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ANALYSIS AND PREDICTION OF SOOT MORPHOLOGY IN POST-DETONATION FIREBALLS

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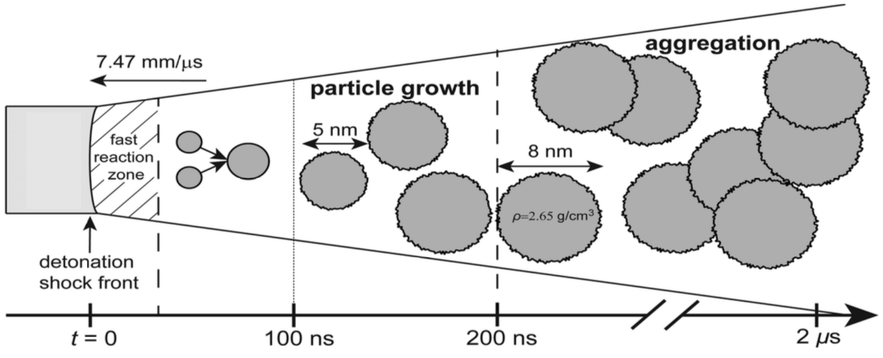
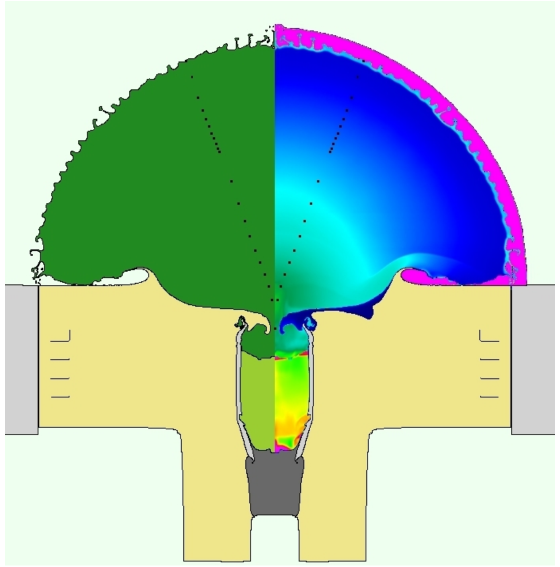
MOTIVATION

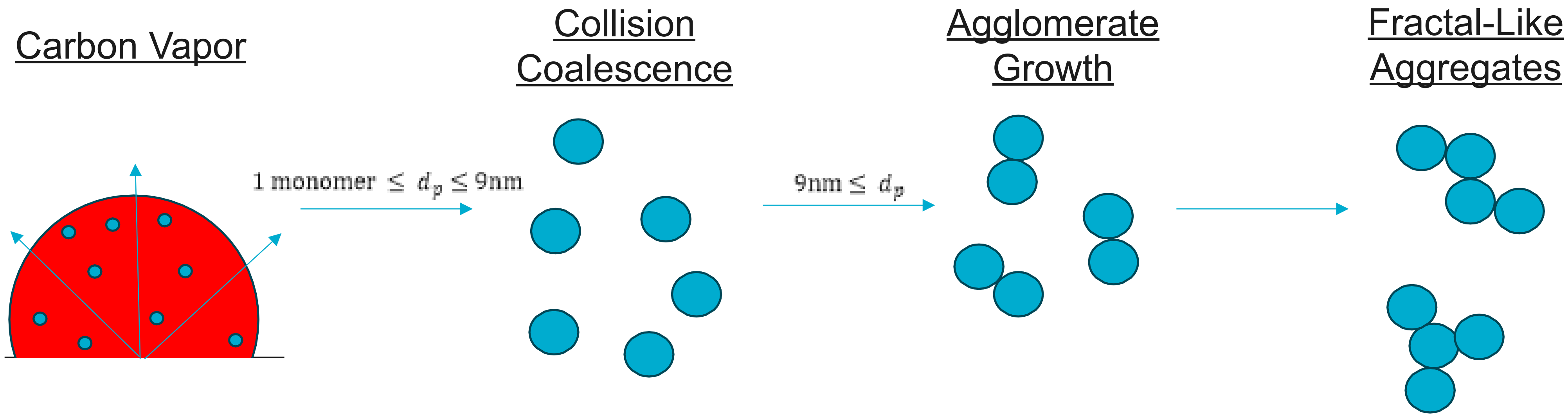
- Interest in improving prediction of light emission and particle production fidelity from simulations of high explosives.
- Uncertainty **<u>in particle size distribution (PSD)</u>** inhibits understanding of light signatures.
  - Where the particles are, and how big they are matters!
- **<u>Particle evolution</u>** in detonations is largely unknown
  - Soot particles have inertia which influences dispersion in a detonation.
  - Performance of the explosive.





