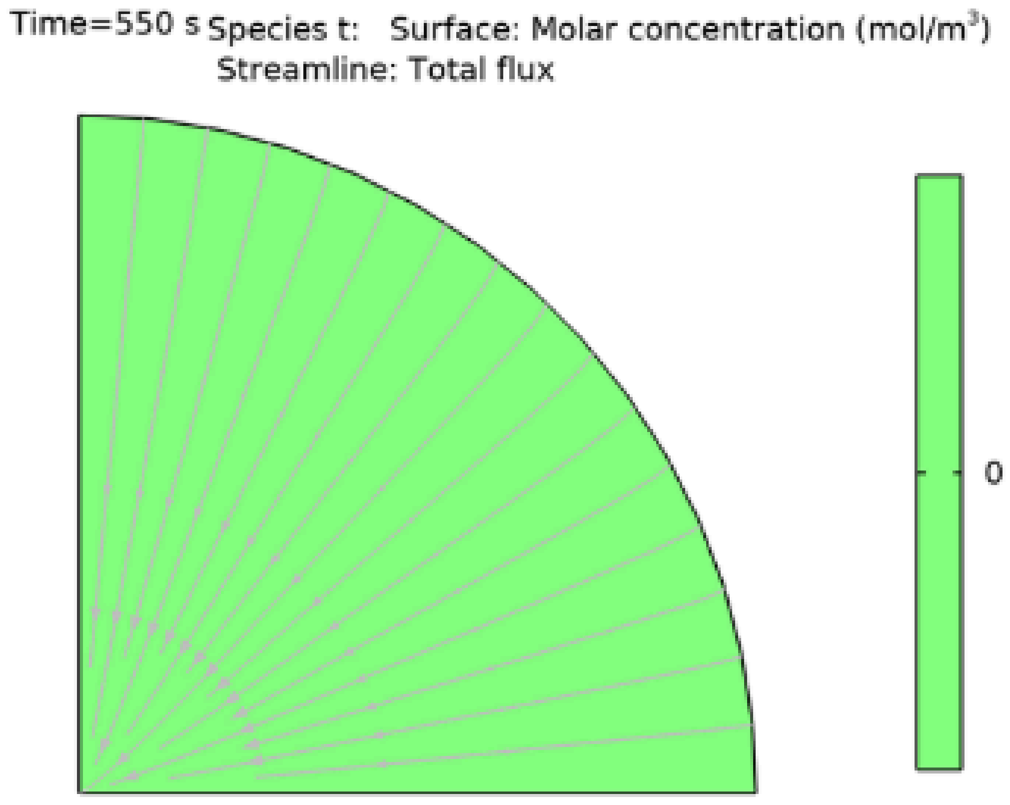
- In the base model, significant amounts of unreacted wood remain, especially in the core.
- In the optimized model, more uniform decomposition is observed, with a thinner unreacted core

