



National Aeronautics and
Space Administration

Aviation Turbine Fuels Combustion Meeting

ANALYSIS OF A SURROGATE JET FUEL SKELETAL MECHANISM WITH PAHCHEMISTRY

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In collaboration
with scientists from



Motivations

- A detailed reaction mechanism for Jet-A fuel is intractable for CFD
- Detailed polycyclic aromatic hydrocarbon (PAH) chemistry is needed for accurate soot modeling
- Soot chemistry is complex, many parameters in nucleation, surface growth, etc.
- Sparse soot model libraries available for integration in CFD software

Objectives

- Develop a skeletal surrogate Jet-A reaction mechanism
- Retain detailed PAH species needed for the soot model as part of the reduction
- Fast convergence of canonical problems to rapidly iterate
- Validate the new OpenNCC Sectional Soot modeling software
- Validate the mechanism against canonical cases and an aeronautics combustor reactor network

Jet-A Fuel Surrogate Mechanism

Comprehensive Kinetic Model

- >12,000 species
- Saggese et al. (LLNL)

Detailed Surrogate Mechanism

- 844 species, Jeta-A A2, C1-C2, and blends
- Pintor et al. (Sandia)

Skeletal Mechanism

- DRG, DRGEP, DRGPFA + Sensitivity
- Limit ranges $P=1\text{-}20\text{atm}$, $T=1000\text{-}1800\text{K}$, $\phi=0.8\text{-}2$
- 308 species, 2291 reactions
- S. Roy et al. (W. Michigan U.)

Species	Formal Name	Mole%
N-tridecane	NC13H28	21.605
Iso-dodecane	XC12H26	27.907
Butylcyclohexane	NBCH	31.75
1,2,4 trimethylbenzene	T124MBZ	13.055
Alpha-methyl naphthalene	A2CH3	5.683

Species targeted for accuracy

C6H6, C2H2, **A4R5**, NBCH, C6H5C2H, NAPH, FULVENE

Other species retained

O2, A2CH3, XC12H26, N2, AR, CO2, NC13H28, T124MBZ, H2O, A3R5, A2R5, ANTHRACENE, C2H3, C2H4, C4H6, CO, IC4H8, PHNTHRN, **PYRENE**