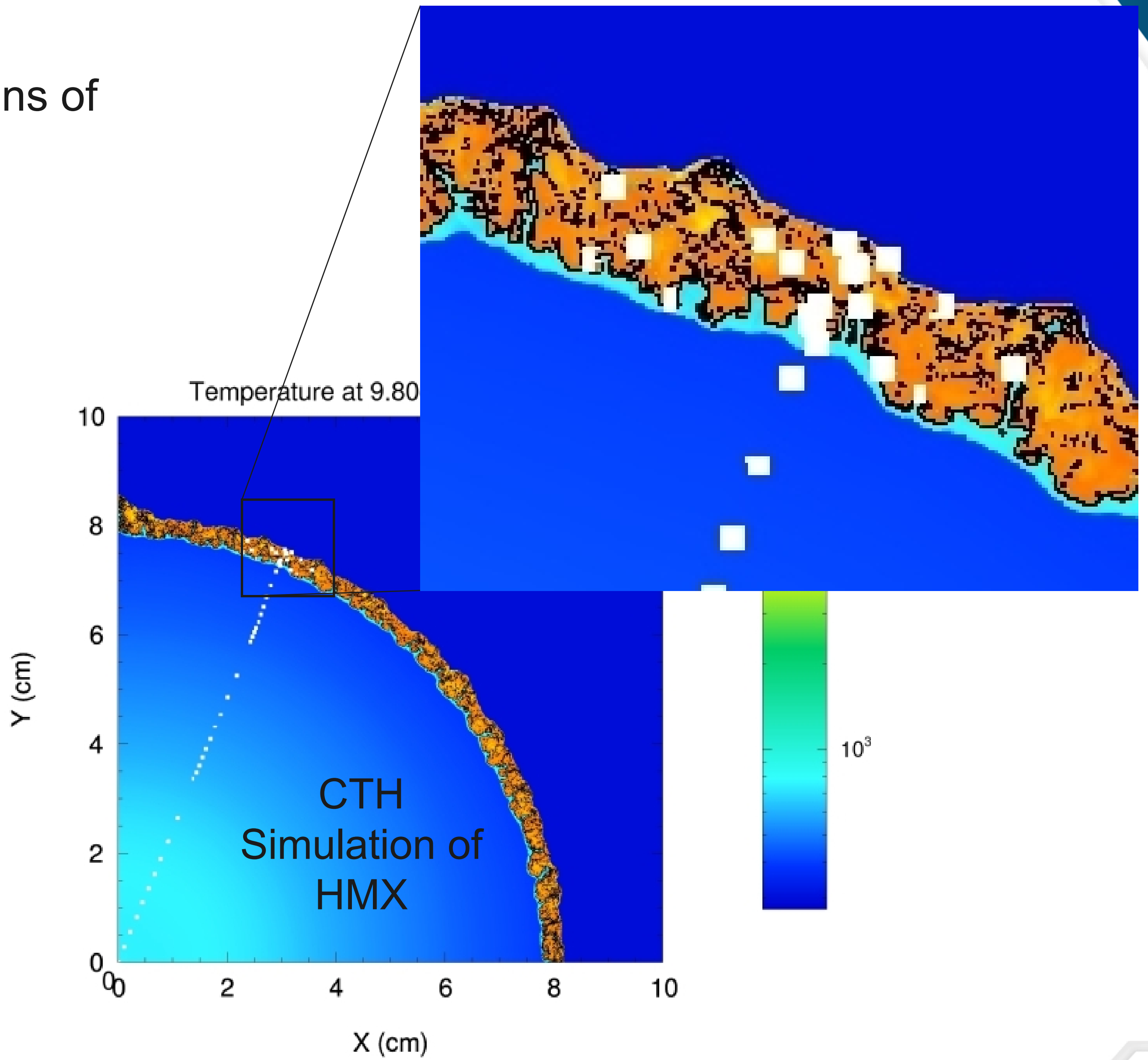
UNDERSTANDING PARTICLE EVOLUTION

- Soot particle evolution is **<u>mainly</u>** governed by:
  - Collision Coalescence
  - Later-time agglomeration
- ANSYS Chemkin Pro can simulate these phenomena!