RESULTS

Tar Concentration Profile



Base Case

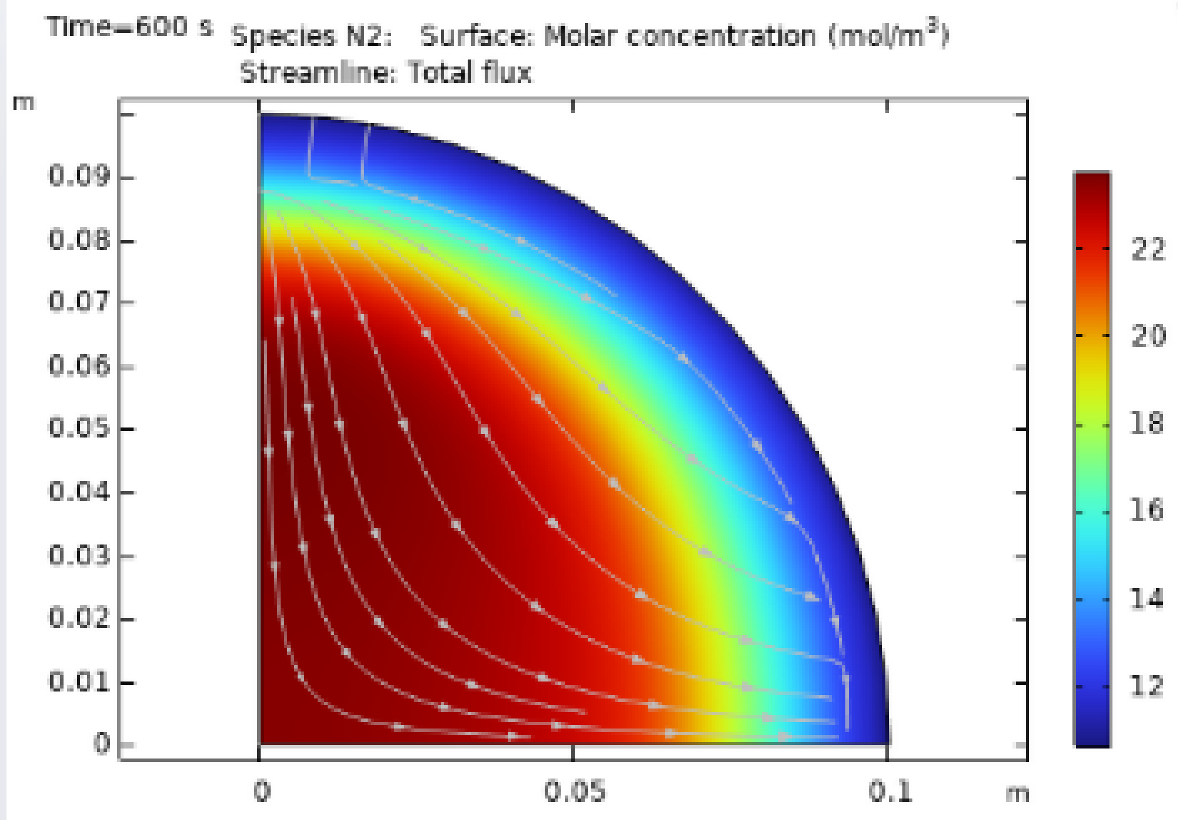


optimised

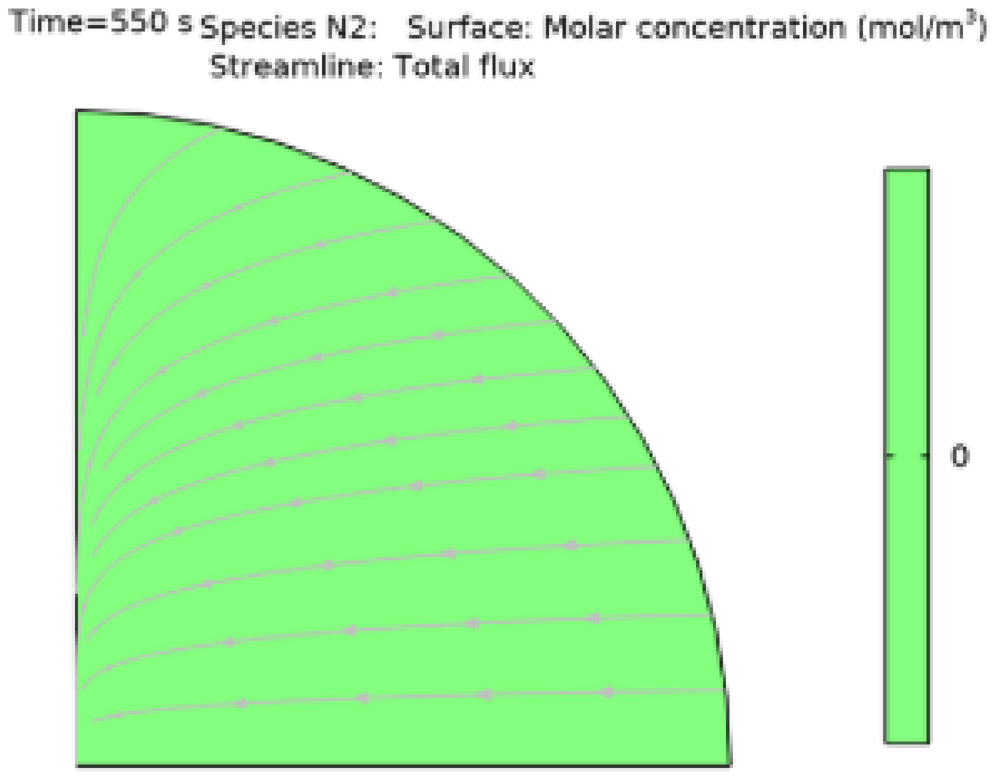
- **Higher tar accumulation near the surface in the base model, due to slow transport and insufficient reaction rates.**
- **In the optimized model, tar is more evenly spread and removed more efficiently via gas flow.**

