Application Models: TRISO Particle Production

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Presentation Outline

An Introduction to TRISO Particles

Application Model Objective

- Barracuda Virtual Reactor solution
- Value of solution

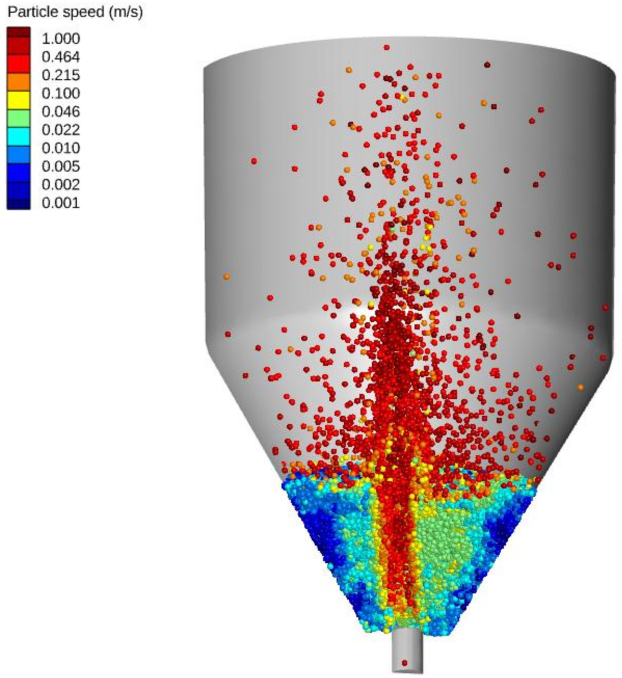
Modeling TRISO Particle Production in a Spouted Bed Reactor

- Model definition / key features
- Key results and conclusions

TRI-structrural ISOtropic (TRISO) Particles

What are TRISO Particles?

- The most robust nuclear fuel in existence, and the fuel choice for advanced 4th-gen nuclear reactors.
- TRISO particles consist of a central core of Uranium fuel, and 3 surrounding layers of deposited carbon and silicon carbide.
- Layers are deposited on the central core via pyrolysis of hydrocarbons and MTS.



Advantages of TRISO particles over traditional fuels?

- Each fuel kernel is self containing, ensuring fission products are sealed even in worst case accident scenarios.
- Micro-containment vs Macro-containment
- TRISO particles are meltdown-proof, allowing for usage in next-gen HTGR's and microreactors.
- Higher burn-up than traditional fuels.

Application Model Objective

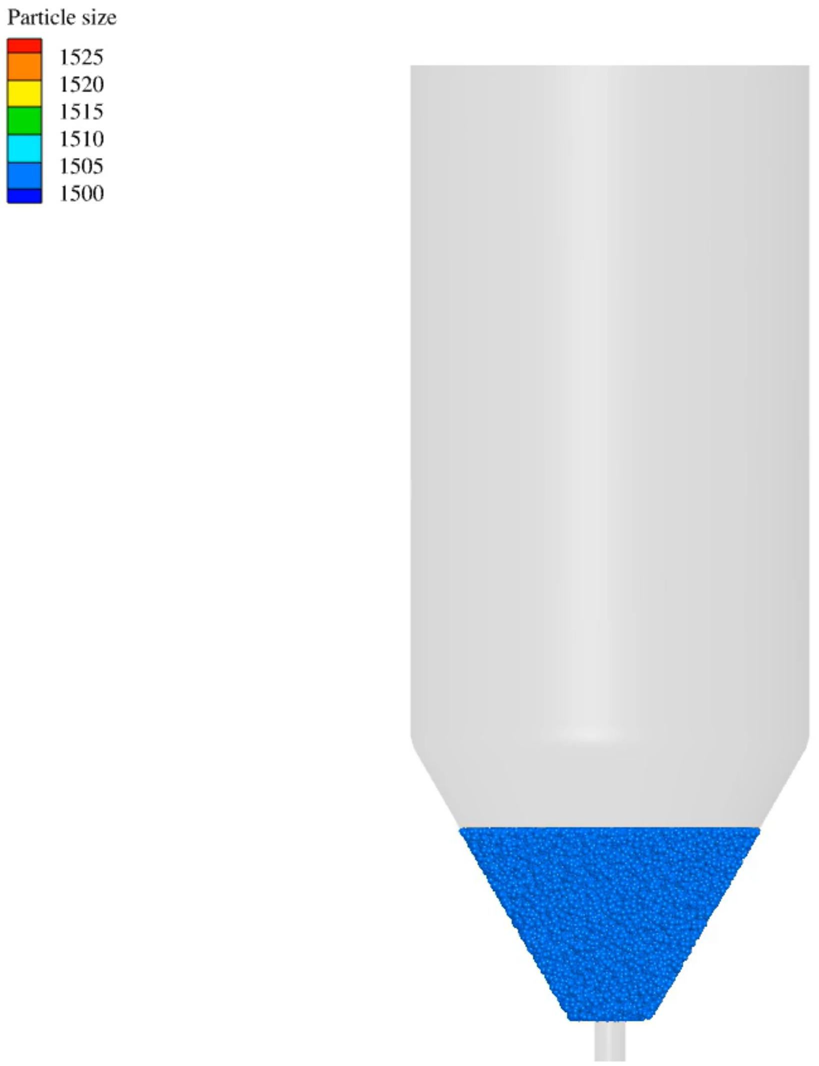
Model the production of TRISO particles in a lab scale spouted bed reactor, targeting growth rates consistent with experimental findings.