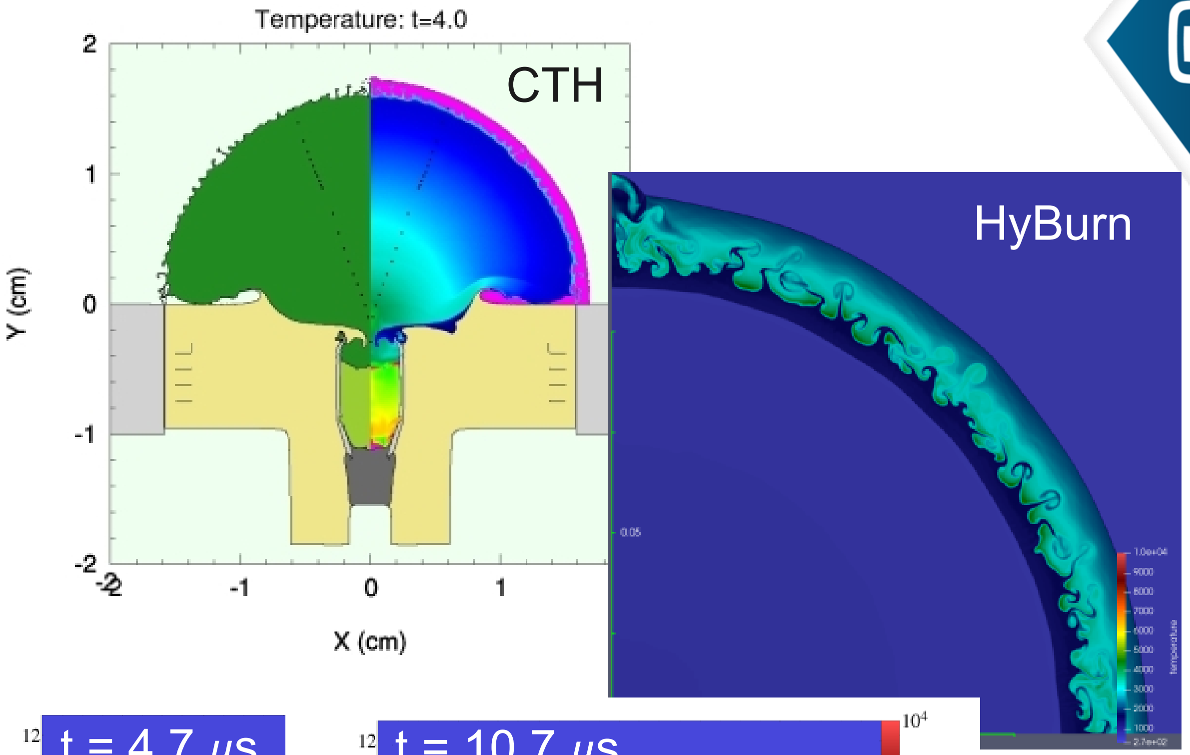
METHODOLOGY

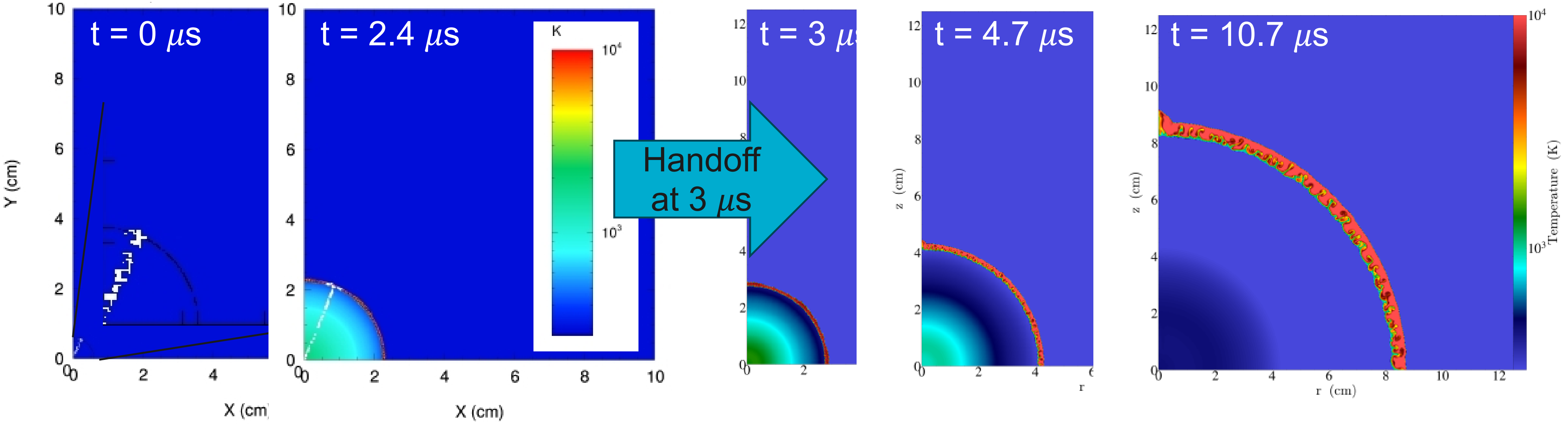
- First, create high-fidelity gasdynamic simulations of explosive detonations.
- Two codes used, CTH and HyBurn.
  - CTH excels at multimaterial modeling.
  - HyBurn excels at turbulent mixing.
- Seeded with Lagrangian tracers.
- HMX, 12mm diameter simplified mini-hemi
  - 90 Pa ambient air pressure