RESULTS

Nitrogen Concentration Profile



Base Case



optimised

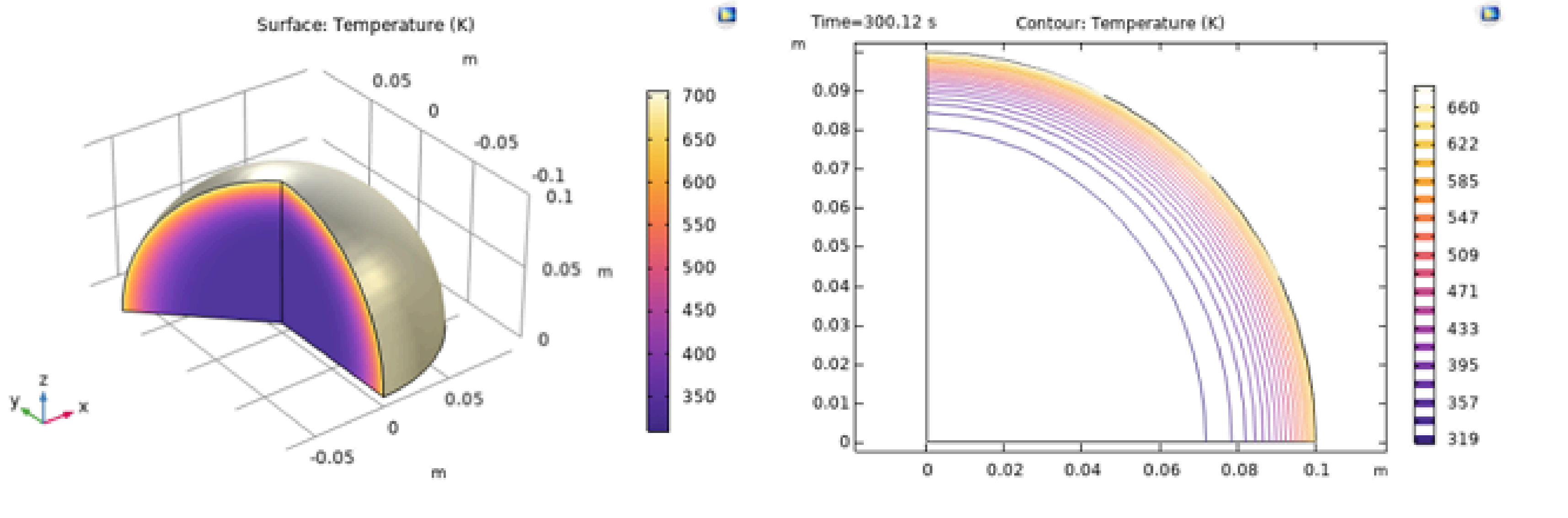
- In the base model, limited nitrogen flux indicates slow convection.
- In the optimized model, nitrogen is better distributed, reflecting enhanced Darcy flow.