Barracuda Virtual Reactor Solution:

- MP-PIC framework applied to multiphase, compressible fluid domain.
- Accurate modeling of discrete and homogeneous reactions for hydrocarbon pyrolysis and solids deposition.
- Detailed understanding of 3D flow fields, local species concentrations, temperature, and particle growth dynamics.

Value of Simulation

- Simulation provides insight into key metrics like PSD evolution, layer thickness, and entrainment, and identifies potential root causes.
- Provides a full fidelity picture of hydrodynamics and chemical reactions at high temperatures, which are difficult understand in lab settings.
- The effects of changing operating conditions and particle loading can be explored from lab, to pilot, and industrial scale



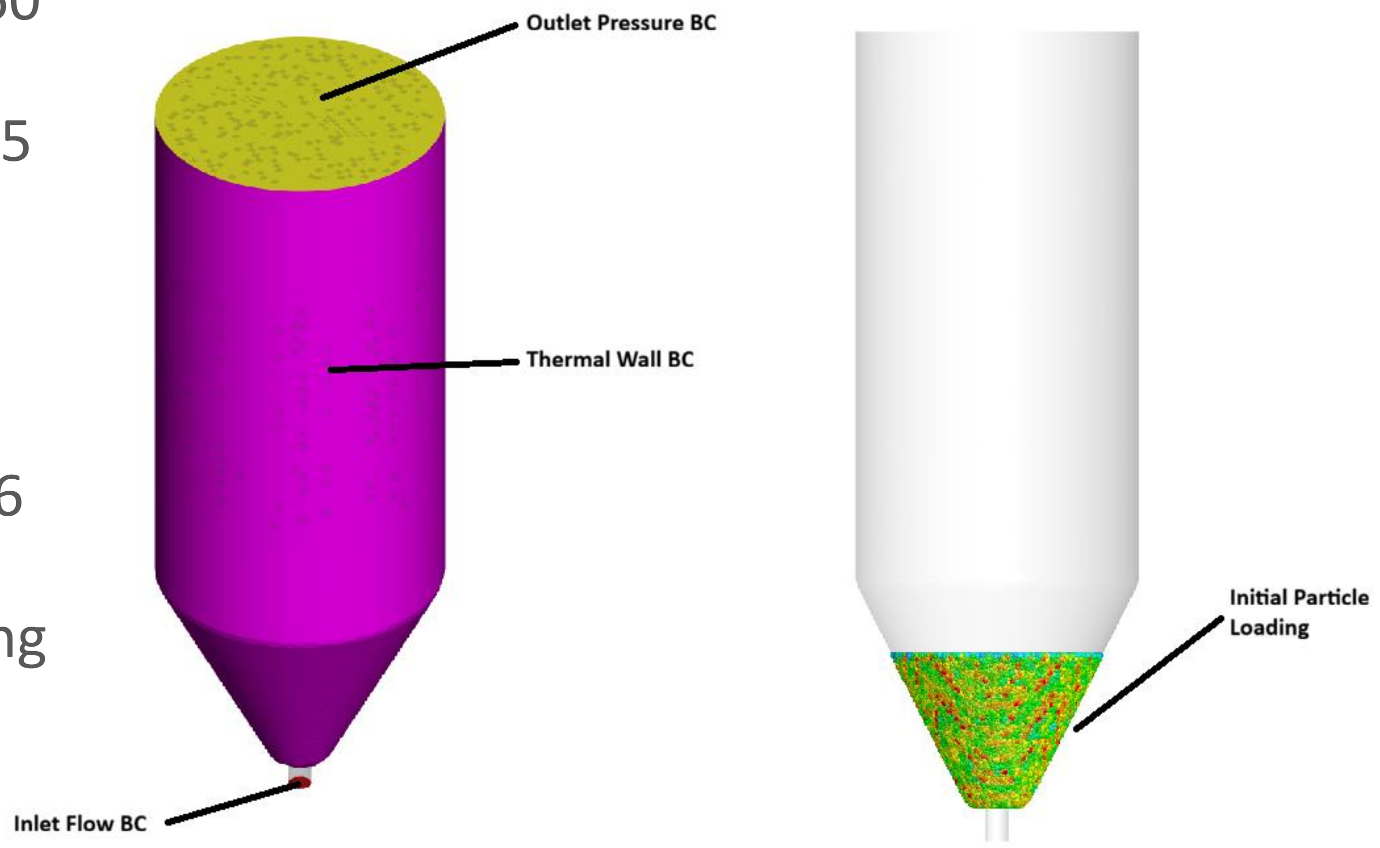
Spouted Bed Reactor Model

Model Domain

- Lab-scale geometry taken from **Liu 2024.**
- 250 mm in height, 100 mm in top diameter, 60° cone angle, and an 8 mm nozzle diameter.
- Initial inventory of 0.35 kg UO_2 particles w/1.5 mm diameter.