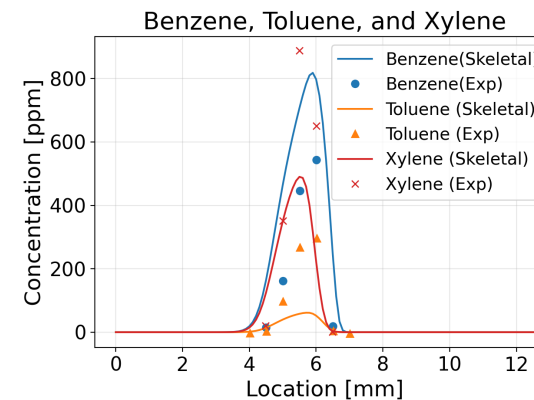
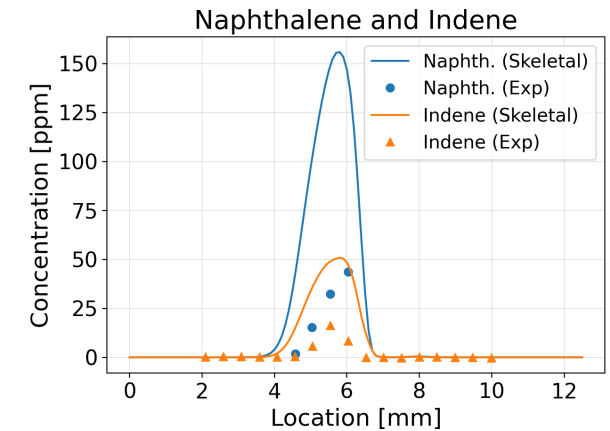
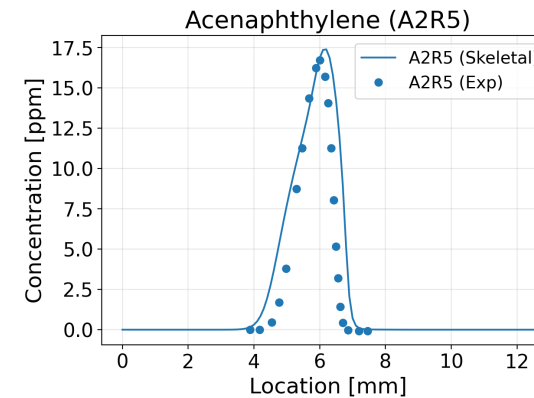
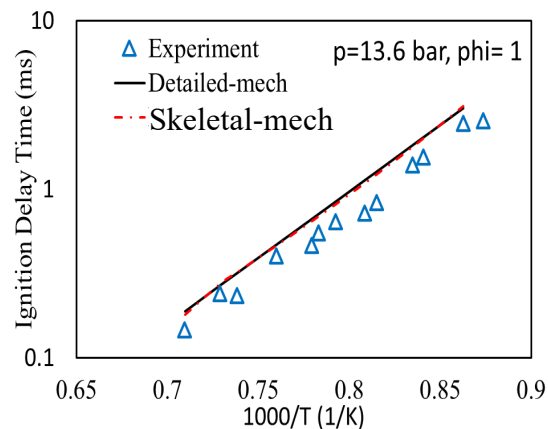
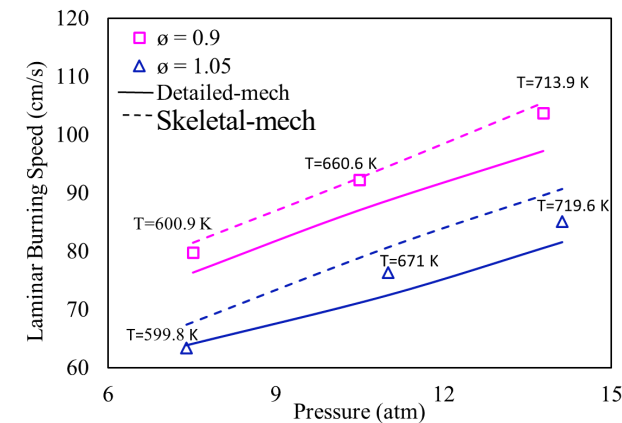
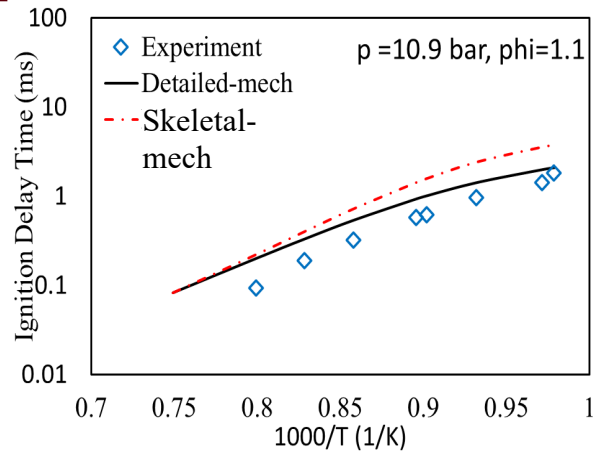
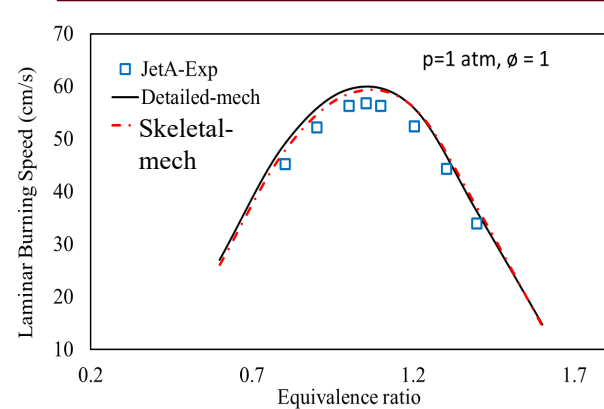
Property	A2 (jet-A)	Surrogate
Formula	$C_{11.4}H_{21.7}$	$C_{11.1}H_{21.8}$
H/C ratio	1.90	1.95
A/F _{stoich}	14.599	14.685
MW [g/mol]	158.6	155.4
LHV [MJ/kg]	43.06	43.33
HoV [MJ/kg]	0.36	0.34
Flash point [°C]	48.0	51.1
Freeze point [°C]	-51.0	-50.2
Derived Cetane #	48.3	46.9
Smoke point [mm]	22.0	23.9

Skeletal Chemistry Validation

LBS studies

IDT studies

Species vs experiment



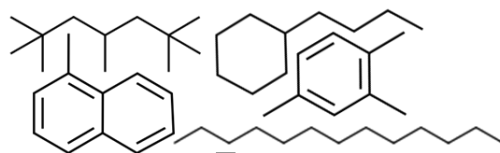
Extensive validation
shows reasonable
agreement

Rate optimizations being
considered for improved
predictions

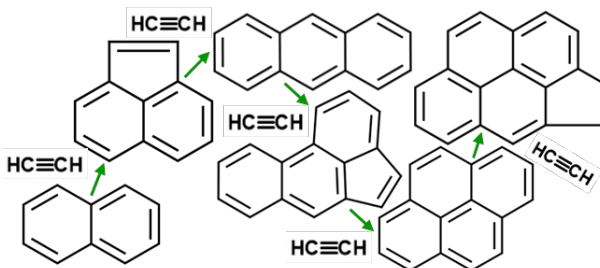
Chemkin Soot Model

- **Nucleation:** Cyclo-penta pyrene collisions form incipient soot particles
 - $2 \text{ A4R5} \rightarrow 36 \text{ C(B)} + 20 \text{ H(s)} + 32.6 \text{ C(sr)}$
- **Condensation:** 9 PAH species
 - $\text{PAH} + n \cdot \text{H(se)} \rightarrow m \cdot \text{C(B)} + n \cdot \text{C(s)} + p \cdot \text{H}_2 + q \cdot \text{C}_2\text{H}_2$
- **Surface Growth:** Hydrogen Abstraction Carbon Addition (HACA) with acetylene and diacetylene
- **Oxidation:** OH and 3-step O_2
- **Coagulation:** Fixed pivot technique
- **Surface radical sites:** Explicitly tracked finite-rate