RESULTS

Temperature Profile

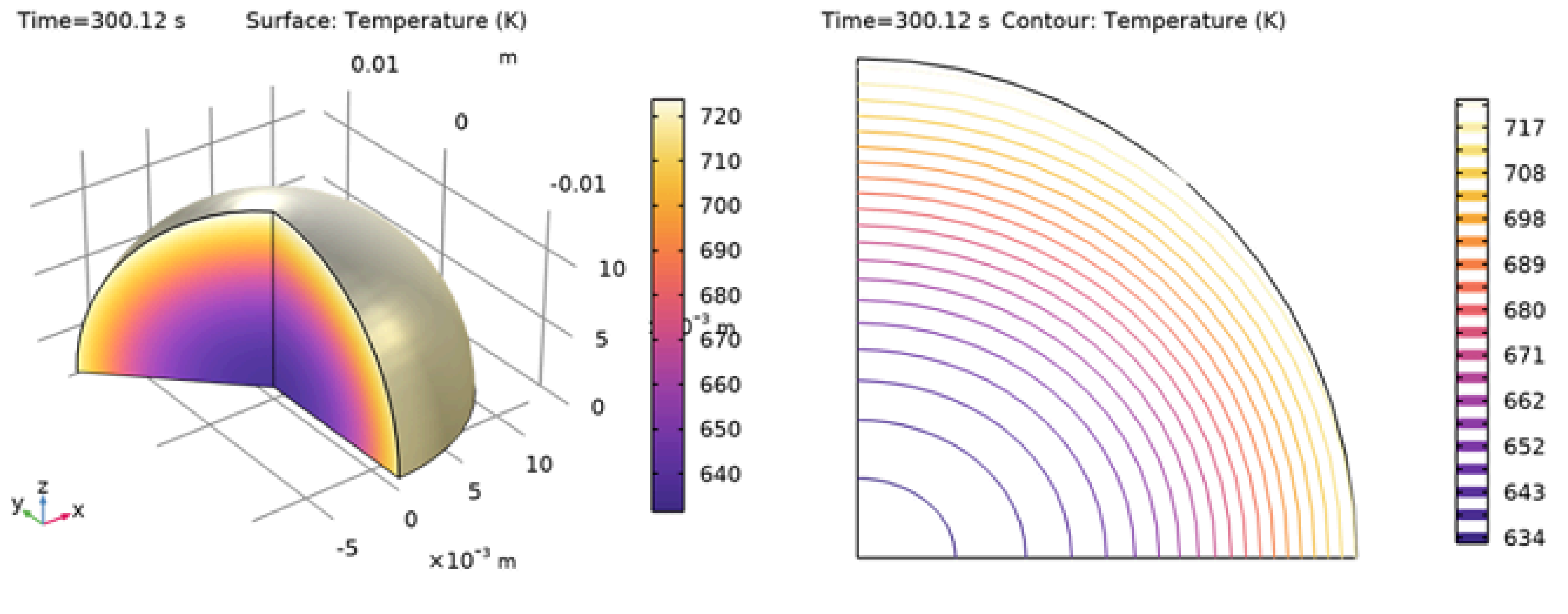
- In the base model, steep temperature gradients exist; the center remains cooler for a long time.

- The optimized model achieves faster, more uniform heating, with higher core temperatures by 600 seconds