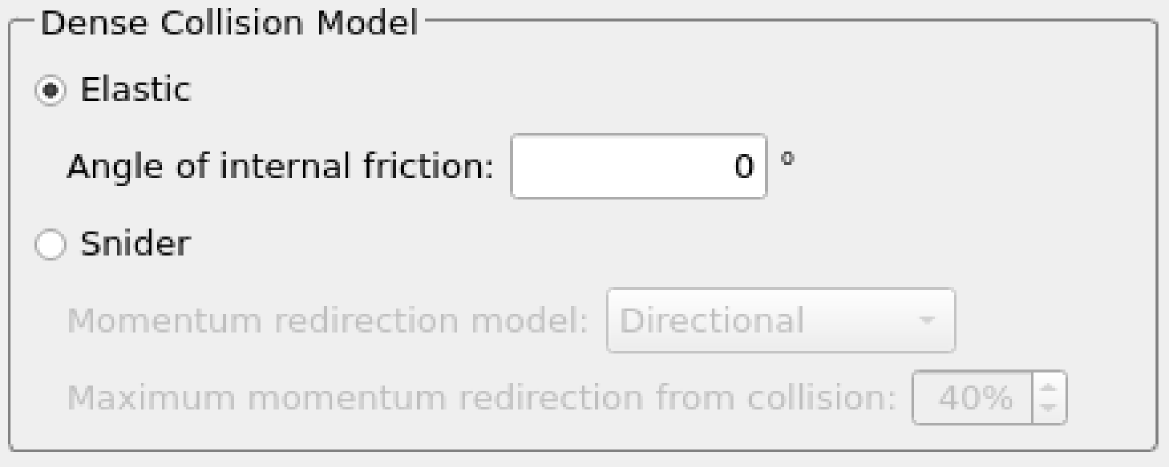
Boundary Conditions and Settings

- Reaction conditions taken from **Chen 2021**.
- An 80/20 argon-acetylene mixture is fed at 26 m/s from the inlet flow BC.
- A wall temperature of 1273 K is specified using a thermal wall BC.
- Convective heat transfer and particle-to-particle heat transfer are enabled.
- Elastic Dense Collision Model Enabled.



Dense Collision Model

- Improved modeling of spouting behavior with the Elastic Collision Model.
- The angle of internal friction significantly impacts spouting behavior.
- For TRISO particles, an IF value of 0-10 is recommended.



