# 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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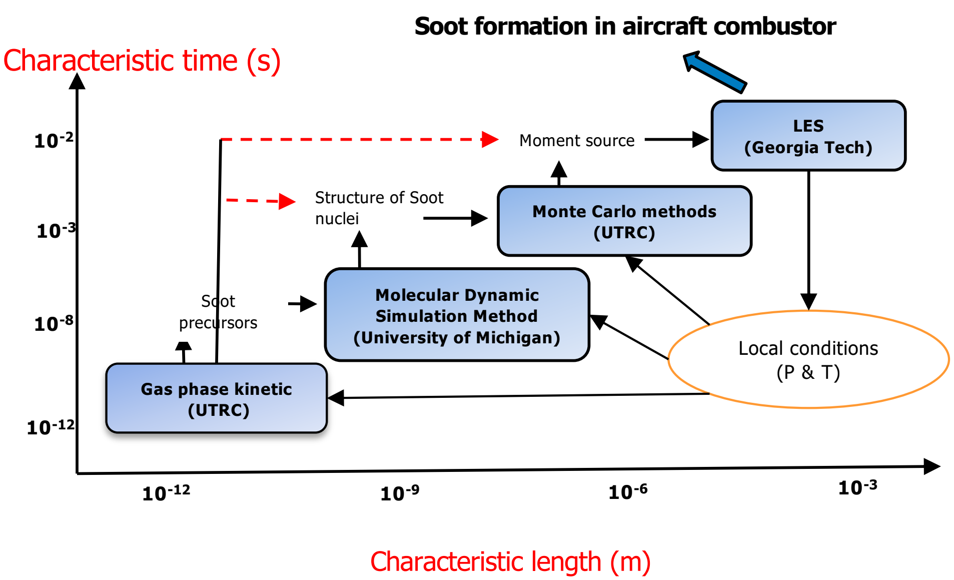
## Objective:

- 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 using multi-scale analysis for coupling physics at disparate scales
- New CFD to simulate emission from turbulent flames using these multi-scale models




## Major Accomplishments (as of April 2022):

- Reduced order model for soot inception and surface growth, Reduced kinetic mechanism for PAH species now being tested in LES
- Free energy calculations of PAH dimer stability as function of temperature – towards nucleation model
- Coupling between surface growth model and LES being tested for couple analysis
- LEMLES-Method of Moment for canonical turbulent combustion to evaluate new models operational

## Future Work / Schedule:

- Complete Assessment of PAH based soot kinetics
- Couple particle growth model with nucleation and inception-growth model for use in LES
- Reduced models testing for LES application

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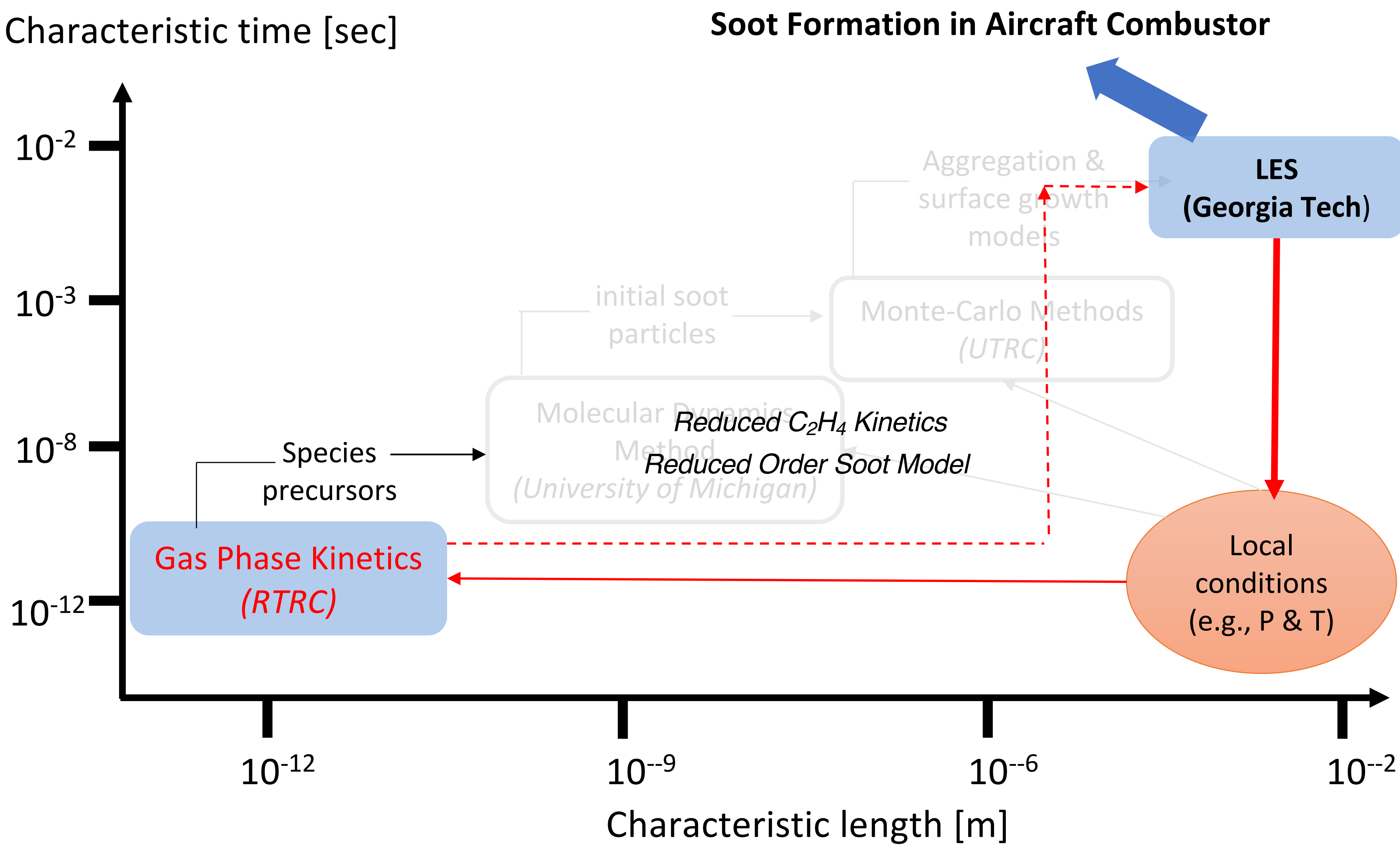
# Kinetics of Soot formation (RTRC)