Temperature *isothermal contours*

Base Case

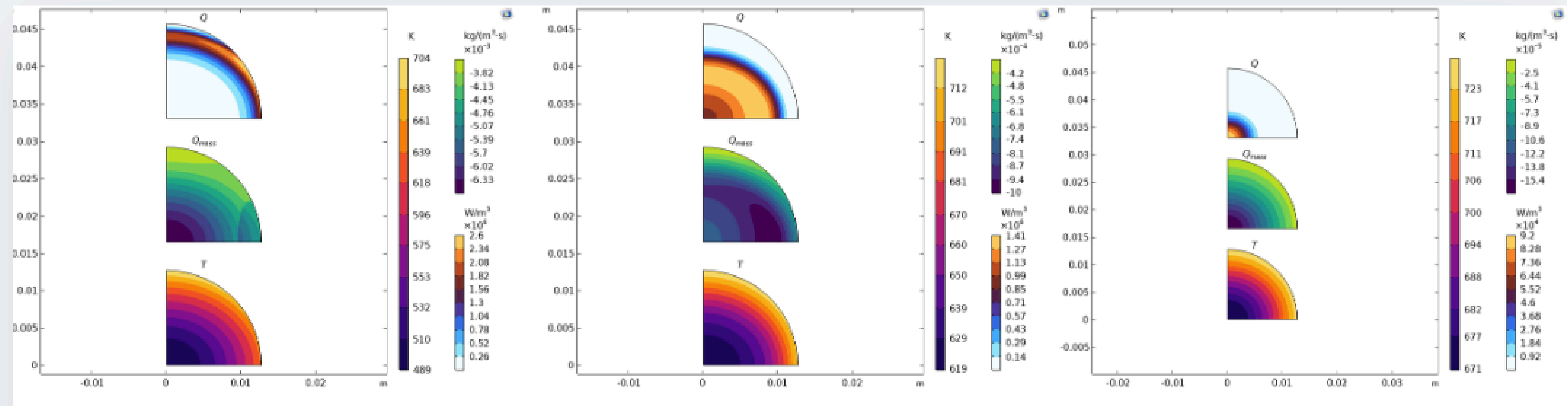


Temperature *isothermal contours*

optimised

RESULTS

Spatial Distributions of Temperature (T), Mass Source (Qmass), and Heat Source (Q) at Different Times