Dense Collision Model

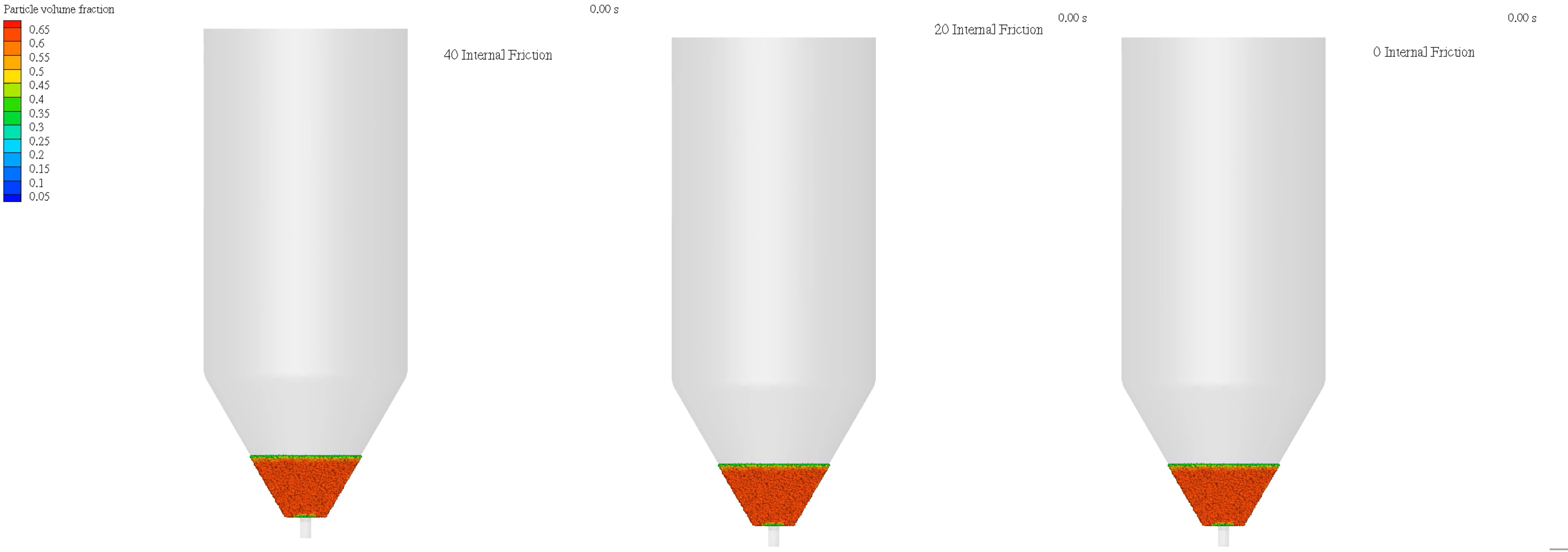
● Elastic

Angle of internal friction: 0 °

○ Snider

Momentum redirection model: Directional

Maximum momentum redirection from collision: 40%



Stage 1: Acetylene Pyrolysis Reaction Kinetics

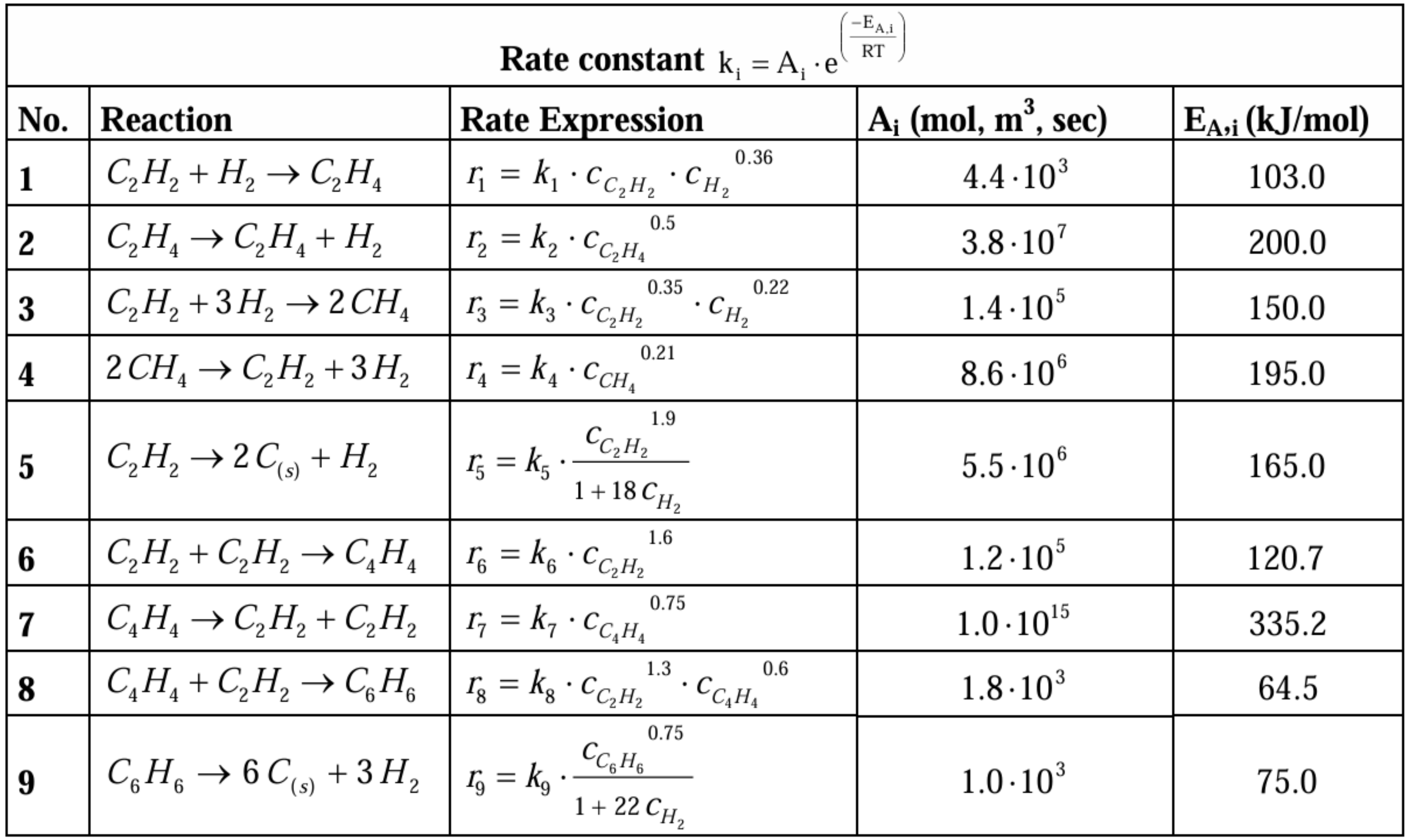


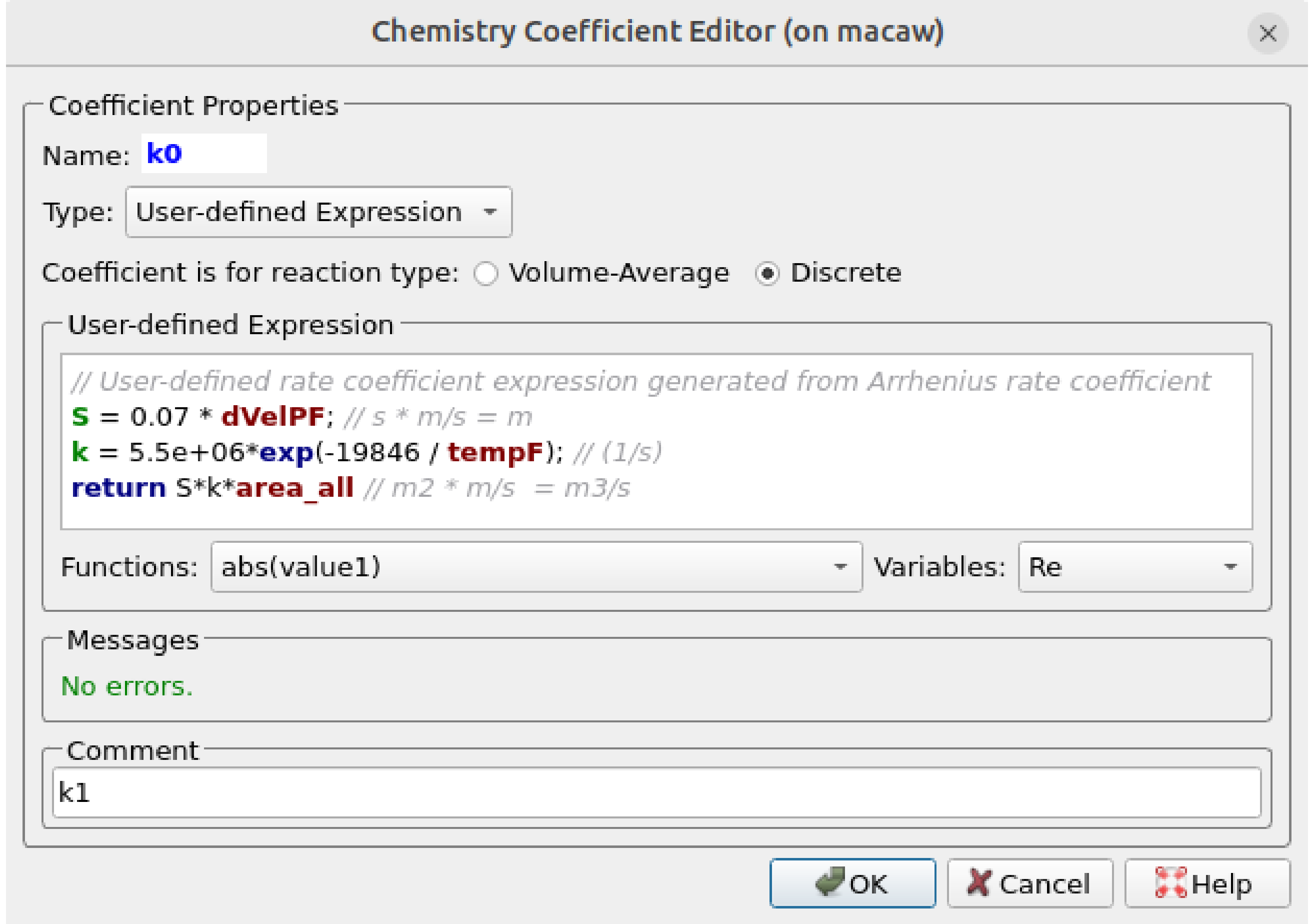
Table 1. Proposed reaction mechanism and kinetic parameters of acetylene pyrolysis.

