ASCENT Project: 071

Predictive Simulations of nvPM Aircraft Emissions

Georgia Institute of Technology

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Cost Share Partners: [1]Georgia Institute of Technology, [2]University of Michigan, and [3]Raytheon Technology Research Center.

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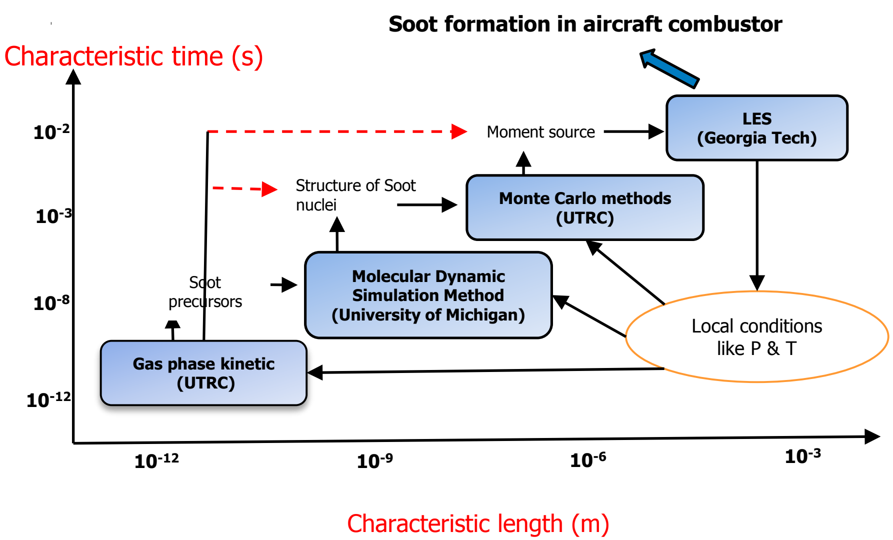
Objective:

- Reliable soot kinetics for complex polyaromatic hydrocarbons (PAHs) jet-fuel systems
- Develop a new model for nanoparticle inception
- Link kinetics and particle inception to growth models
- Apply models within large-eddy simulations (LES)

Project Benefits:

- Predictive model for aeroengine combustor emission
- New predictive inception and growth models for soot formation in PAHs dominated fuels
- New CFD to simulate emission from flames using these multi-scale models



Major Accomplishments:

- Reduced order model for soot inception and surface growth, Reduced kinetic mechanism for ethene with PAH species
- Free energy calculations of PAH dimer stability as function of temperature
- LEMLES-Method of Moment for canonical turbulent combustion to evaluate new models

Future Work / Schedule (2-Year Plan):

- Complete validation of PAH based soot kinetics
- Couple particle growth model with nucleation and inception-growth mode with validation
- Reduced models for LES application
- To LES of canonical and relevant problems