T, Qmass and Q at 150 s

T, Qmass and Q at 270 s

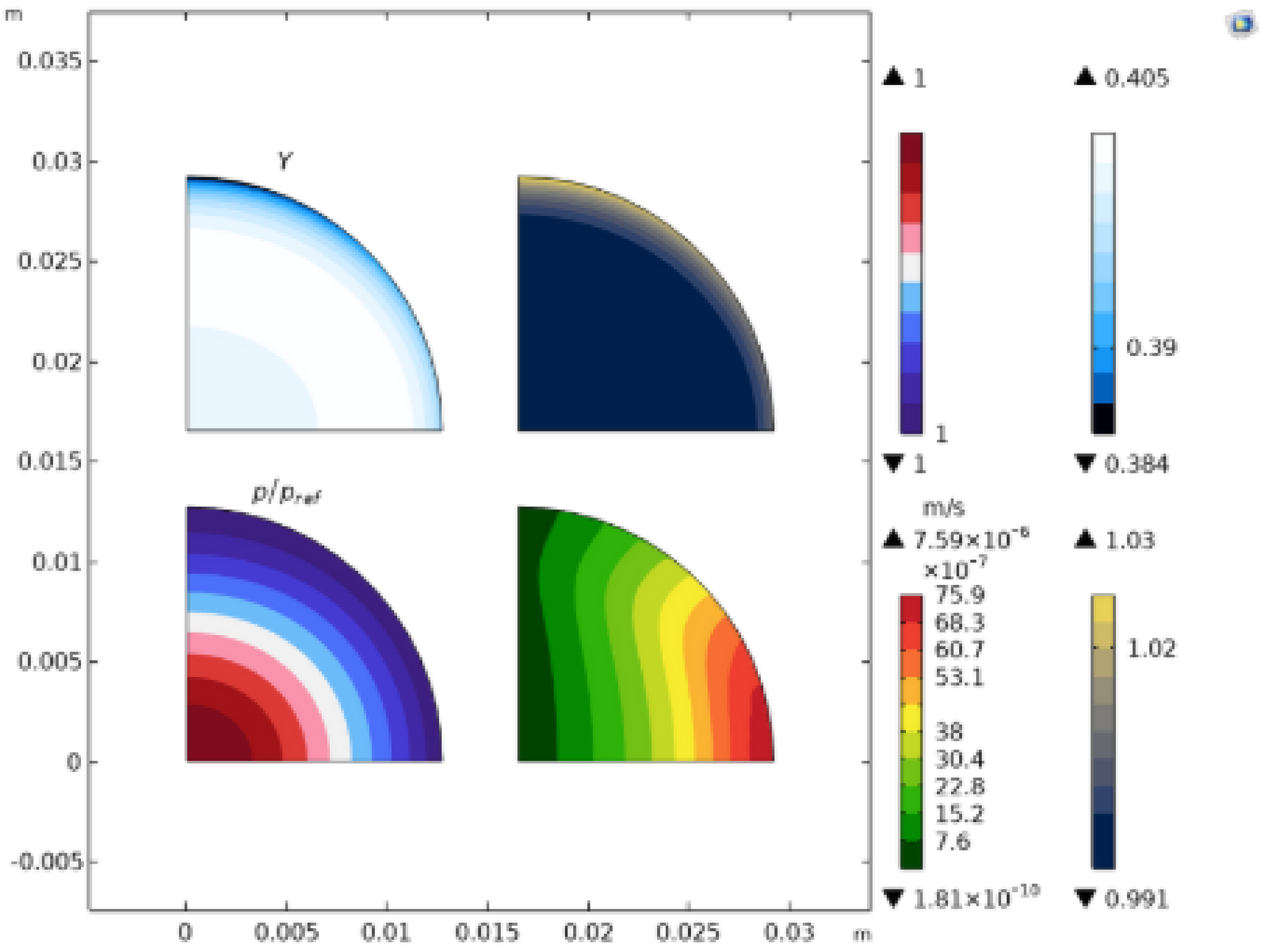
T, Qmass and Q at 433 s

At 150 s:- High endothermic heat sink (Q < 0) near the sur face; mass generation (Qmass > 0) is concentrated at the surface; temperature gradients are steep.- At 270 s:- The heat source (Q) becomes less negative, indicating decreasing endothermicity; mass generation shifts deeper.- At 433 s:- Q becomes slightly positive (exothermic char formation), and the temperature f ield becomes more uniform across the particle.

RESULTS

Pressure, Velocity, Porosity, and Normalized Solid Mass at 270 Secs

Pressure field: Smooth gradient indicating outward gas flow.
Velocity field: Strong radial flow showing efficient volatile transport.
Porosity field: Porosity near the surface increases due to decomposition.
Normalized Solid Mass (Y): Mass loss progresses from the surface inward.