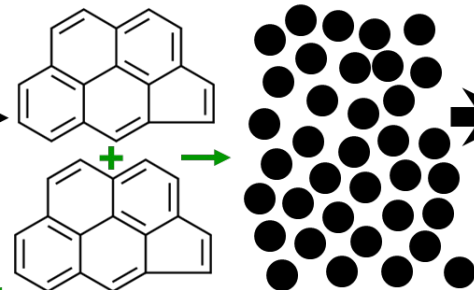
Jet-A



PAH formation



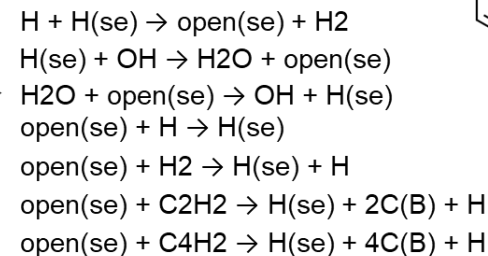
Nucleation



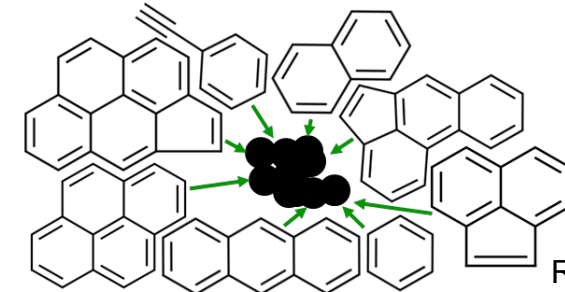
Aggregation
& coagulation



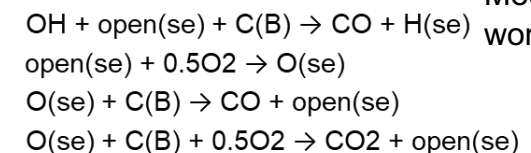
HACA growth



PAH condensation



Oxidation

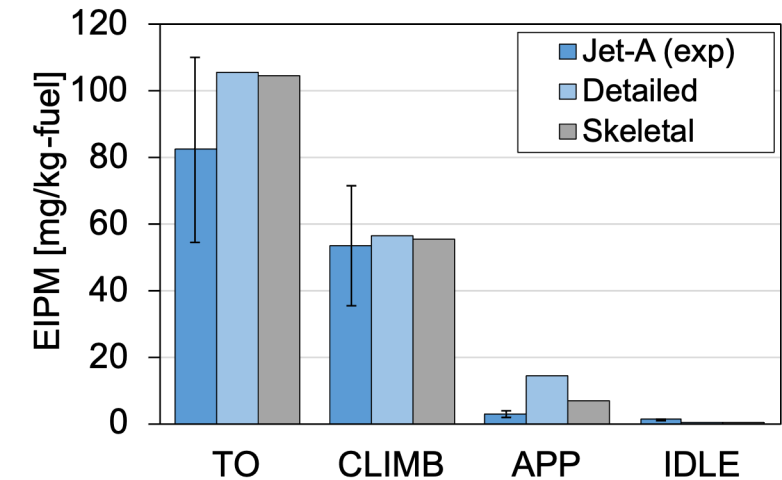
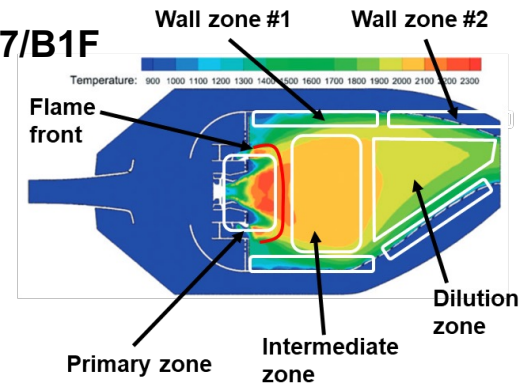