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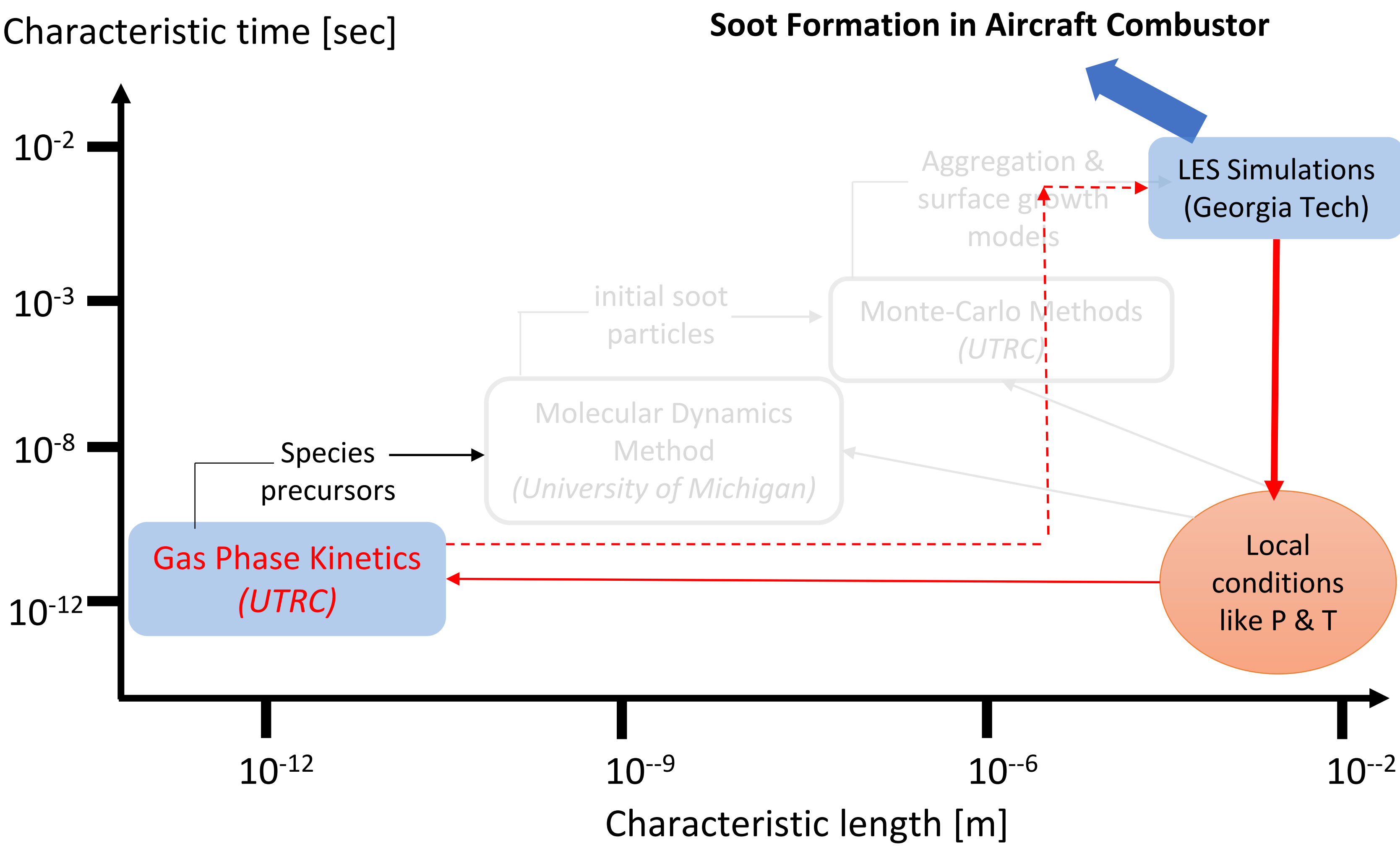
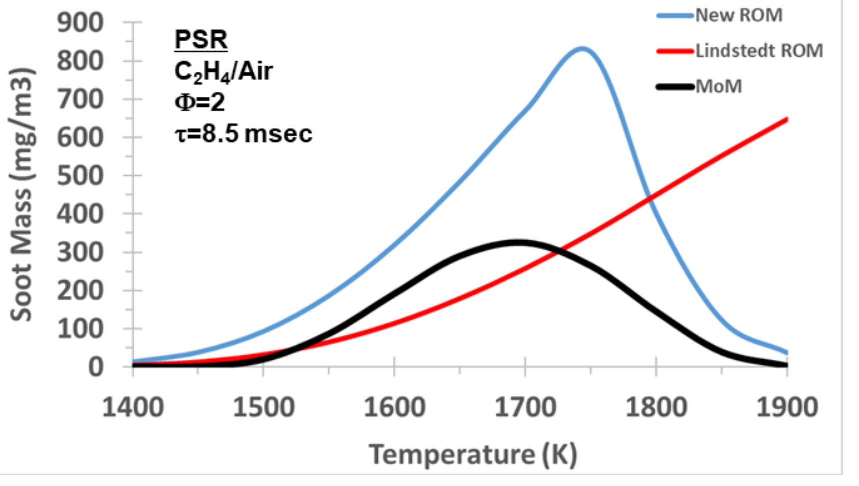
Kinetics of Soot formation