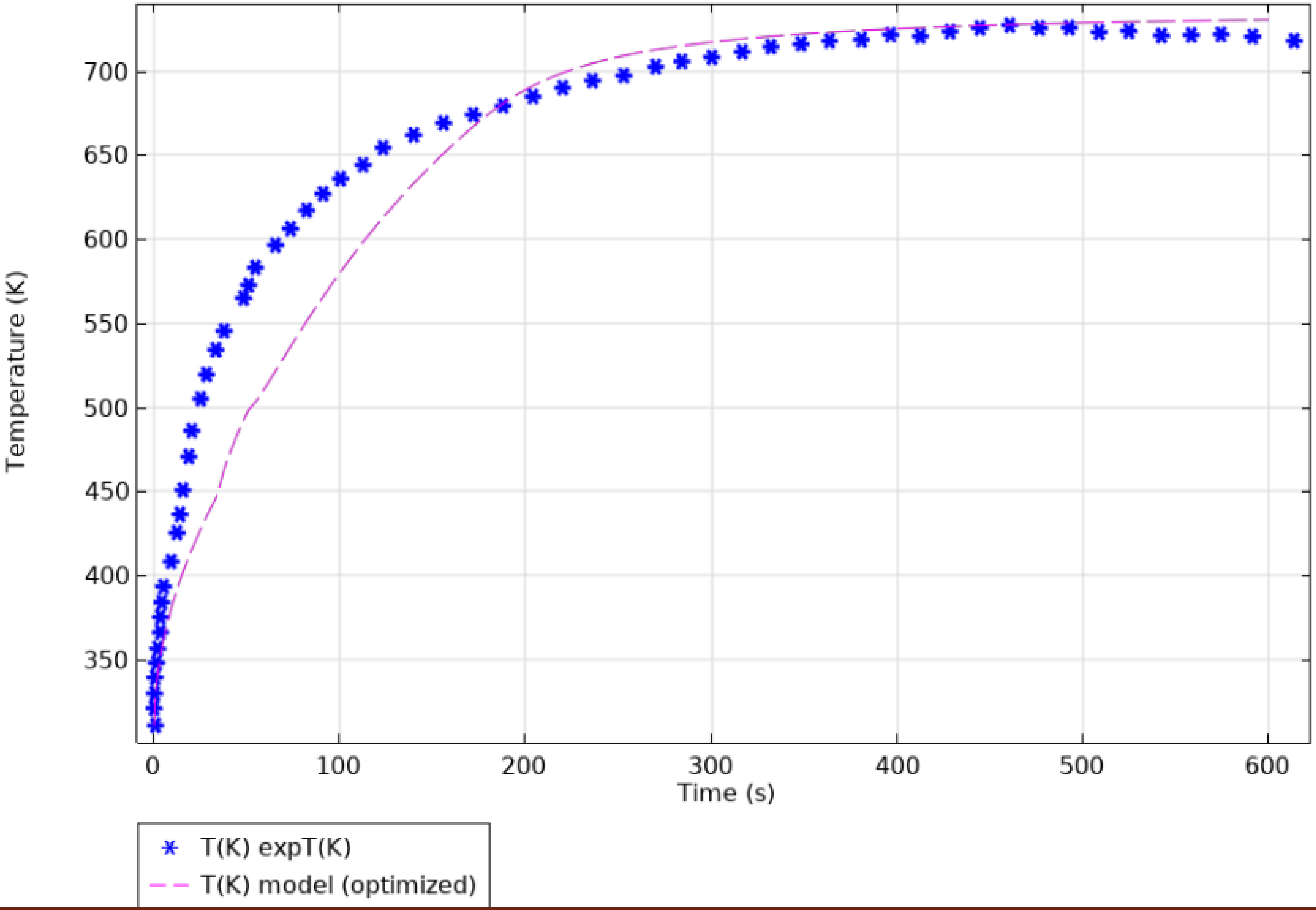
Pressure, velocity, porosity, and normalized solid mass at 270 s

RESULTS

Model vs Experimental Data for Surface Temperature

- In the base model, steep temperature gradients exist; the center remains cooler for a long time.