Rate constant $k_i = A_i \cdot e^{\left(\frac{-E_{A,i}}{RT}\right)}$				
No.	**Reaction**	**Rate Expression**	**A_i (mol, m^3, sec)**	**$E_{A,i}$ (kJ/mol)**
1	$C_2H_2 + H_2 \rightarrow C_2H_4$	$r_1 = k_1 \cdot c_{C_2H_2} \cdot c_{H_2}^{0.36}$	$4.4 \cdot 10^3$	103.0
2	$C_2H_4 \rightarrow C_2H_4 + H_2$	$r_2 = k_2 \cdot c_{C_2H_4}^{0.5}$	$3.8 \cdot 10^7$	200.0
3	$C_2H_2 + 3H_2 \rightarrow 2CH_4$	$r_3 = k_3 \cdot c_{C_2H_2}^{0.35} \cdot c_{H_2}^{0.22}$	$1.4 \cdot 10^5$	150.0
4	$2CH_4 \rightarrow C_2H_2 + 3H_2$	$r_4 = k_4 \cdot c_{CH_4}^{0.21}$	$8.6 \cdot 10^6$	195.0
5	$C_2H_2 \rightarrow 2C_{(s)} + H_2$	$r_5 = k_5 \cdot \frac{c_{C_2H_2}^{1.9}}{1 + 18\,c_{H_2}}$	$5.5 \cdot 10^6$	165.0
6	$C_2H_2 + C_2H_2 \rightarrow C_4H_4$	$r_6 = k_6 \cdot c_{C_2H_2}^{1.6}$	$1.2 \cdot 10^5$	120.7
7	$C_4H_4 \rightarrow C_2H_2 + C_2H_2$	$r_7 = k_7 \cdot c_{C_4H_4}^{0.75}$	$1.0 \cdot 10^{15}$	335.2
8	$C_4H_4 + C_2H_2 \rightarrow C_6H_6$	$r_8 = k_8 \cdot c_{C_2H_2}^{1.3} \cdot c_{C_4H_4}^{0.6}$	$1.8 \cdot 10^3$	64.5
9	$C_6H_6 \rightarrow 6C_{(s)} + 3H_2$	$r_9 = k_9 \cdot \frac{c_{C_6H_6}^{0.75}}{1 + 22\,c_{H_2}}$	$1.0 \cdot 10^3$	75.0

The included kinetic model for the first stage acetylene pyrolysis and deposition is from the work of **Khan 2008**.

User Defined Chemistry

- The rate of deposition is controlled by the scavenging coefficient, “S”.
- Scavenging models soot deposition, accounting for the difference in gas / solids velocity, as well as the surface area of particles.
- With this user defined expression, the rate of deposition can be fine tuned to match those of physical systems.



Chemistry Coefficient Editor (on macaw)

Coefficient Properties

Name: **k0**

Type: User-defined Expression

Coefficient is for reaction type: ○ Volume-Average ● Discrete

User-defined Expression

```
// User-defined rate coefficient expression generated from Arrhenius rate coefficient
S = 0.07 * dVelPF; // s * m/s = m
k = 5.5e+06*exp(-19846 / tempF); // (1/s)
return S*k*area_all // m2 * m/s  = m3/s
```

Functions: abs(value1)

Variables: Re

Messages

No errors.