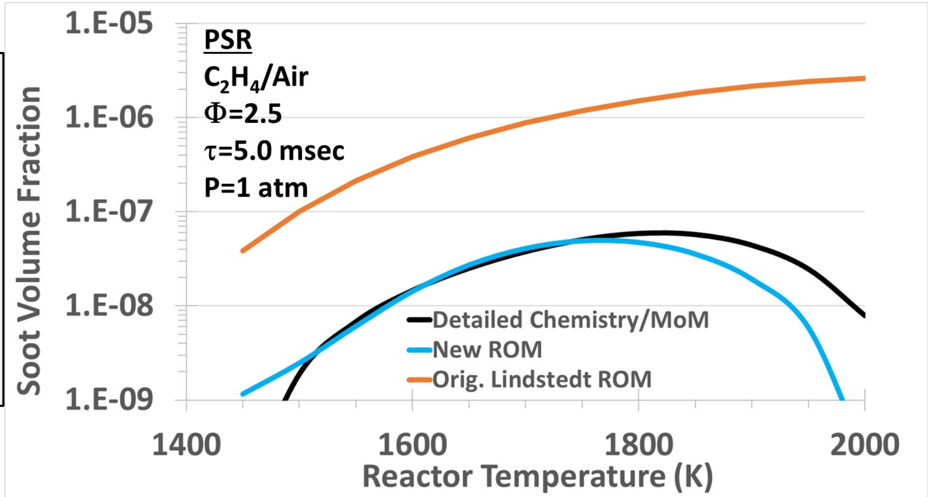


# Kinetics of Soot formation (RTRC)

**Current :**
- Improvements in global simplified soot model to match predictions with detailed model
- New ethylene (ROM) kinetic mechanisms (25 species) capturing PAH species important for soot formation (e.g., pyrene ) developed and is now being tested in LES