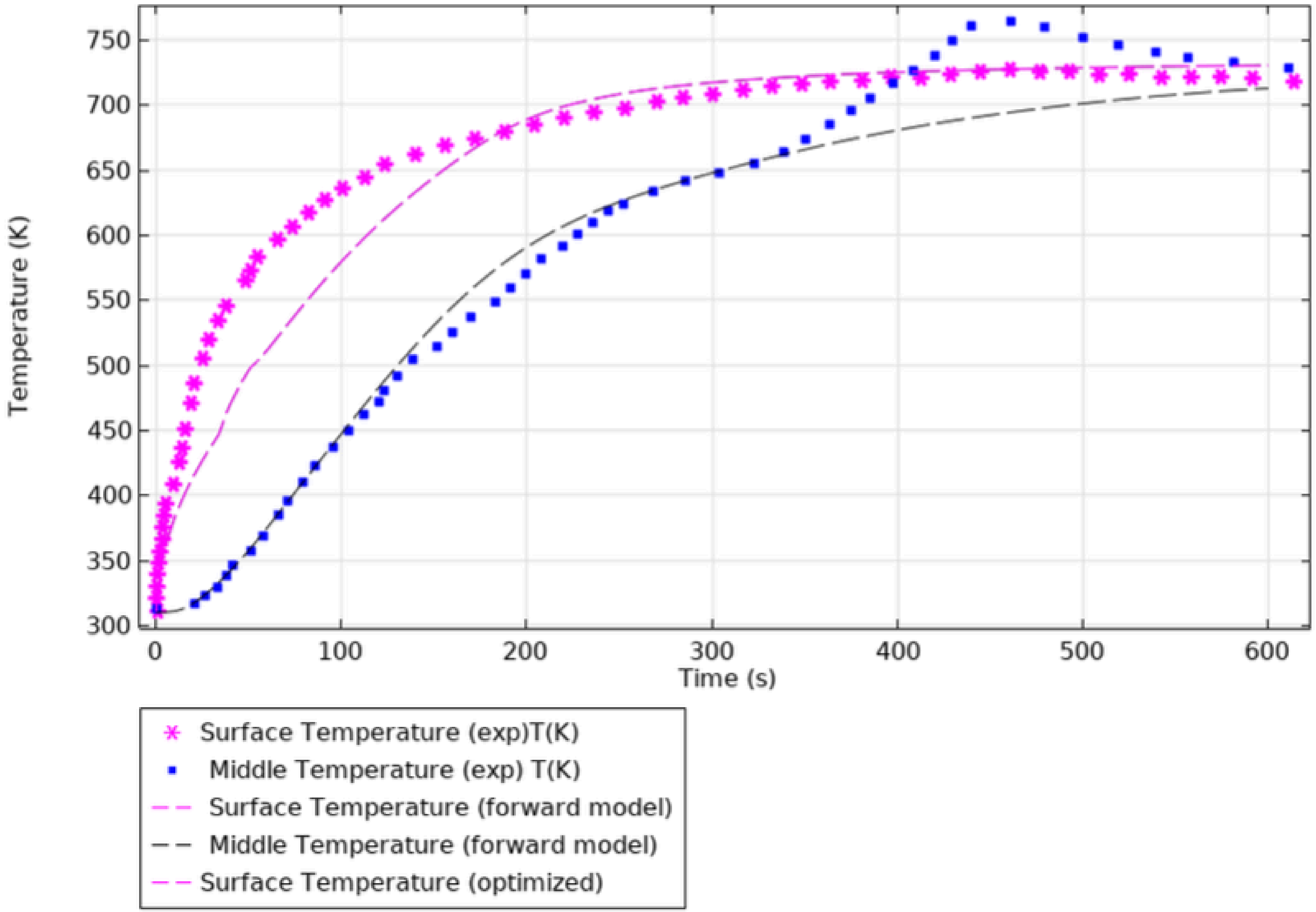
- The optimized model achieves faster, more uniform heating, with higher core temperatures by 600 seconds



RESULTS

COMPARISON OF SURFACE AND MIDDLE TEMPERATURES FOR FORWARD AND OPTIMIZED MODELS

In the forward model (dashed lines), surface and center temper atures rise too slowly and stay under experimental measurements. In the optimized model (solid lines with markers), surface temperature reaches 720 K, matching experiment; center temperature reaches 650 K by 600 seconds.



RESULT

COMPARISON OF INITIAL AND OPTIMIZED PARAMETERS

Parameters	Initial Guess	Optimized Value
Arrhenius pre-exponential factor, A_{is} [1/s]	1.0×10^7	2.0×10^7
Heat of reaction (wood → tar), ΔH_t [J/kg]	-2.0×10^5	-1.0×10^5
Heat of reaction (inter. solid → char), ΔH_c [J/kg]	$+5.0 \times 10^4$	-1.1×10^5
External conv. heat-transfer coeff., h_{conv} [W/m2K]	5.0	5.005

CONCLUSION

- **Parametric studies revealed critical insights:**

1. Decreasing the size of the particle rapidly increased porosity process.
2. Increasing porosity improved heat penetration, volatile transport, and pyrolysis uniformity.
3. Lower activation energies accelerated decomposition, while higher activation energies slowed it.
4. Raising the ambient temperature enhanced the rate of heating, volatile release, and mass loss.

- **Model calibration (parameter estimation) significantly enhanced accuracy:**

5. Optimized reaction kinetics and heat transfer parameters led to excellent agreement with experimental mass loss and temperature profiles.
6. Initial models underpredicted decomposition and temperature rise; optimization corrected these discrepancies.

THANK YOU