Comment

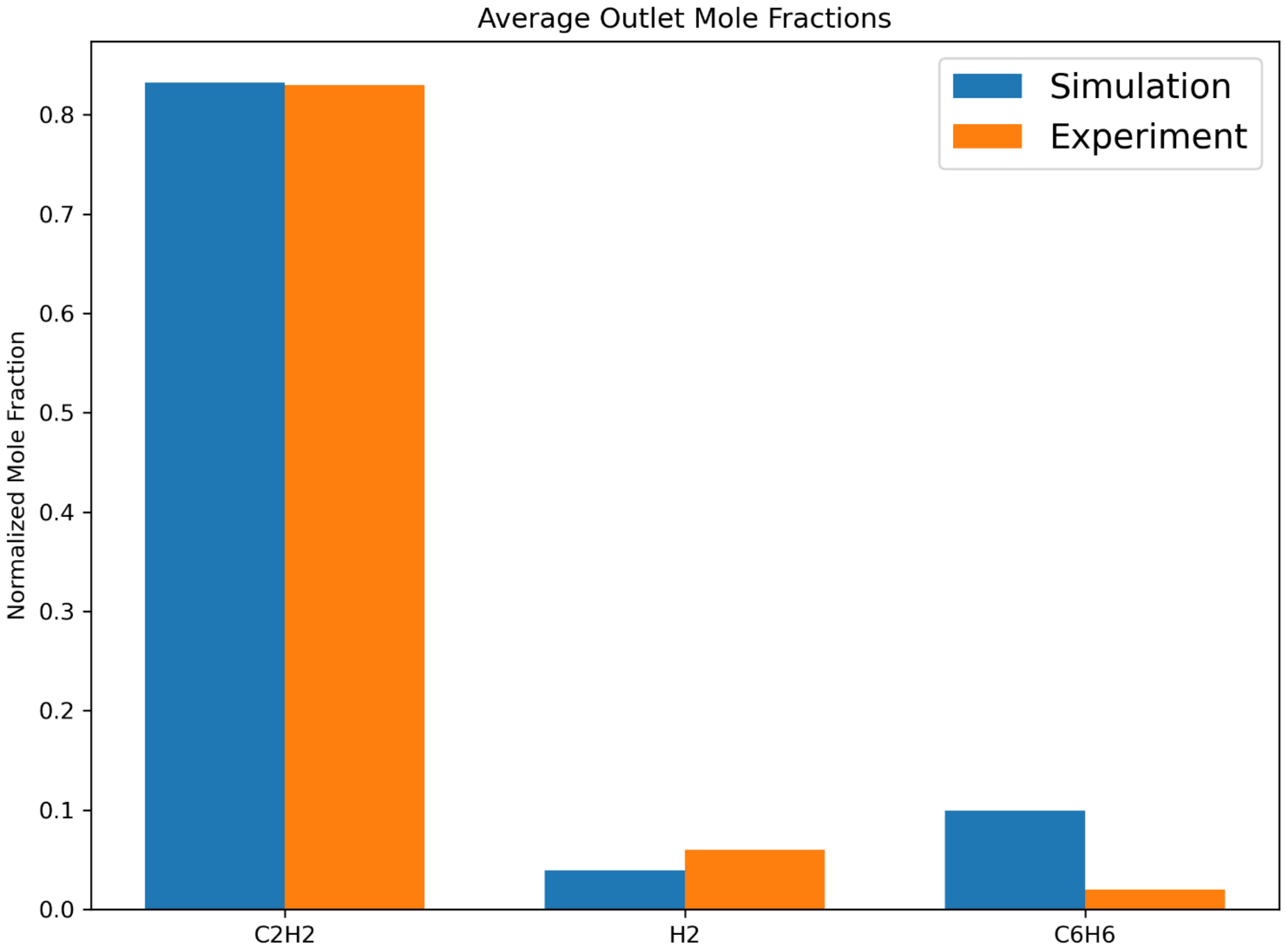
k1

Model Validation

Barracuda Results vs. Experimental Findings

- Barracuda results of outlet gas mole fractions showed good agreement with experimental data at 1273 degrees K.
- Outlet gas compositions matched as a consequence of tuning the deposition rate to match experimental findings.

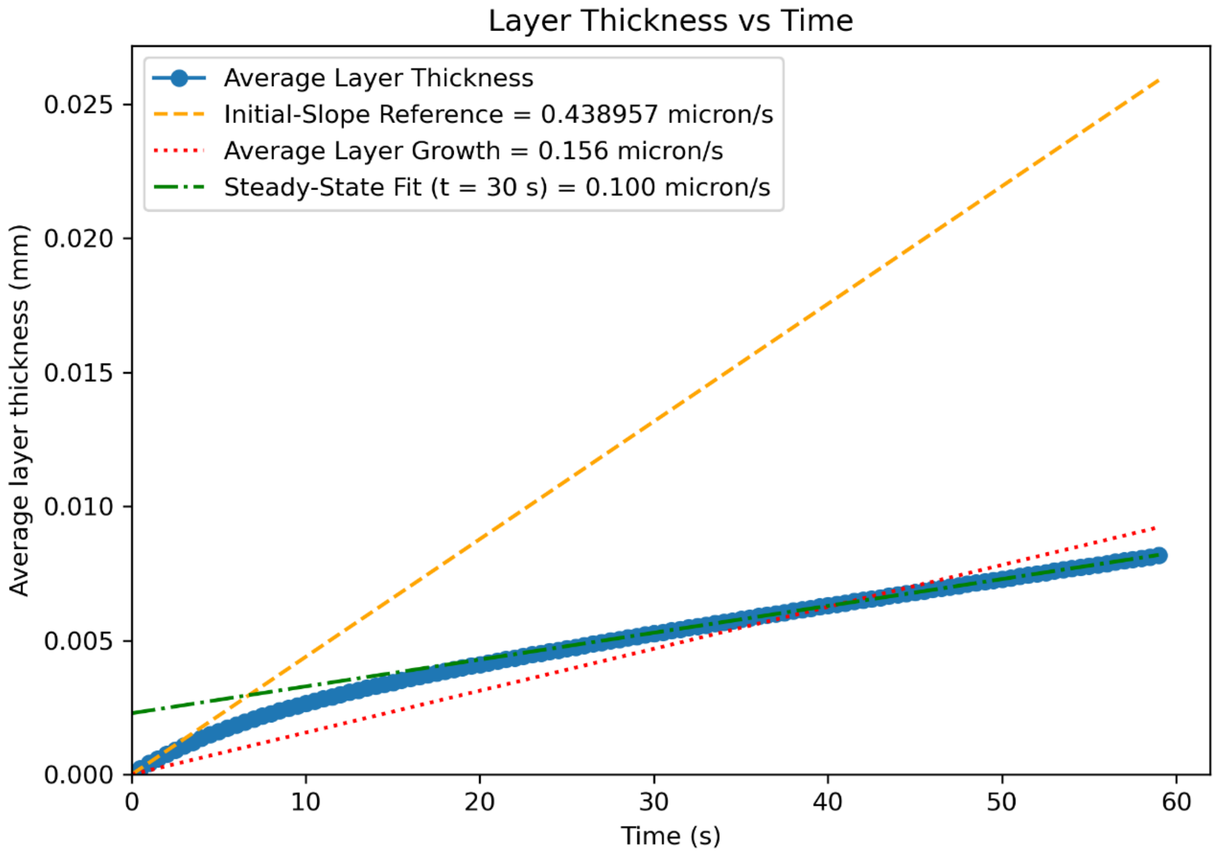
At the reaction temperature of 1273 K, the model results were deemed reasonable to proceed with further analysis of particle growth rate characteristics.