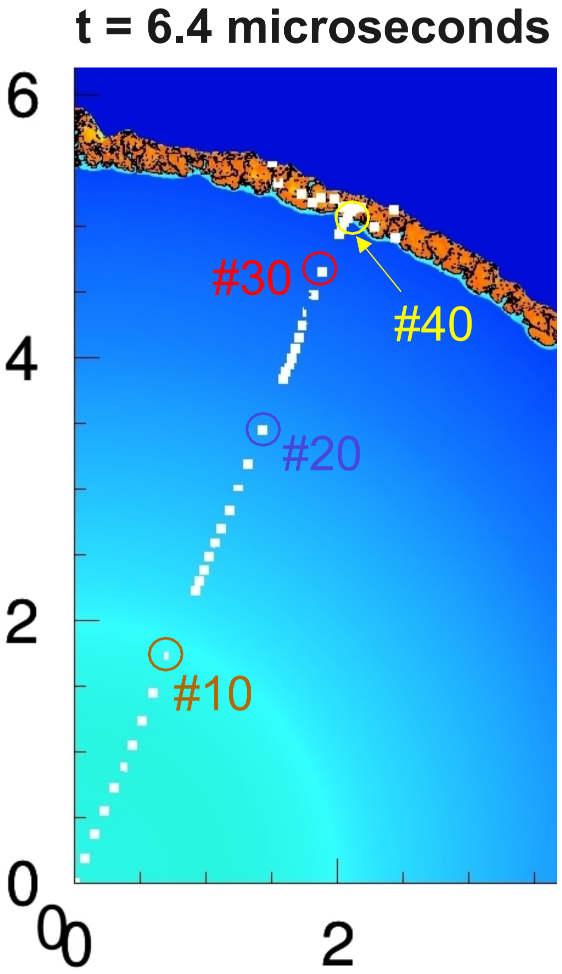
HANDOFF

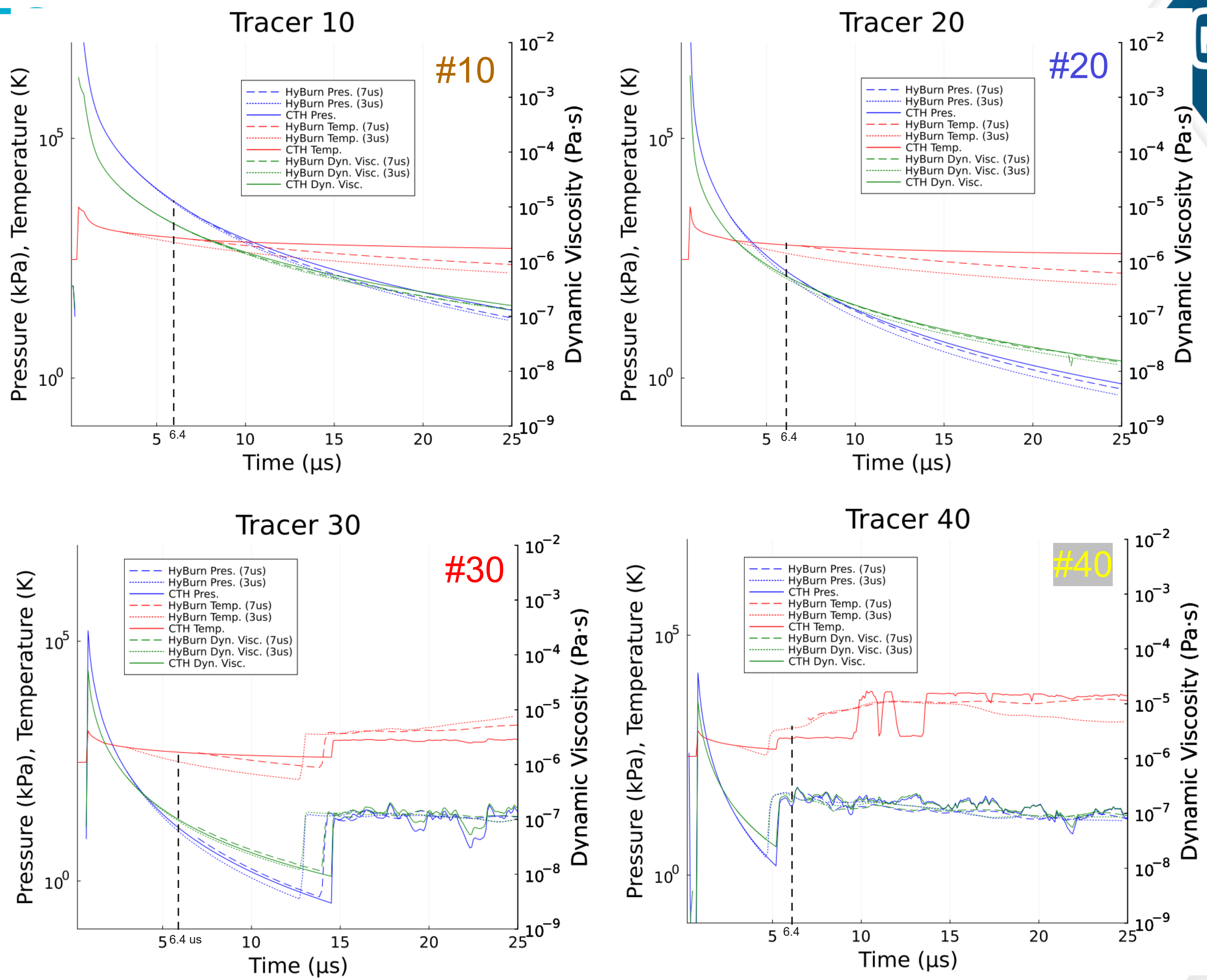
- Handoff CTH to HyBurn to take advantage of the capabilities of both softwares.
- Two handoff-times: 3μs and 7 μs.