Ref: Presentation by
Dario Pintor,
Meeting2023 end user
workshop

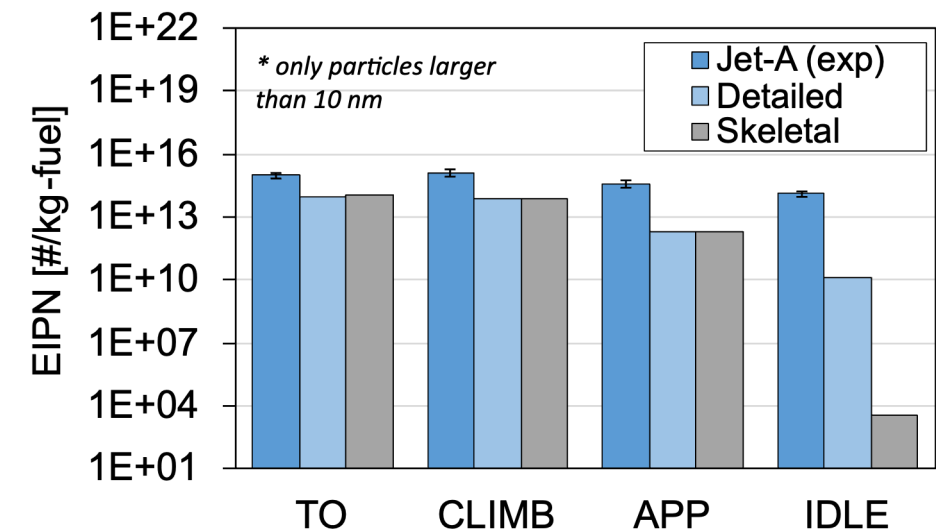
Validation case: Reactor network of CFM56 Engine

Reasonable agreement in an aeronautics combustor reactor network

CFM56 -7B27/B1F



Properties	Unit	Take off	Climb	Approach	Idle
$\dot{m}_{air}$	[Kg/s]	44.52	39.1	20.87	12.12
$\dot{m}_{fuel}$	[Kg/s]	1.28	1.04	0.349	0.119
P_{in}	[Mpa]	2.9	2.48	1.13	0.559
$T_{a,in}$	[K]	800	764	613	505
ϕ_{global}	[-]	0.42	0.39	0.245	0.144



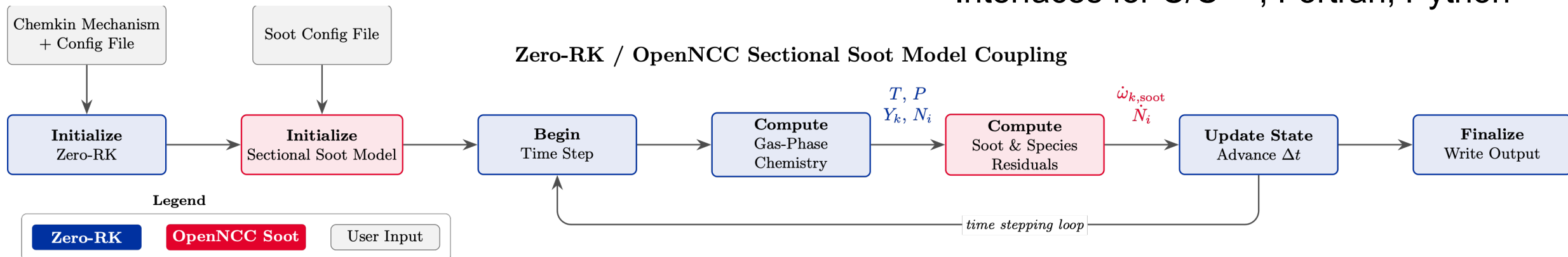
Zero-RK + OpenNCC Sectional Soot Model

• Zero-RK

- McNenly, Whitesides, Lapointe, Saggese and more from Lawrence Livermore National Laboratory
- Thermo-physics, 0D reactors, 1D flames, more (à la Cantera, Chemkin)
- Sparse adaptive preconditioning provides at least a 10x speedup vs Chemkin for large mechanisms

• OpenNCC Sectional Soot Model

- Fixed pivot method conserving first two moments (number, mass)
- Built for use in CFD solvers
- Fully coupled gas and soot phase → conserves mass
- Coupled to several solvers: Chemkin, Cantera, Zero-RK, OpenNCC
- Interfaces for C/C++, Fortran, Python



Adapting the Soot Model

Goal: Convert to “as-similar-as-possible” Chemkin → OpenNCC Soot

Challenge: OpenNCC Soot does not support explicitly tracked surface-site radicals