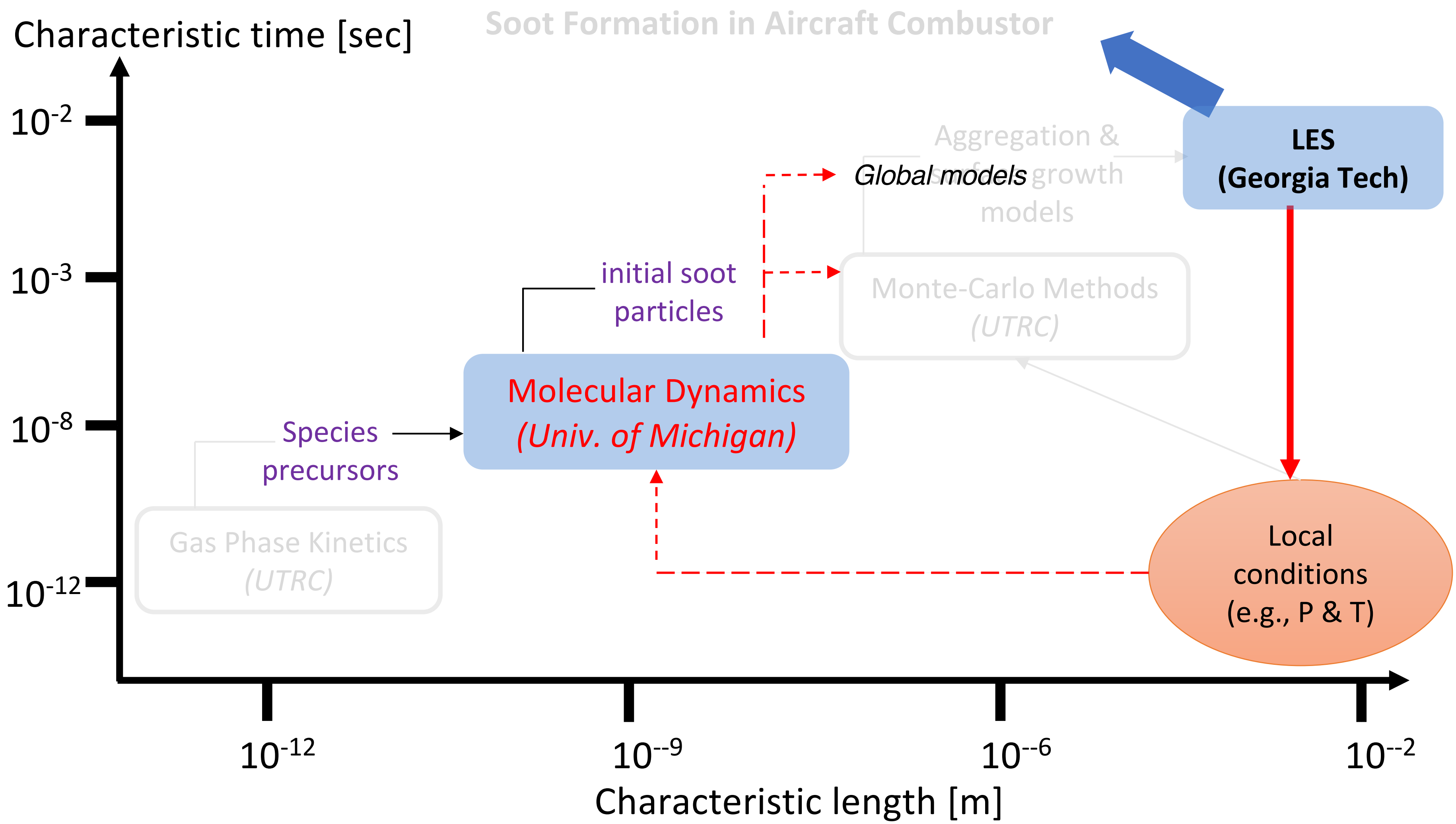
*ROM: Reduced Order Model*

**Future :**
- Assessment of PAH based reduced kinetics for Jet-A type fuels
- *GT: Output for integration within LES*
- *UM: Input to Nucleation model*
- *RTRC: Input to Aggregation model*




Assessment of soot model in PSR

# Particle Inception from Gas-phase Species (U. Mich.)

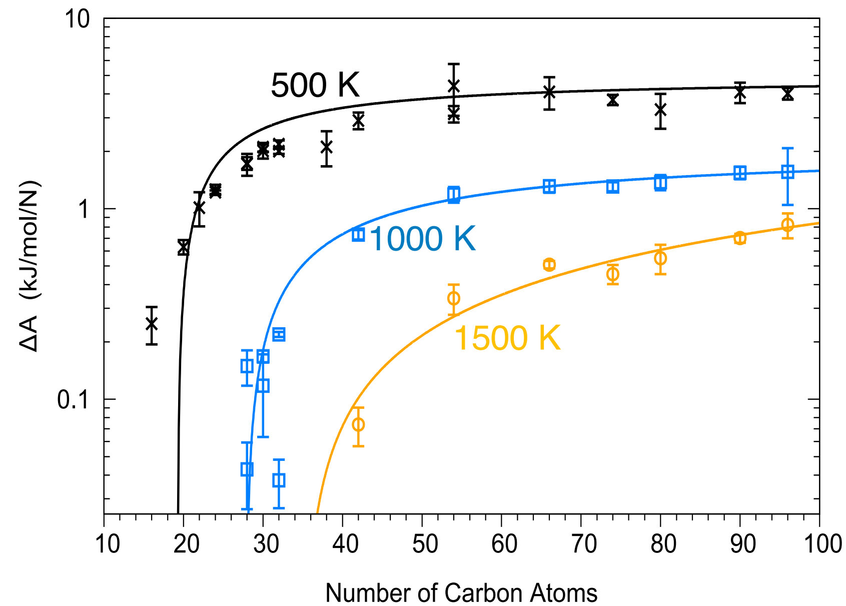


# Particle Inception from Gas-phase Species (U. Mich.)

**Current :**
- Identified PAHs characteristics that are critical to inception
- Molecular Dynamics (MD) simulations for free energy analysis to identify dimer stability
- Formation of aromatic dimers that lead to soot inception investigated