Kinetics of Soot formation

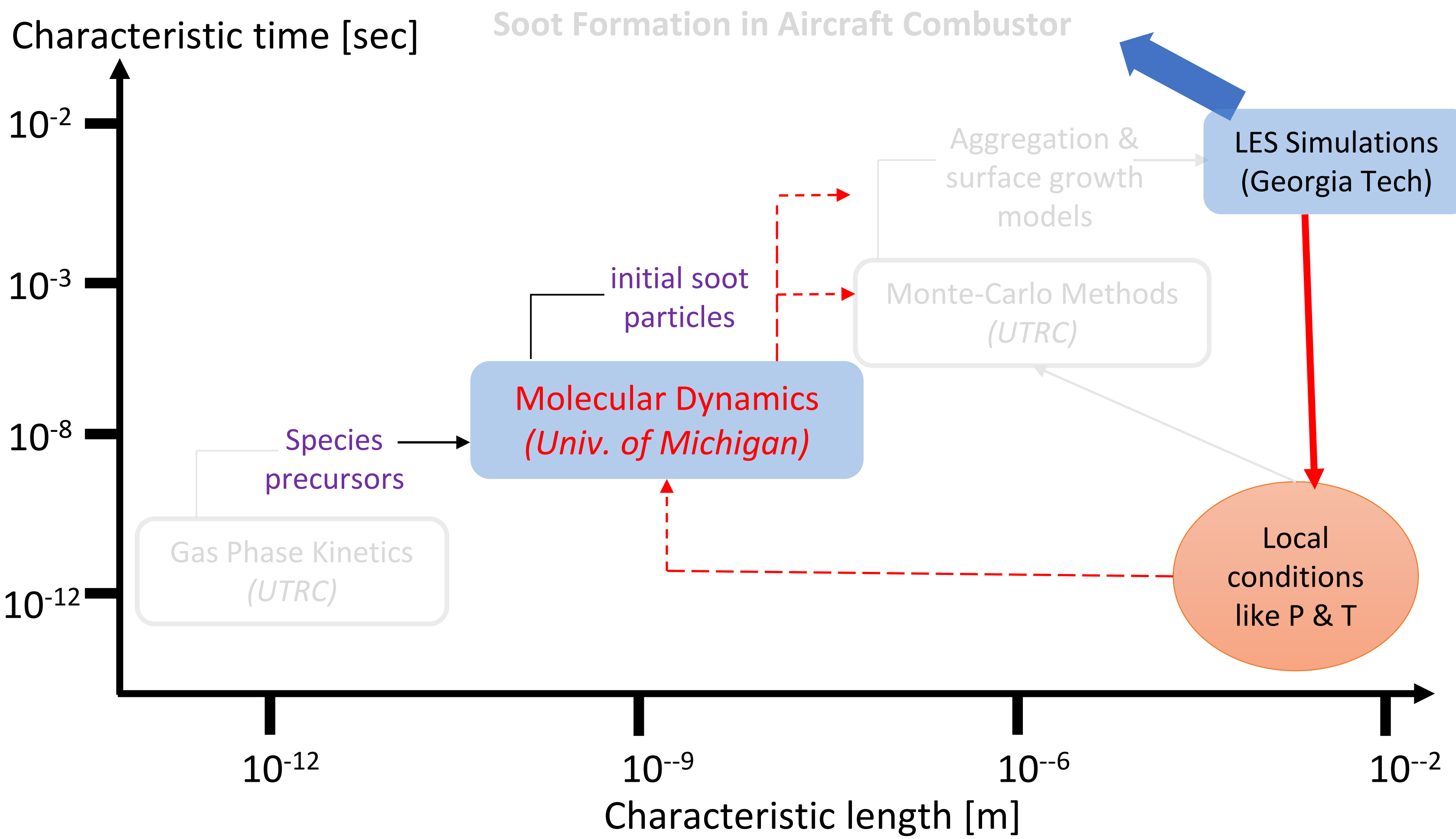
Current :
- New PM kinetics model formulated to account for reduced rates at elevated temperatures (bell-shaped growth curves)
- Reduced C_2H_4 kinetic mechanisms (~24 species) capturing PAH species important for soot formation (i.e., benzene, naphthalene, pyrene) developed



Assessment of soot model in PSR calculations

Future :
- Optimize coefficients in new PM model
- Continue development of reduced mechanisms
- Develop and verify reduced kinetics for simulations
- Input from LES and data for operating conditions
- Output to Nucleation, Aggregation and LES methods