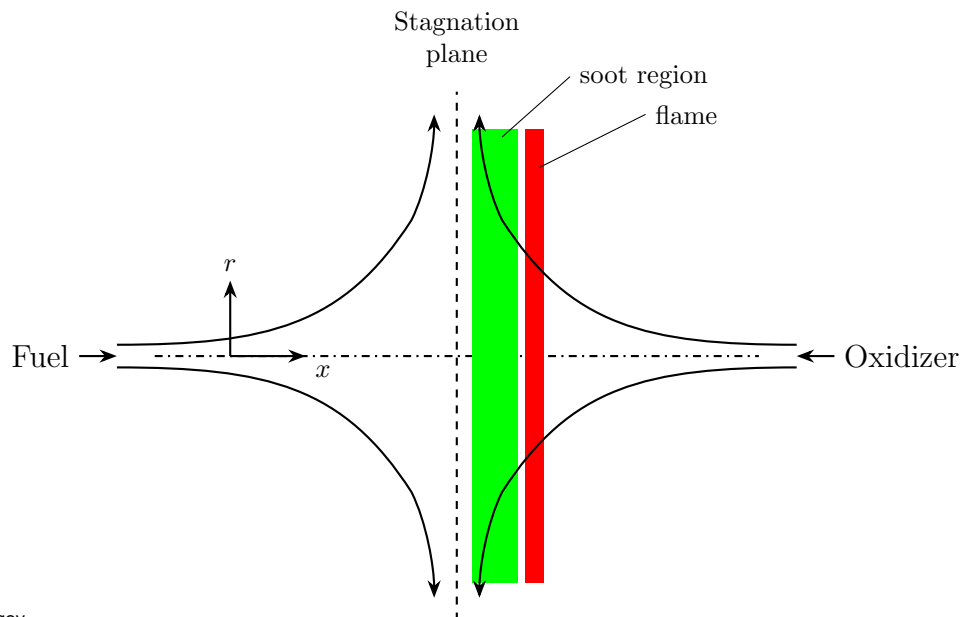
Approach: Use steady state approximation from Frenklach and Wang (1990)

Symbol	Meaning
C(B)	Bulk carbon
H(s)	Hydrogenated edge site
C(sr)	Radical edge site
O(s)	Oxygenated edge site

Process	Chemkin Soot Model	OpenNCC Soot Model
Surface Growth	$C(sr) + C_2H_2 \rightarrow H(s) + C(B) + H$ $r = k(T)[C(sr)][C_2H_2]$	$C_2H_2 + C(B) \rightarrow C(B) + H$ $r = k(T)\alpha\chi_{C(sr)}S_i[C(B)][C_2H_2]$
Oxidation	$O(s) + C(B) + O_2 \rightarrow CO_2 + C(sr)$ $r = k(T)[O(s)][C(B)][O_2]$	$C(B) + O_2 \rightarrow CO_2$ $r = k(T)\alpha\chi_{O(s)}S_i[C(B)][O_2]$

Validation case: Counterflow Diffusion

- Zero-RK provided gas-phase chemistry + CDF solver
 - 1st-order upwind spatial discretization