TRACER RESULT

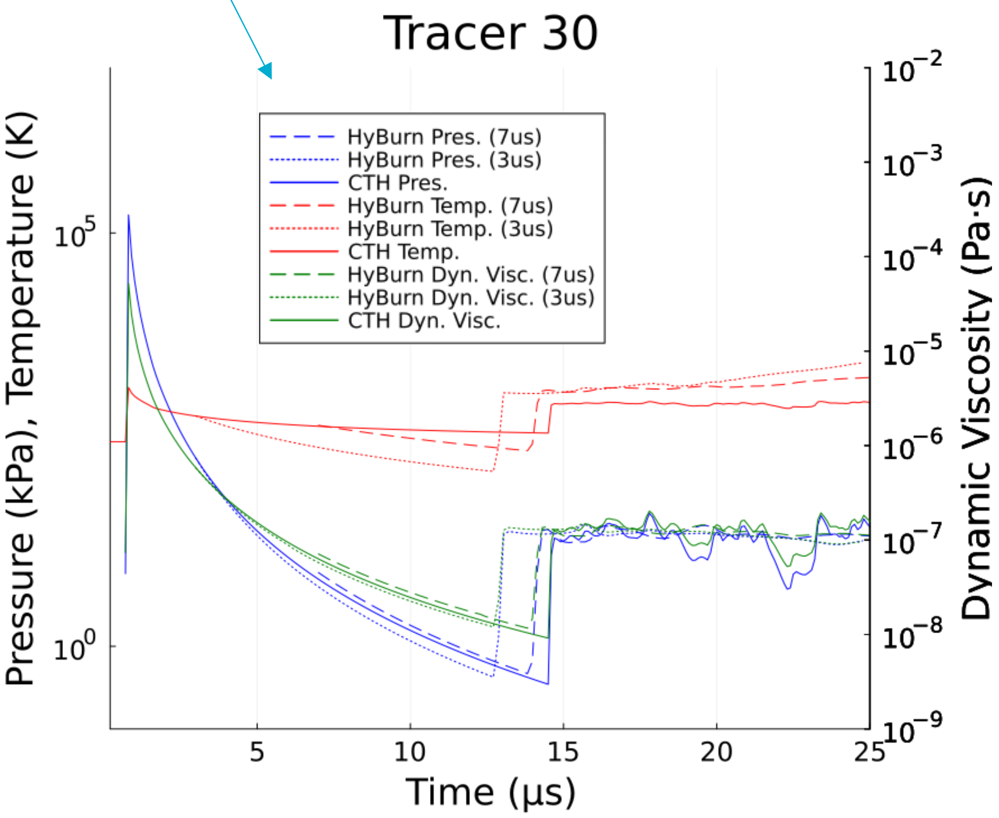




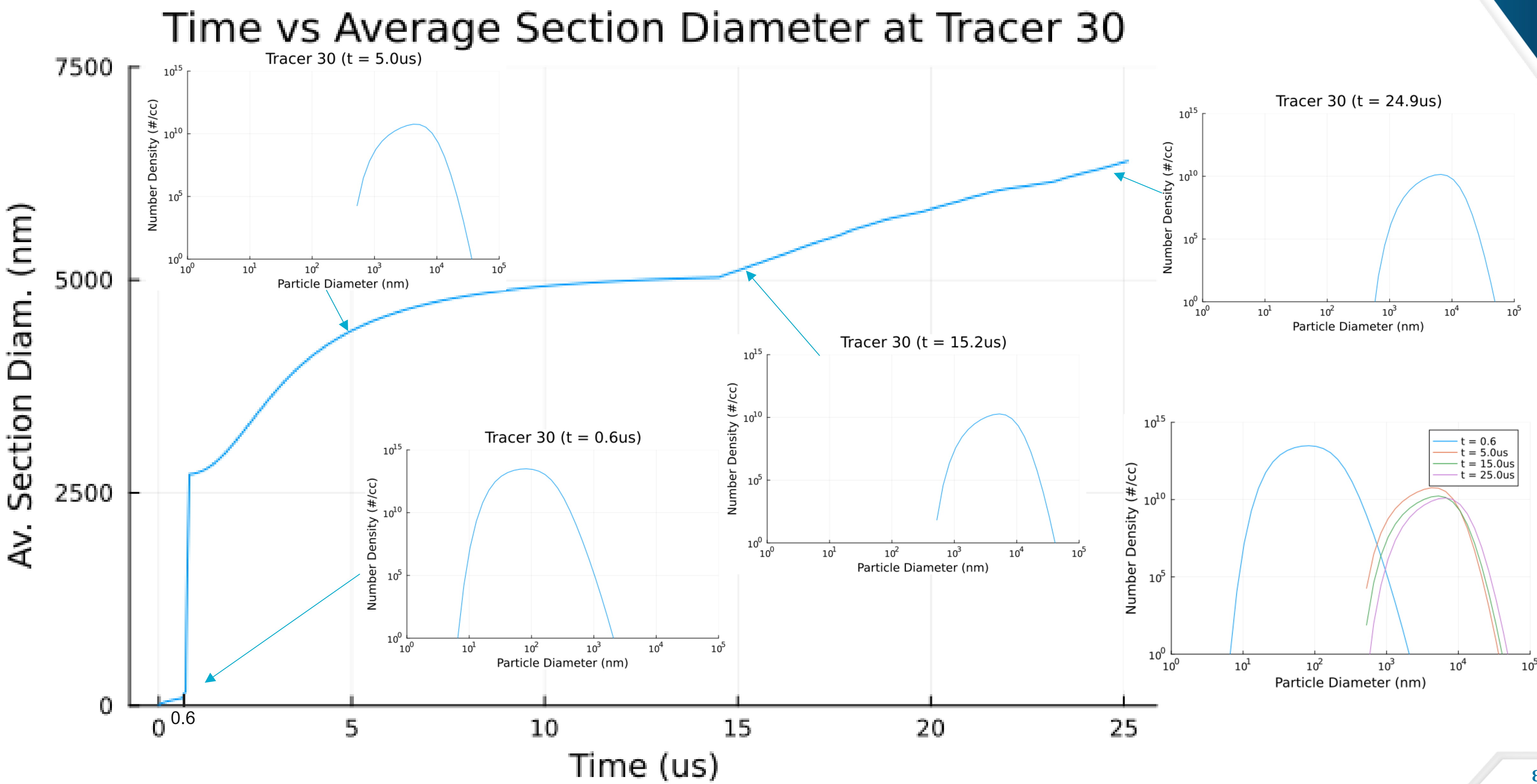
CHEMKIN

- Use ANSYS Chemkin Pro to solve for particle size distribution.
- Tracer data were used as constraints for Chemkin.
- Only **<u>Coagulation and Aggregation</u>** are considered.
- Sectional method.
  - Seed section 1 with 1e^{22} carbon monomers.