**Future :**
- PAHs to be investigated under gas turbine conditions on dimer formation and stability
- Collision rates as a function of chemical and physical properties of PAHs for LES model use
- *RTRC: Input of ROM kinetics*
- *RTRC: Output to aggregation model*
- *GT: Output to particle inception model for LES*

ΔA = Free energy difference between monomer and dimer
ΔA > 0 represents dimers more stable than monomer

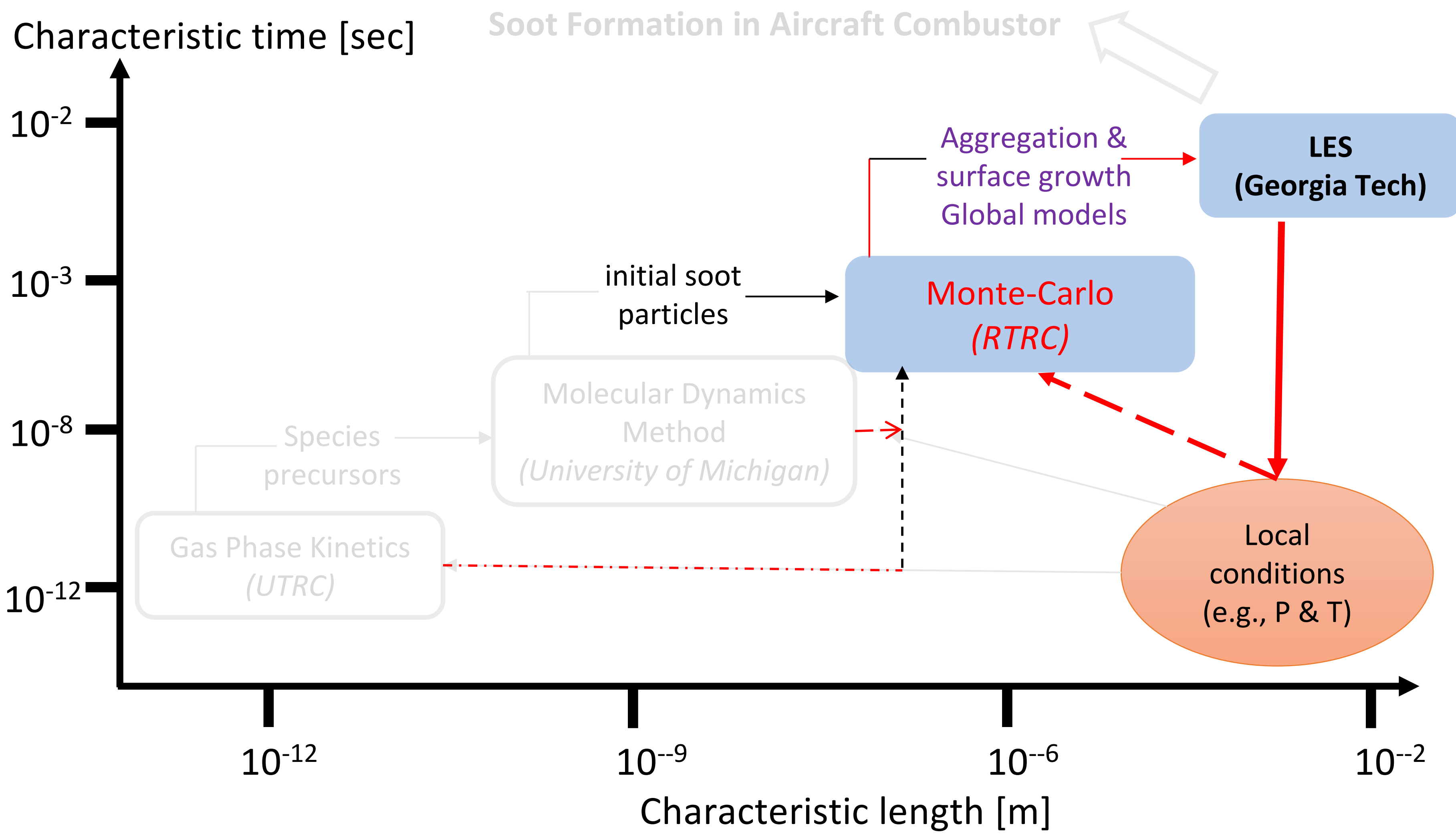



Stable dimers can potentially lead to initial soot nuclei.