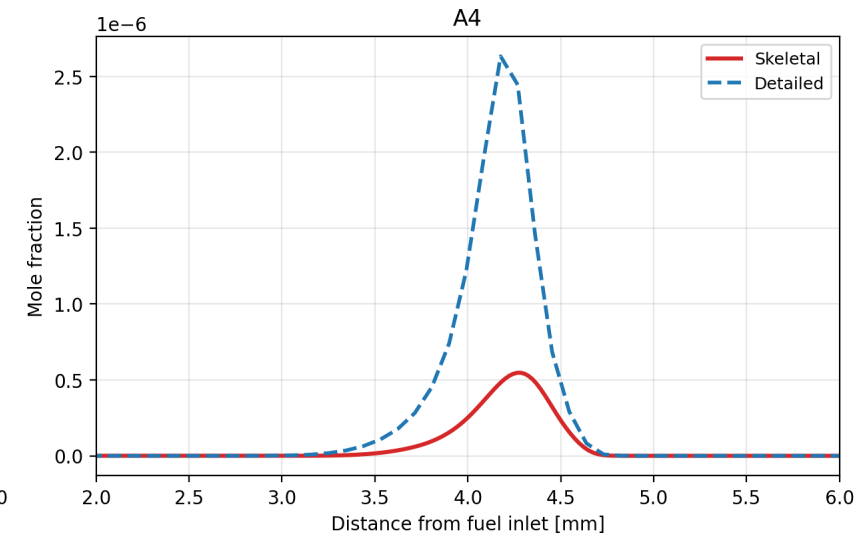
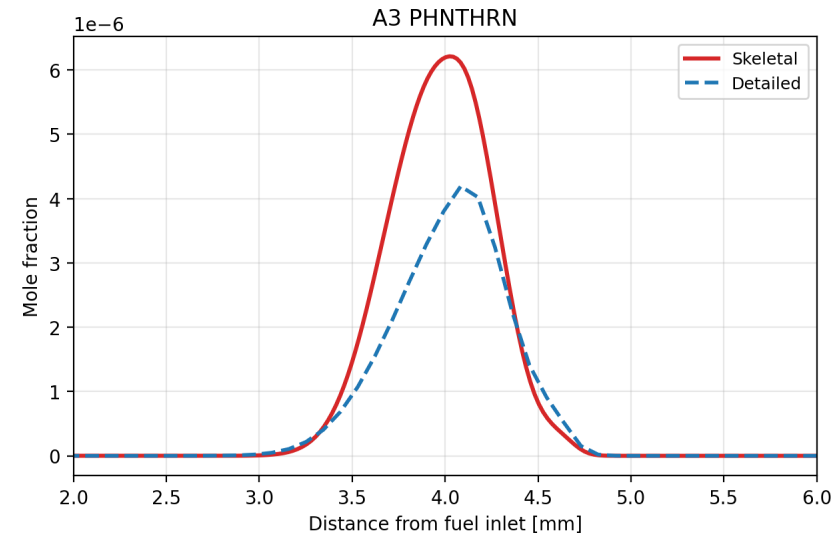
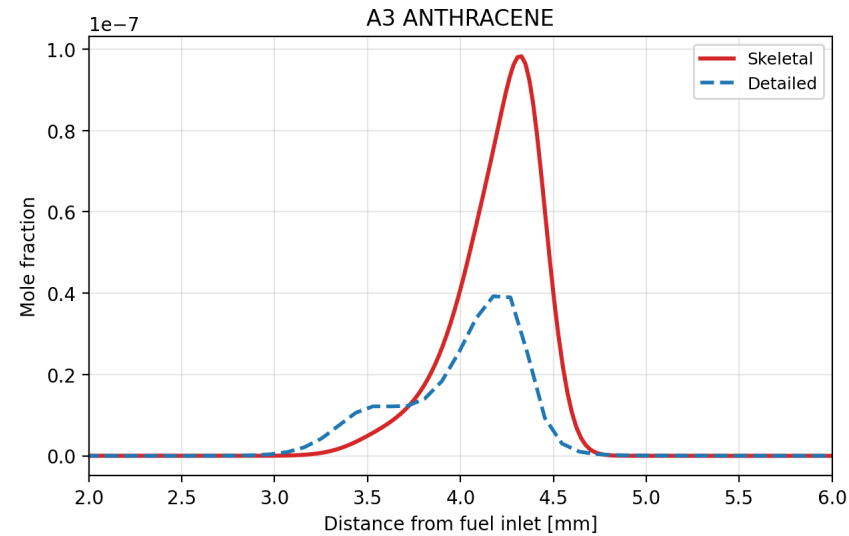
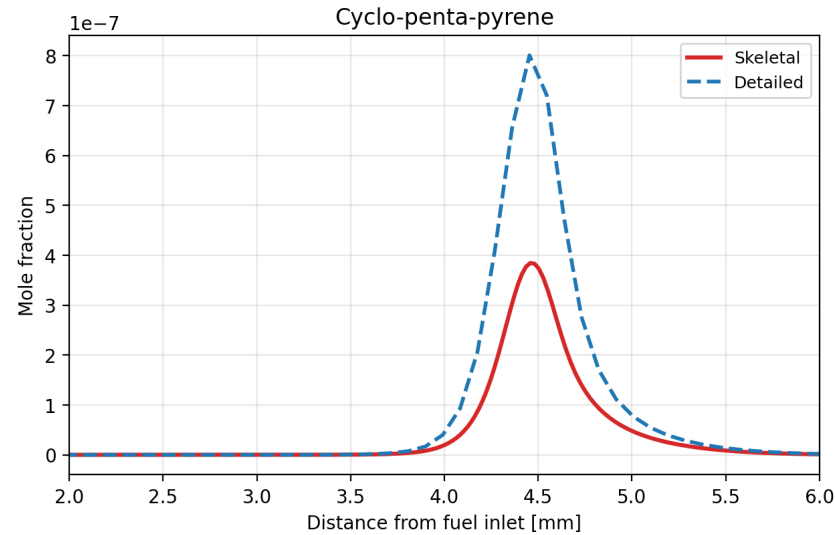
Parameter	Value
Number of bins	60
Growth Factor	1.4
Diameter range	1nm – 1 μ m
Soot density	1,800 kg/m ³

Parameter	Value
Spatial grid points	250
Domain length [mm]	11
Strain rate [1/s]	200
O ₂ mole fraction (remainder N ₂)	40%
Fuel mole fraction (remainder N ₂)	10%
Fuel temperature [K]	473
Oxidizer temperature [K]	473
Global equivalence ratio [ϕ]	4.15