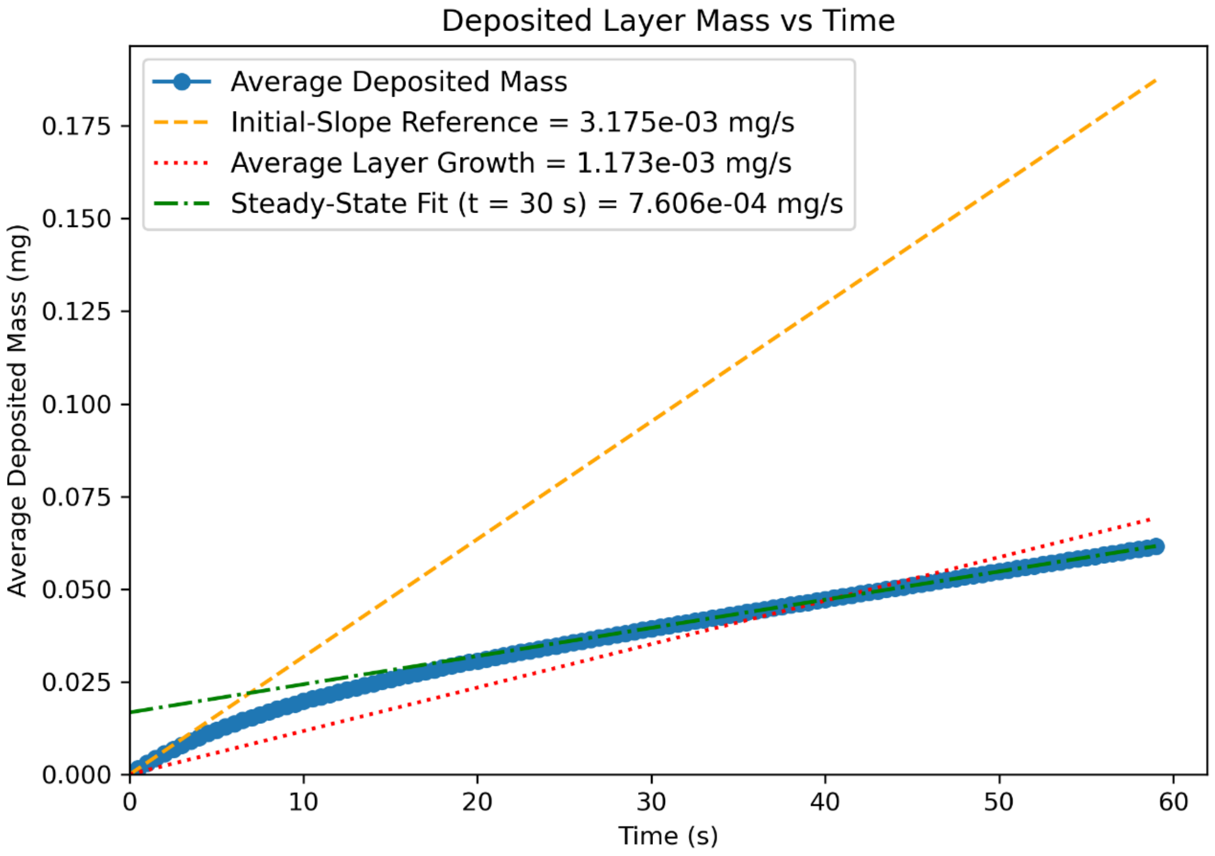


Particle Layer and Mass Growth Rate

Growth Rates

- Steady state growth rates were of the same order of magnitude as the experimental results.
- Inclusion of competing gas phase reactions is necessary to accurately model the transition to steady state deposition.
- Barracuda provides a truly representative view of sustained operation, a unique capability other common modeling approaches do not have due to high computational overhead.