**Publication supported by ASCENT FAA:**

Di Liddo, Saldinger, Jadidi, Elvati, **Violi,** Dworkin. Proc. Combust. Inst. 2022, *Submitted*
Saldinger, Raymond, Elvati, **Violi** Proc. Combust. Inst. 2022, *Submitted*
Saldinger, Elvati, and **Violi**, *Phys. Chem. Chem. Phys., 2021, 23, 4326.*

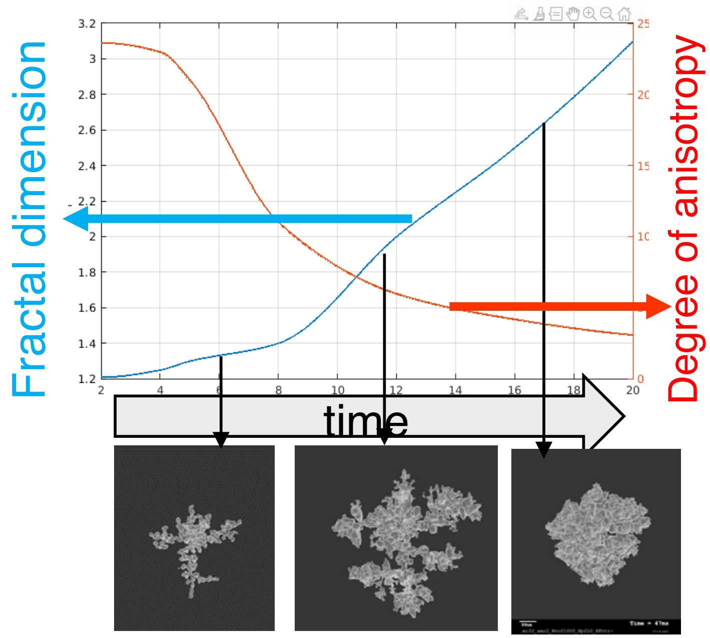
# Post-inception growth of particles (RTRC)



# Post-inception growth of particles (RTRC)

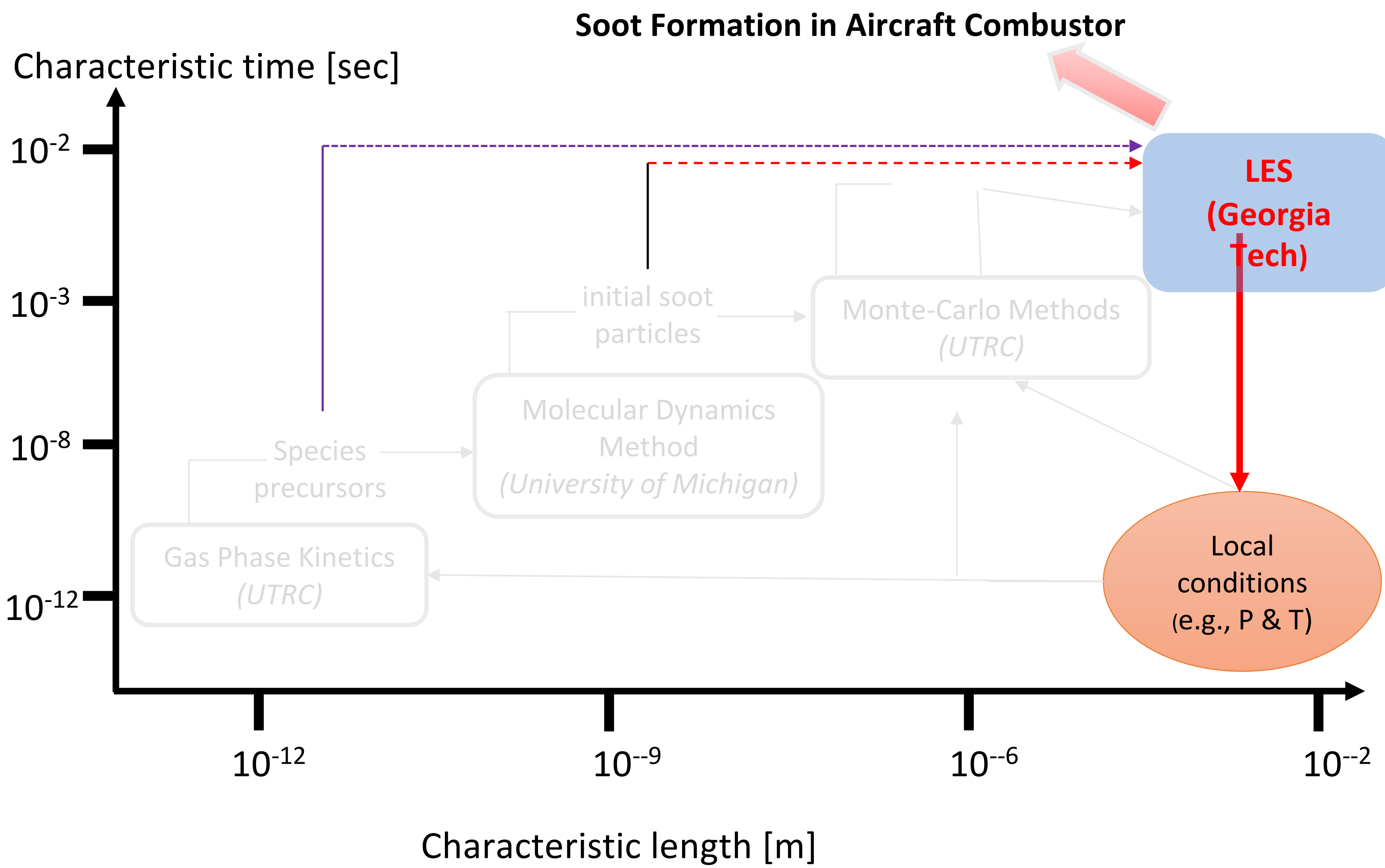
**Current :**
- Monte Carlo simulations for Aggregation to account for short range forces (e.g., VdW)
- Blended model for transition from reaction limited to transport limited growth developed
- Strategy to use the model to analyze LES data (GT) established (one-way coupled)