Species results

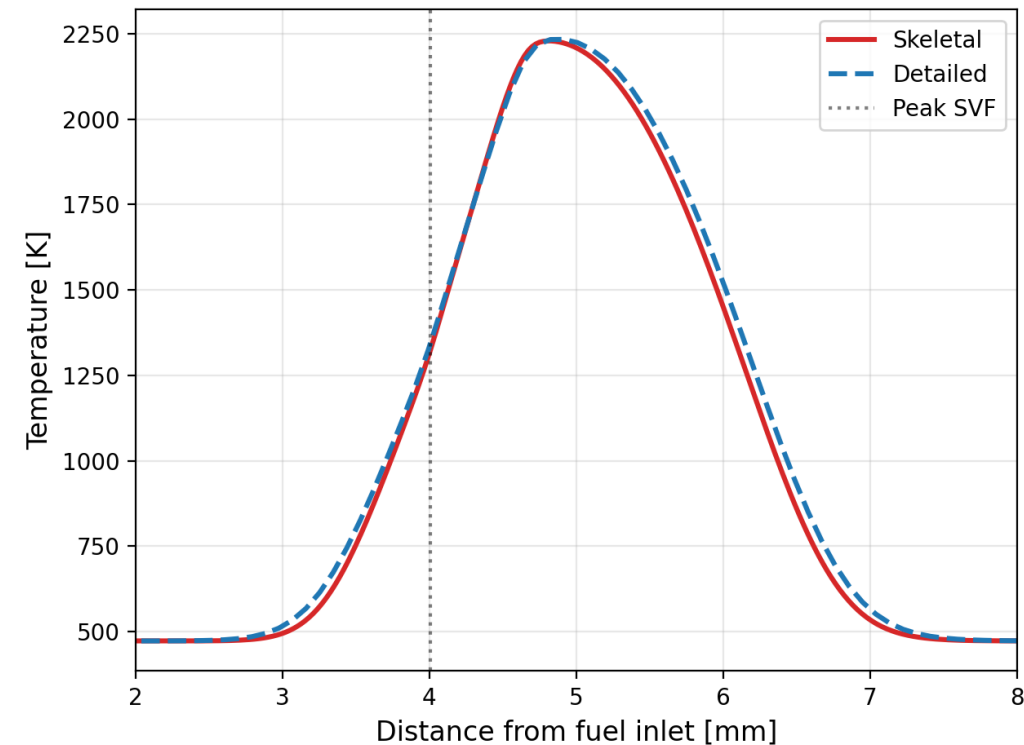
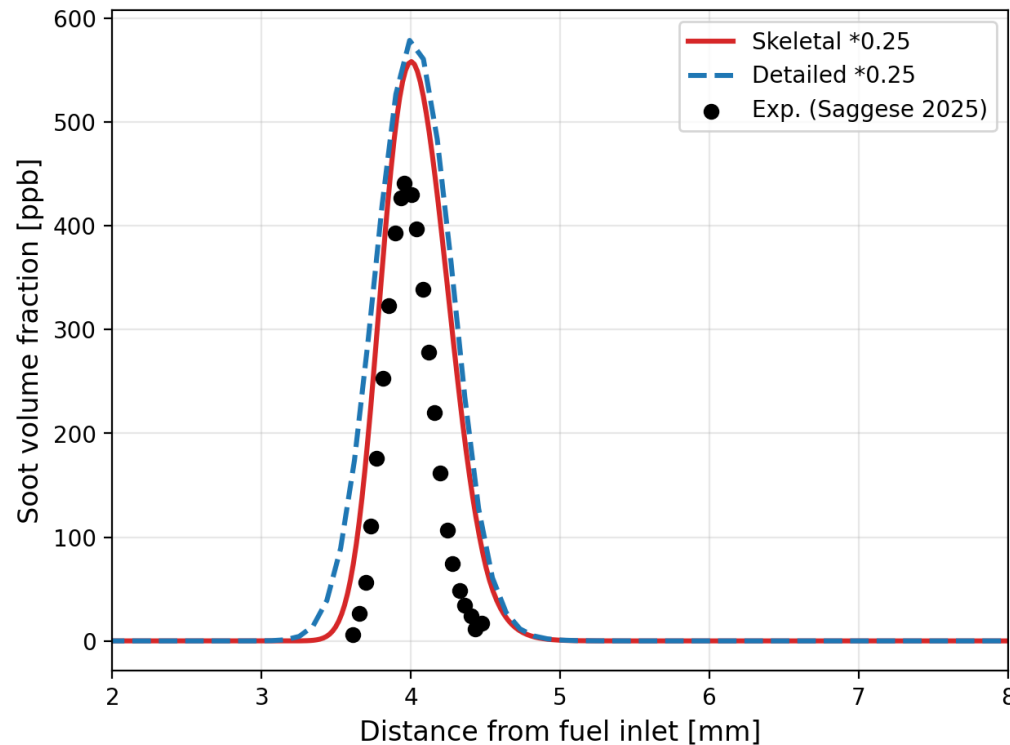
- Mechanism reduction targeted PAH species for retention