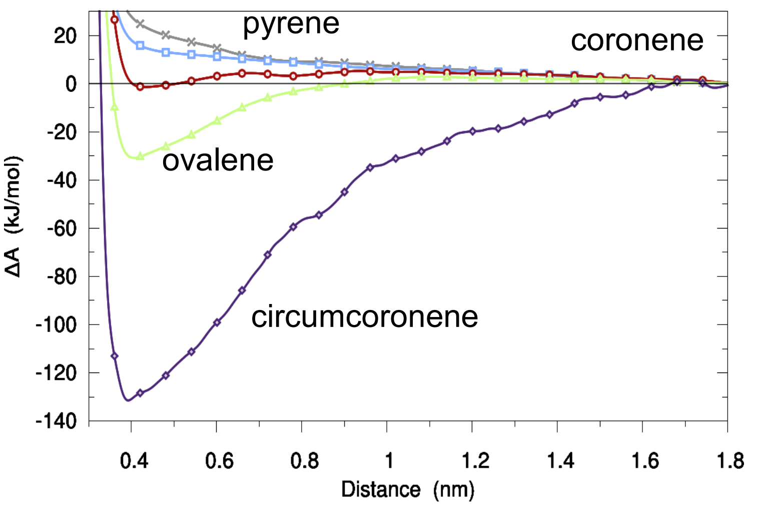
Particle Inception from Gas-phase Species



Particle Inception from Gas-phase Species

Current :
- Identified PAHs that are critical to inception.
- Molecular Dynamics (MD) based computational framework for free energy analysis to identify dimer stability
- Study the collisions of PAHs and formation of aromatic dimers that lead to soot inception.

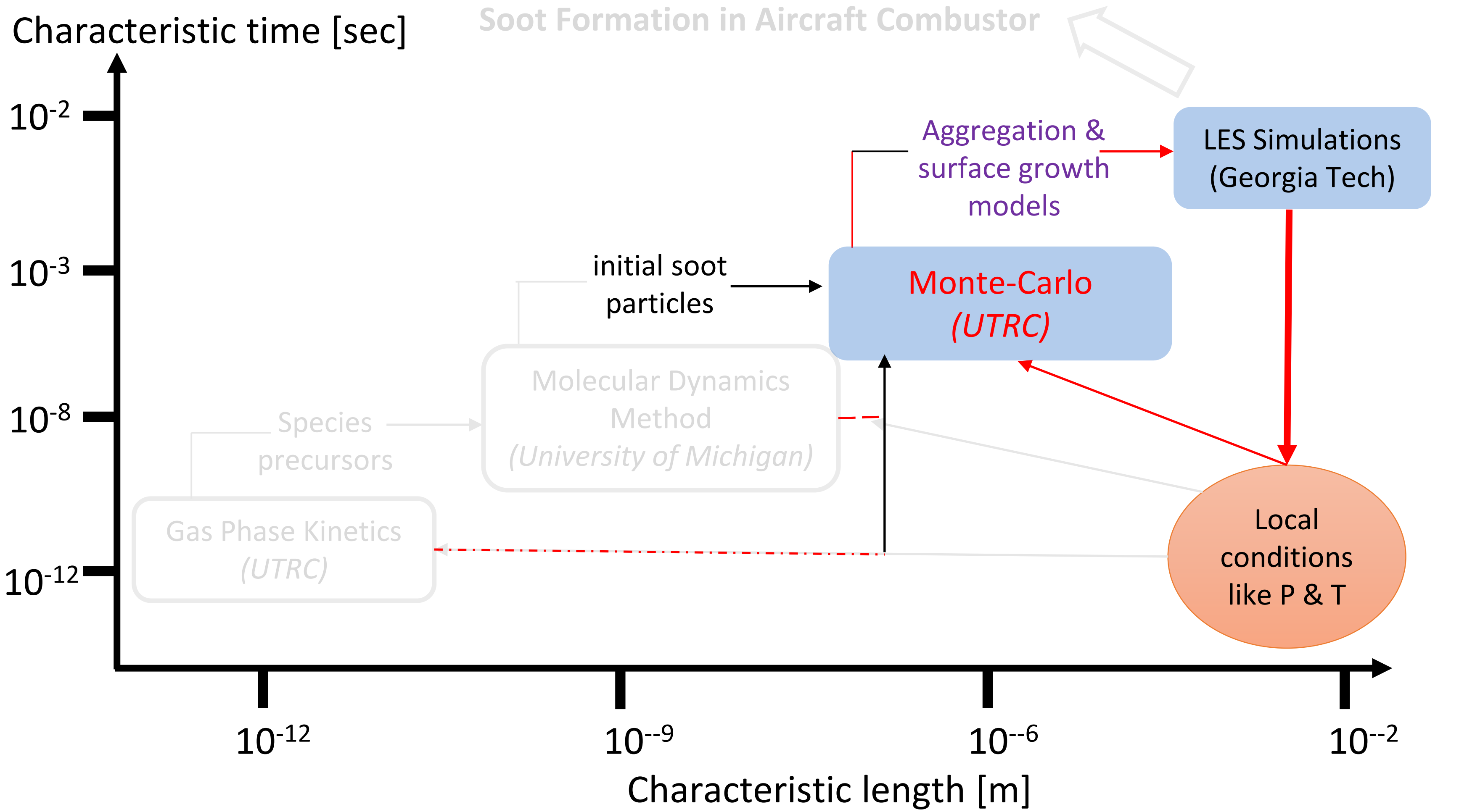
Future :
- Effect of shape and chemical composition of PAHs on dimer formation and stability
- Rate of collisions as a function of chemical and physical properties of PAHs
- Output to aggregation and large scale LES
- Reduced rate models for particle inception