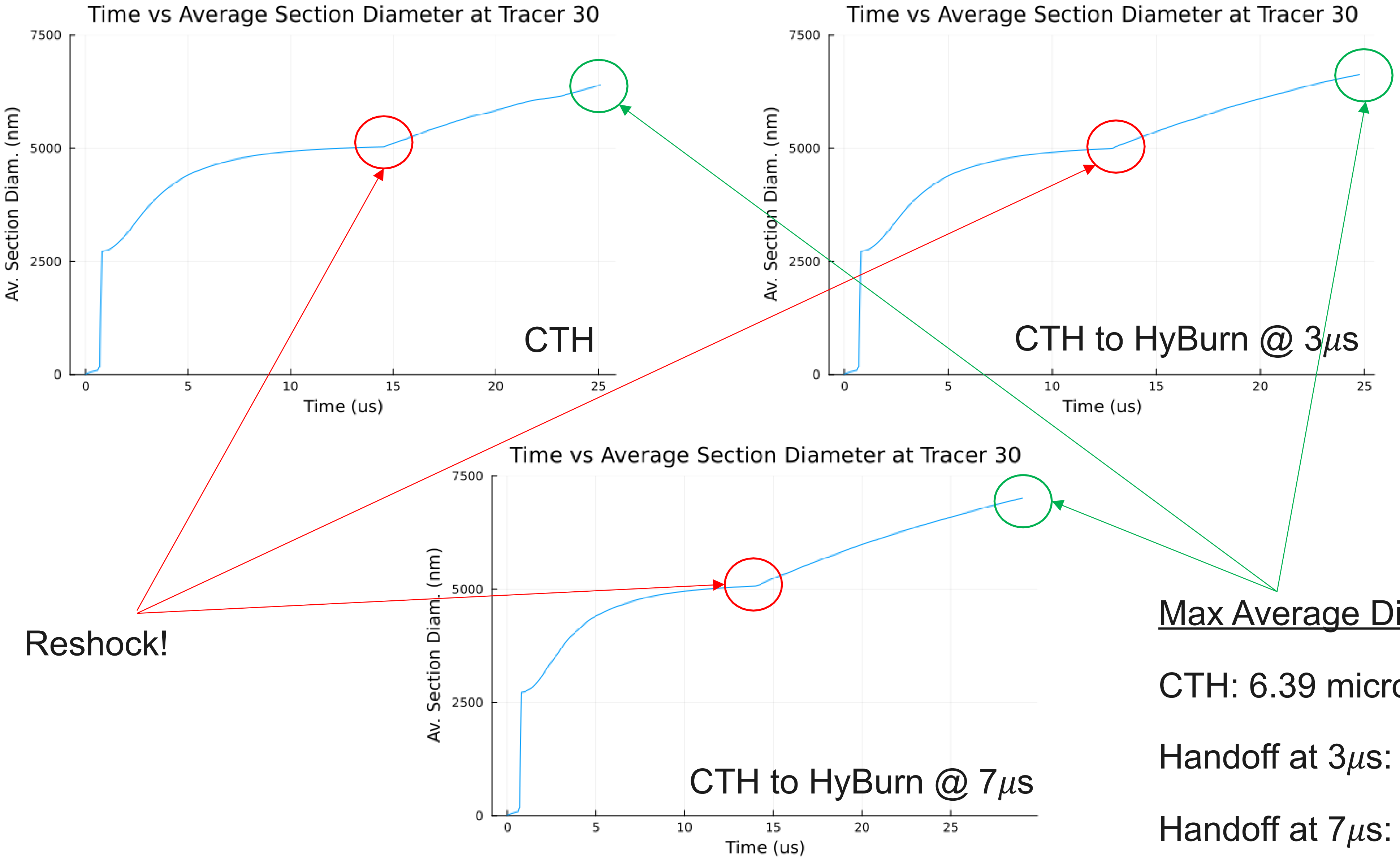
Use this tracer to do Chemkin Simulations!



CHEMKIN RESULTS – CTH ONLY



CHEMKIN RESULTS



<u>Max Average Diameter:</u>

CTH: 6.39 microns

Handoff at 3μs: 6.63 microns

Handoff at 7μs: 7.01 microns

CONCLUSIONS AND FUTURE WORK

- Developed a simulation pipeline to model soot growth via:
  - Fluid dynamic simulations
    - CTH Early-time
    - HyBurn Later-time
  - Chemkin Pro
    - Coagulation
    - Agglomeration
- Obtained particle size distributions to compare with experimental data!
- A need to implement a new collision kernel:
  - Existing relies on solely Brownian motion.
  - Implement new collision kernel based on hydrodynamic drift by shocks.

THANK YOU!