**Future :**
- "in-situ" (2-way) ability to simulate growth (surface growth and aggregation) as function of temporally varying ambient conditions (e.g., equivalence ratio, P, T in LES)
- *RTRC: Input of ROM kinetics*
- *UM: Input of coupling with nucleation model*
- *GT: Output of models for LES*




**Growth from Fractal to Spherical Aggregates modeled**

# Large-scale soot combustion in LES (GT)



# Large-scale soot combustion in LES (GT)

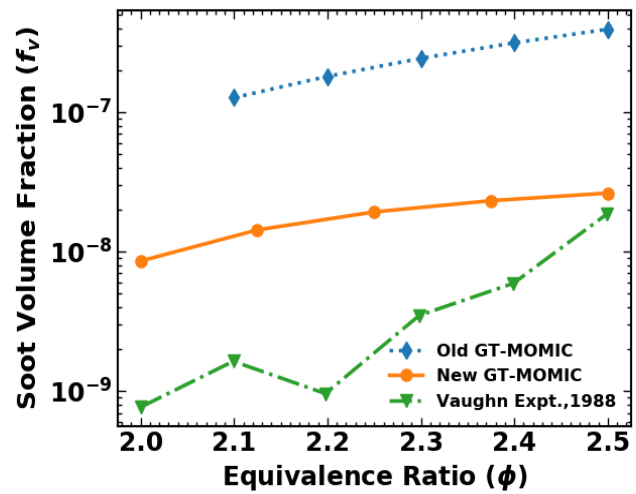
**Current :**

- PAH inception, condensation and surface growth implemented in the 6-MOMIC
- Linear-eddy Mixing (LEM)-6MOMIC chosen as baseline sub-model to study high-Re turbulent mixing-combustion with soot formation – ability to test different models
- New ROM kinetics from RTRC being evaluated using LEM-MOMIC