Free Energy Calculations for PAH

Publication supported by ASCENT FAA:
Saldinger, Elvati, and Violi, *Phys. Chem. Chem. Phys., 2021, 23, 4326.*

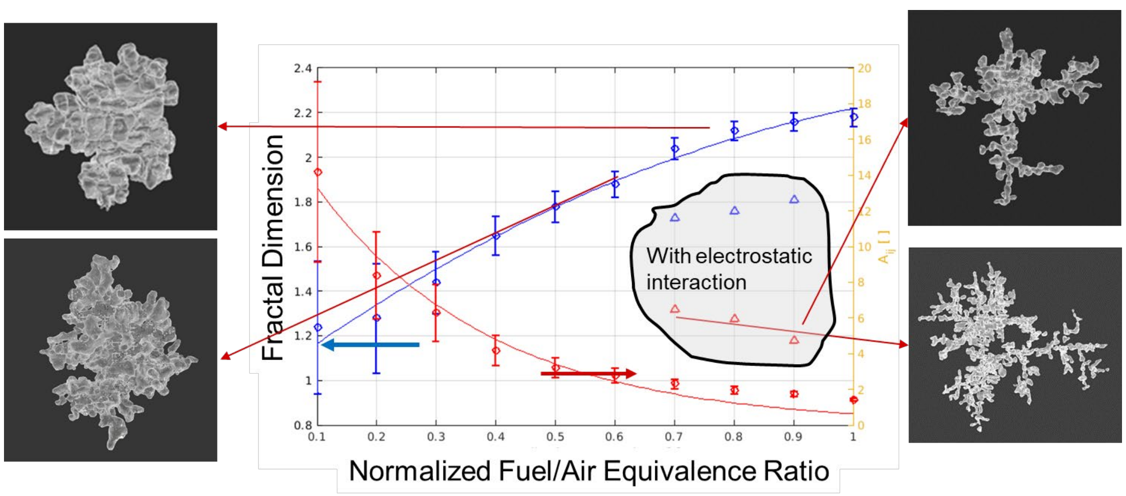
Post-inception growth of particles



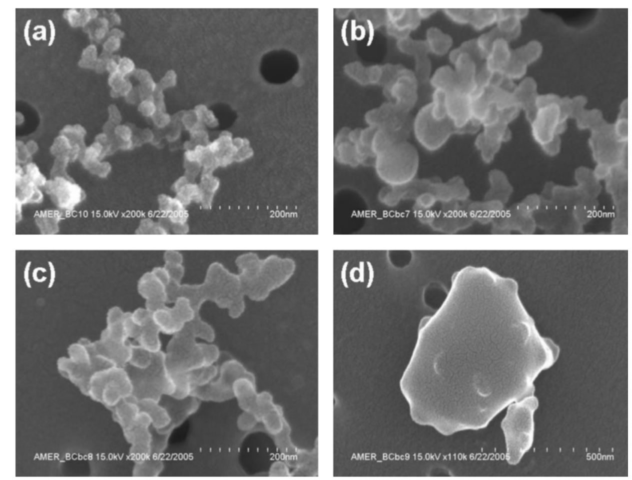
Post-inception growth of particles

Current :
- Surface growth modeling of soot through phase field
- Agglomeration of post-inception particles through Monte Carlo (MC) simulations
- Physics-based transition from reaction-limited to transport-limited growth
- Model to account for cluster-cluster aggregation and regime-based surface growth

Future :
- Validation to coupled wth nucleation physics
- Transition models to MOMLES for large-scale prediction