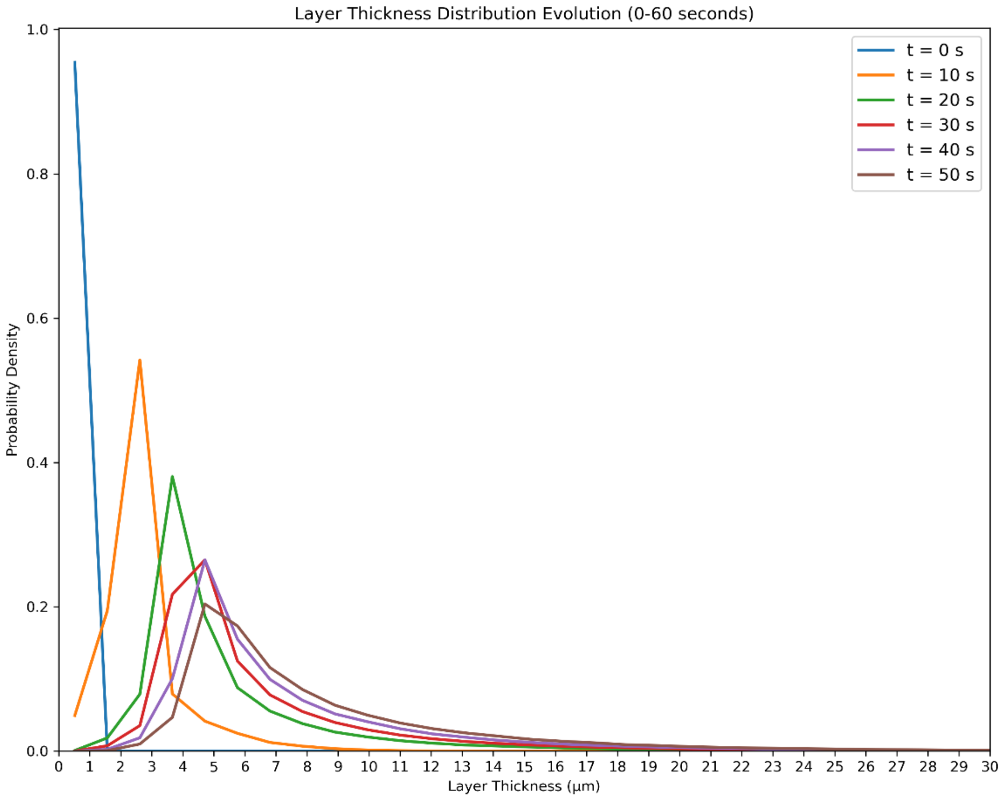


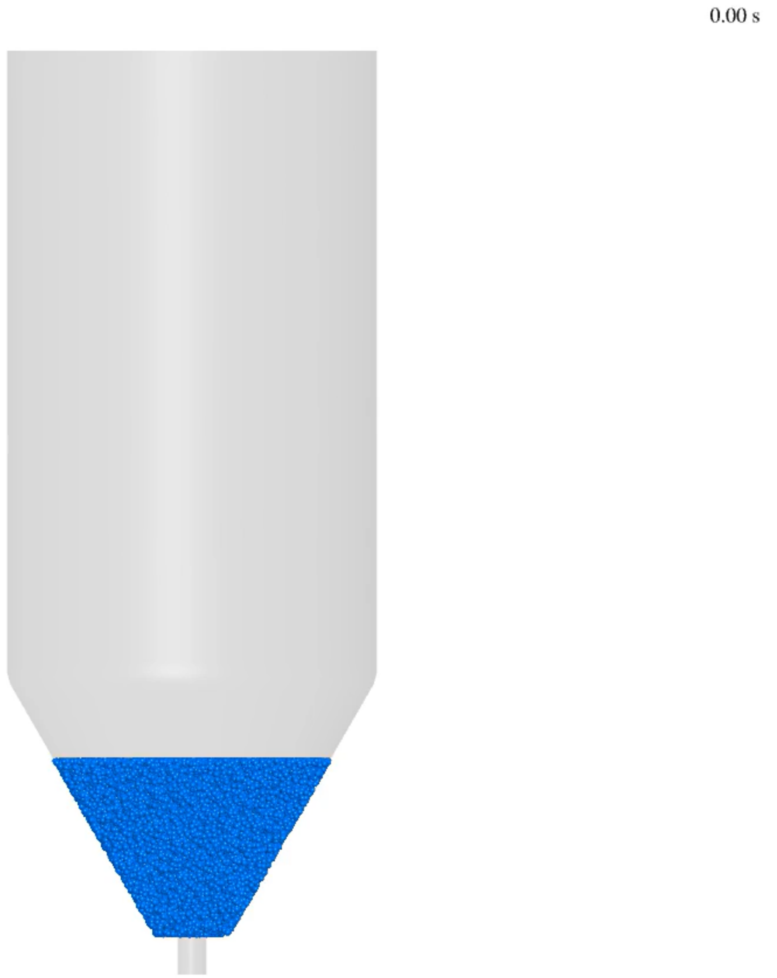


PSD evolution

PSD Growth Characteristics

- Heterogeneity in particle size is seen to develop early in runtime.
- PDF shows incremental shifts of layer thickness distribution, eventually exhibiting a rightward skew.
- Growth rate decreases and maintains consistency past 30 seconds, consistent with growth plots.
- Growth rate is uniform, while particle layer thickness is not.
- CFD use case for optimizing layer thickness uniformity.


Layer Thickness Distribution Evolution (0-60 seconds)



Entrainment

Density Change Over Time

- Density decreases as more carbon is deposited.
- From beginning to end stage in this model, density decreases by 4000 kg/m^3 after just 18 minutes.
- At the same gas velocity, entrainment of "end stage" particles becomes an issue, with 3.6 kg/hr exiting the system.
- Loss of particles is both expensive and problematic due to the radioactive nature of the entrained species.

Barracuda can pinpoint root causes of entrainment and identify ideal conditions to mitigate losses.