**Karpe et. al.,** ***18th Int. Conf. on Numerical Combustion, 2022***

**Future :**

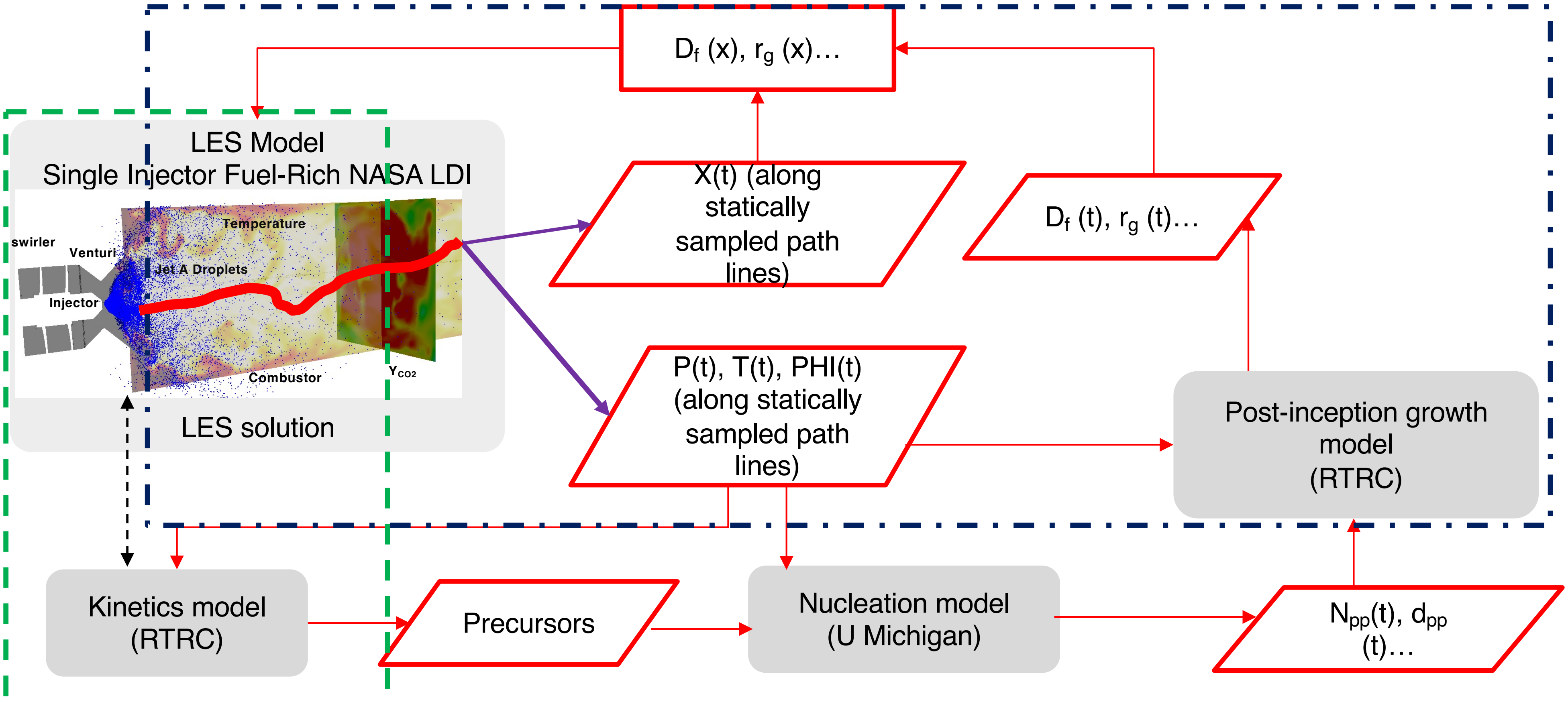
- LEM-6MOMIC assessment in turbulent flames
- *RTRC: Input of ROM kinetics with PAH*
- *RTRC: Input of aggregation model*
- *UM: Input of nucleation rate model*
- Multiple test beds for LES evaluation developed
  - LEM-MOMIC as a turbulence-chemistry model
  - 3D canonical premixed and non-premixed flames
  - 3D LES of single element liquid fueled direct injection (NASA-LDI) combustor