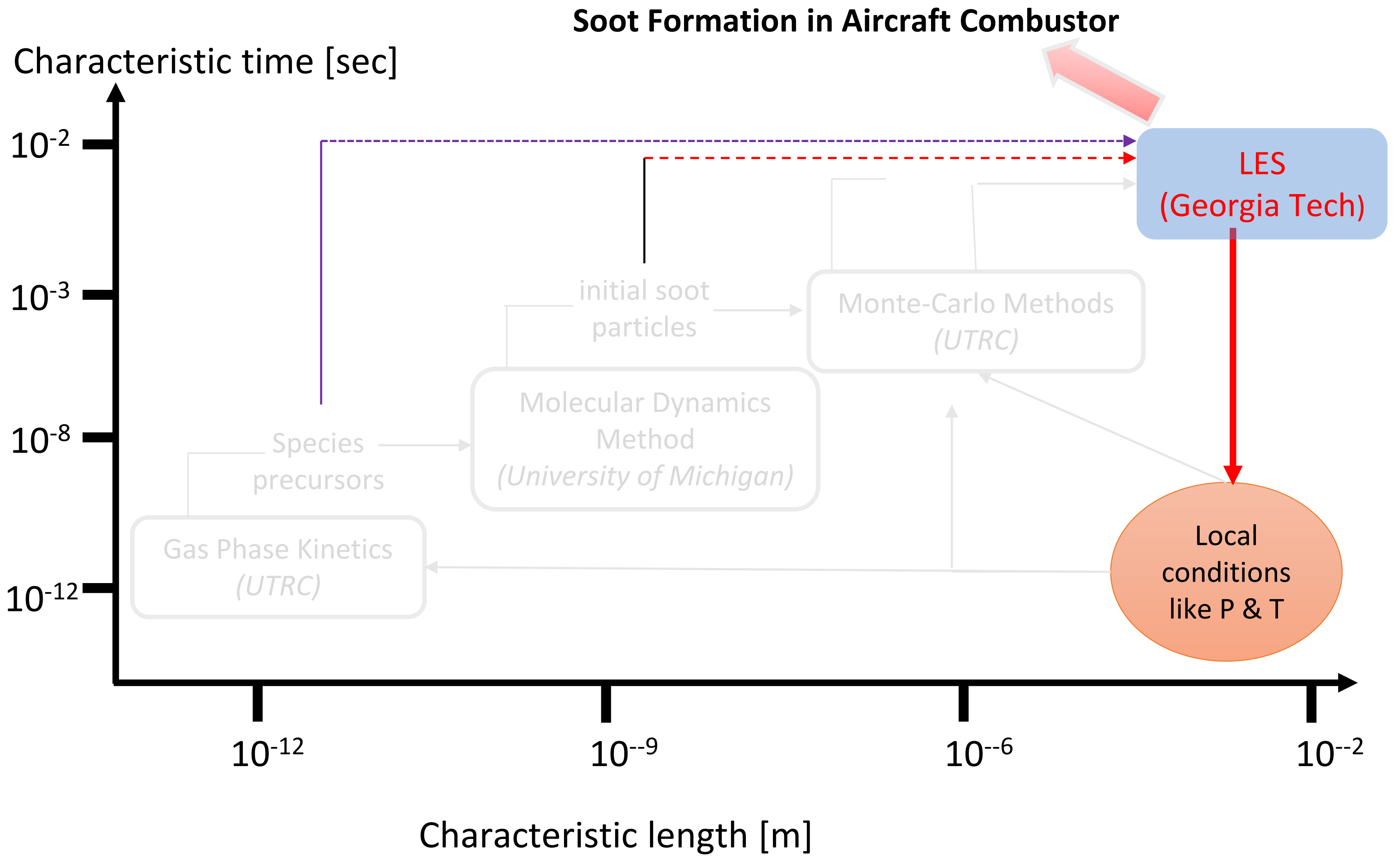


Phase field simulation to predict aggregate structures



Experimental observation of soot morphology

Large-scale soot combustion in LES



Large-scale soot combustion in LES

Current :

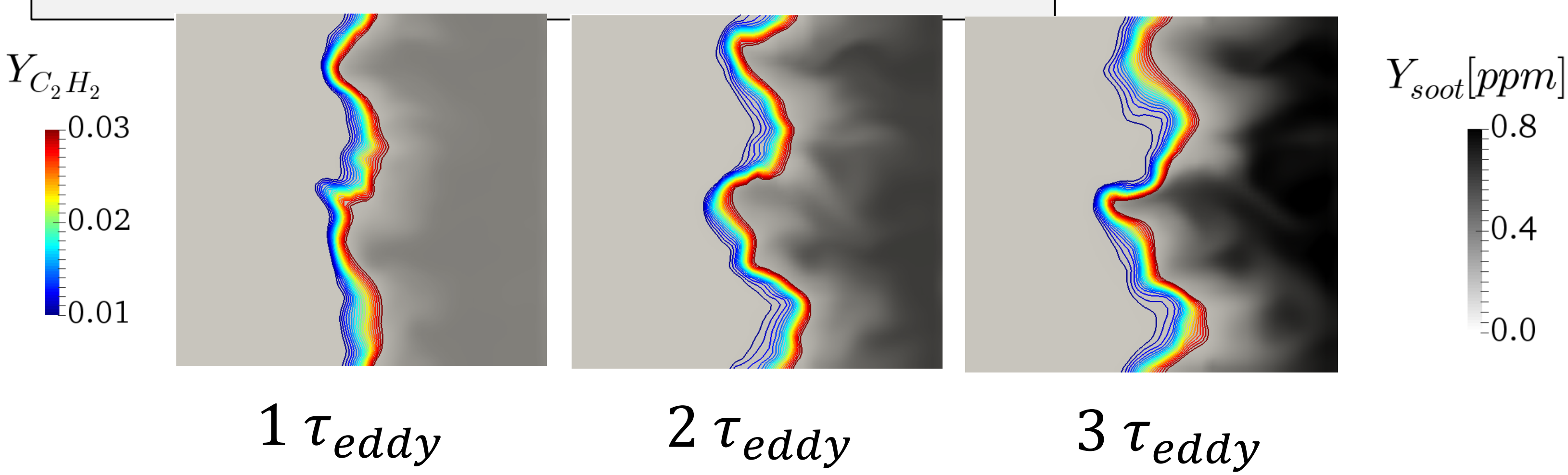
- Assessment of detailed (99 species), skeletal (34 species) and reduced chemistry (19 species) models within the LES framework to predict uncertainties in precursor concentrations
- Linear eddy model (LEM) for soot evolution within sub-grid LES in premixed rich ethylene flames using reduced kinetics and method of moments based on 6 moments
- Canonical extinction-reignition flame to evaluate the soot formation and transport in non-premixed ethylene jet flames
- Extend the capability to include MOMIC source terms based on PAH nucleation and PAH condensation on soot surface

Future :

- Integration of aromatic reduced kinetics with PAH species and multiscale inclusion of inputs from nucleation and growth models
- Subgrid soot-turbulence-chemistry assessment in both canonical premixed and non-premixed flames

$$\tau_{eddy} = \frac{l}{u'}$$

l – Turbulent length scale
u'- Turbulent fluctuations



Soot Evolution in Turbulent Rich Premixed C_2H_4/Air Flame as eddy turnover time Overlapped with precursor C_2H_2 precursor