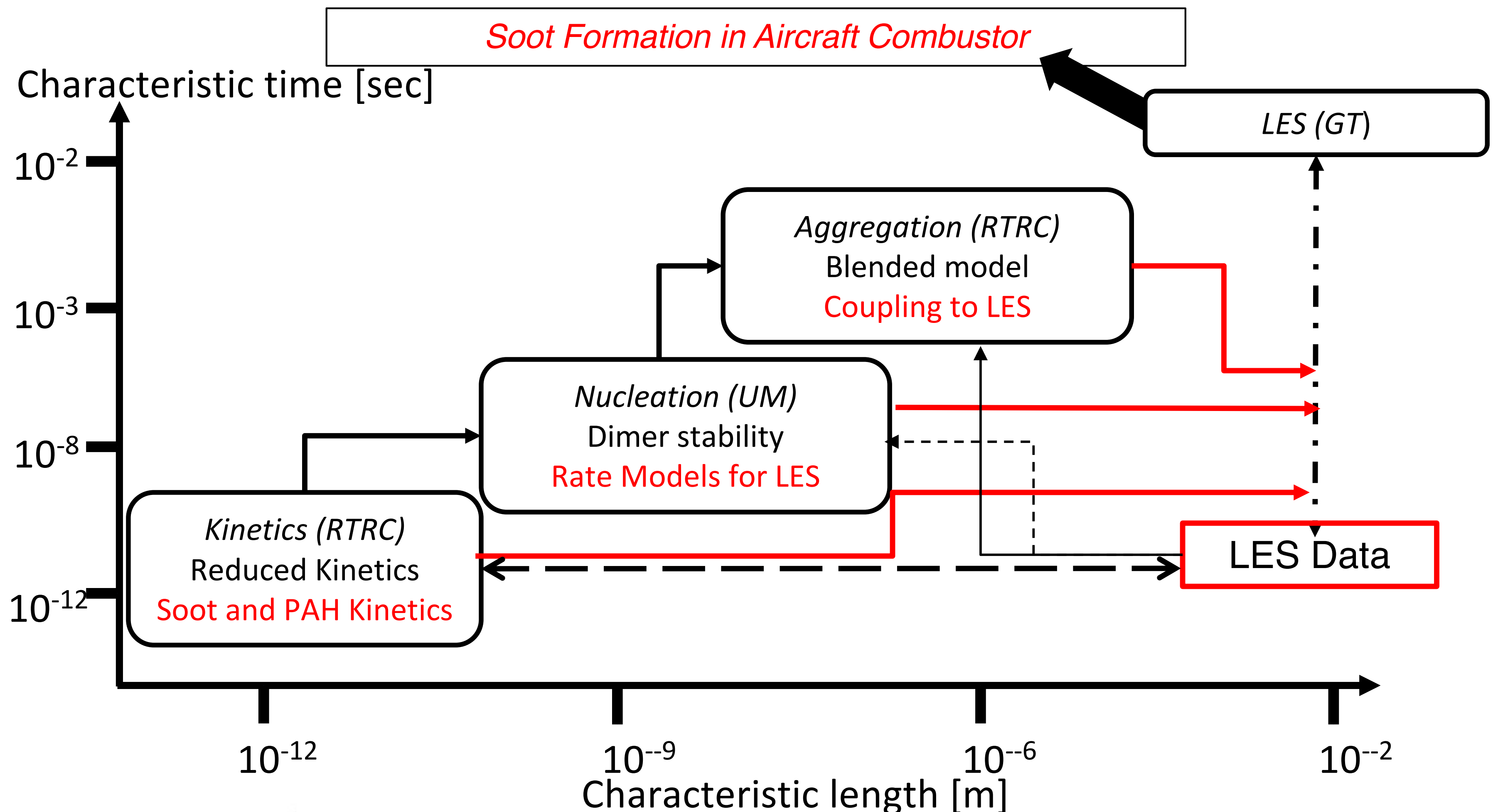

**PSR of rich ethylene-flames, Comparison against Vaughn[1] data**

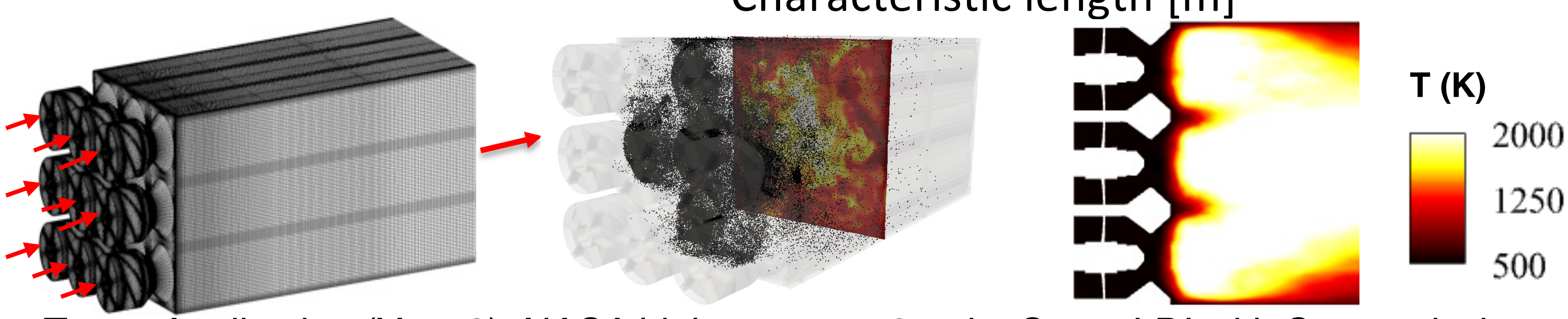
[1]Vaughn, C.B. 1988, PhD thesis, Massachusetts Institute of Technology, Cambridge, MA
[2]Leung, K. M., Lindstedt, R. P., & Jones, W. P. (1991). *Combustion and flame*, *87*(3-4), 289-305
[3]Kroneburg, A. , *Combustion and Flame* 121 (2000): 24-40.

# Example: One-way Coupling LES data on NASA-LDI for Surface Growth Model (GT-RTRC)



# Summary and Future Plans




Some data from NASA (GRC): Raju & Wey. *AIAA-2020-2088.*

*Target Application (Year 3): NASA high-pressure 9-point Spray LDI with Soot emission.*