Reduced mech within
2x of detailed mech



Soot results

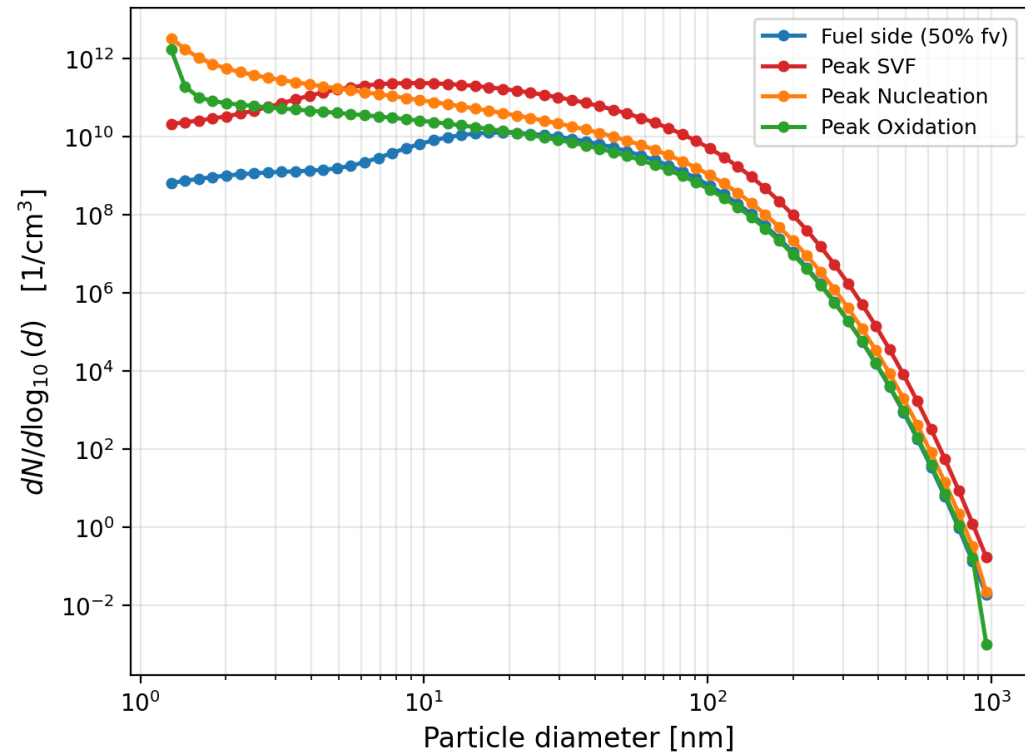
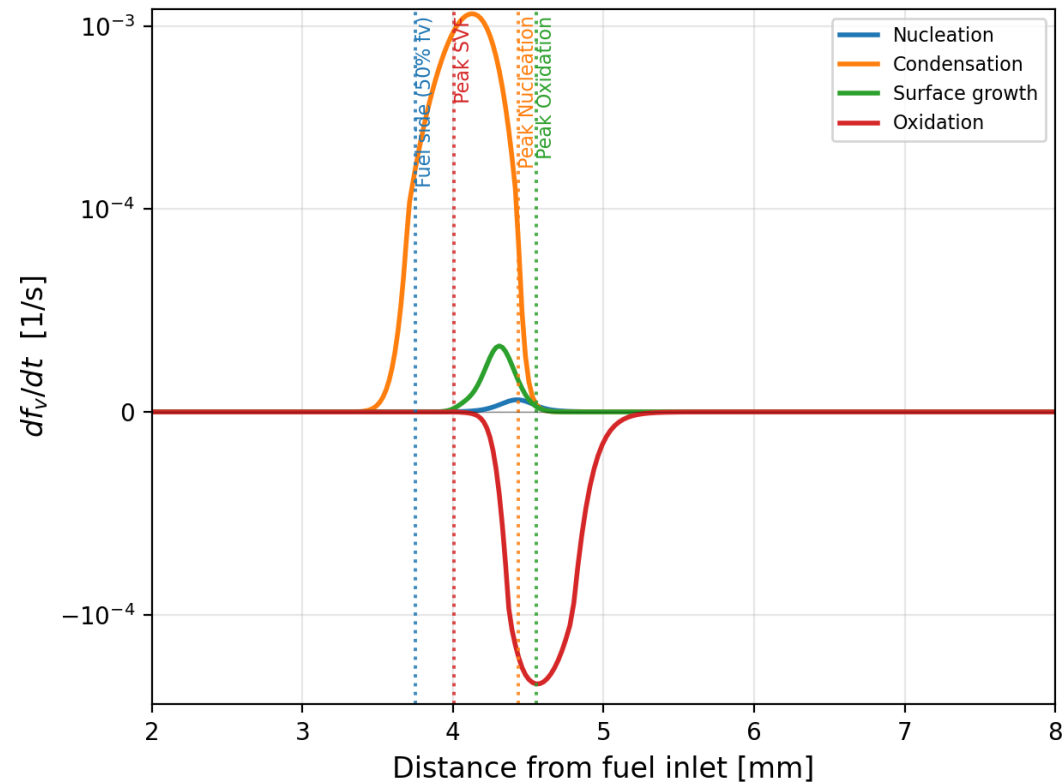
- Skeletal has close agreement with detailed
- Peak SVF location matched



- Following Saggese, numerical results transformed:
 - Shifted 1mm towards fuel inlet
 - SVF scaled by 0.25

Exp data: Saggese et al. 2025, Proceedings of the Combustion Institute

Soot PSD results



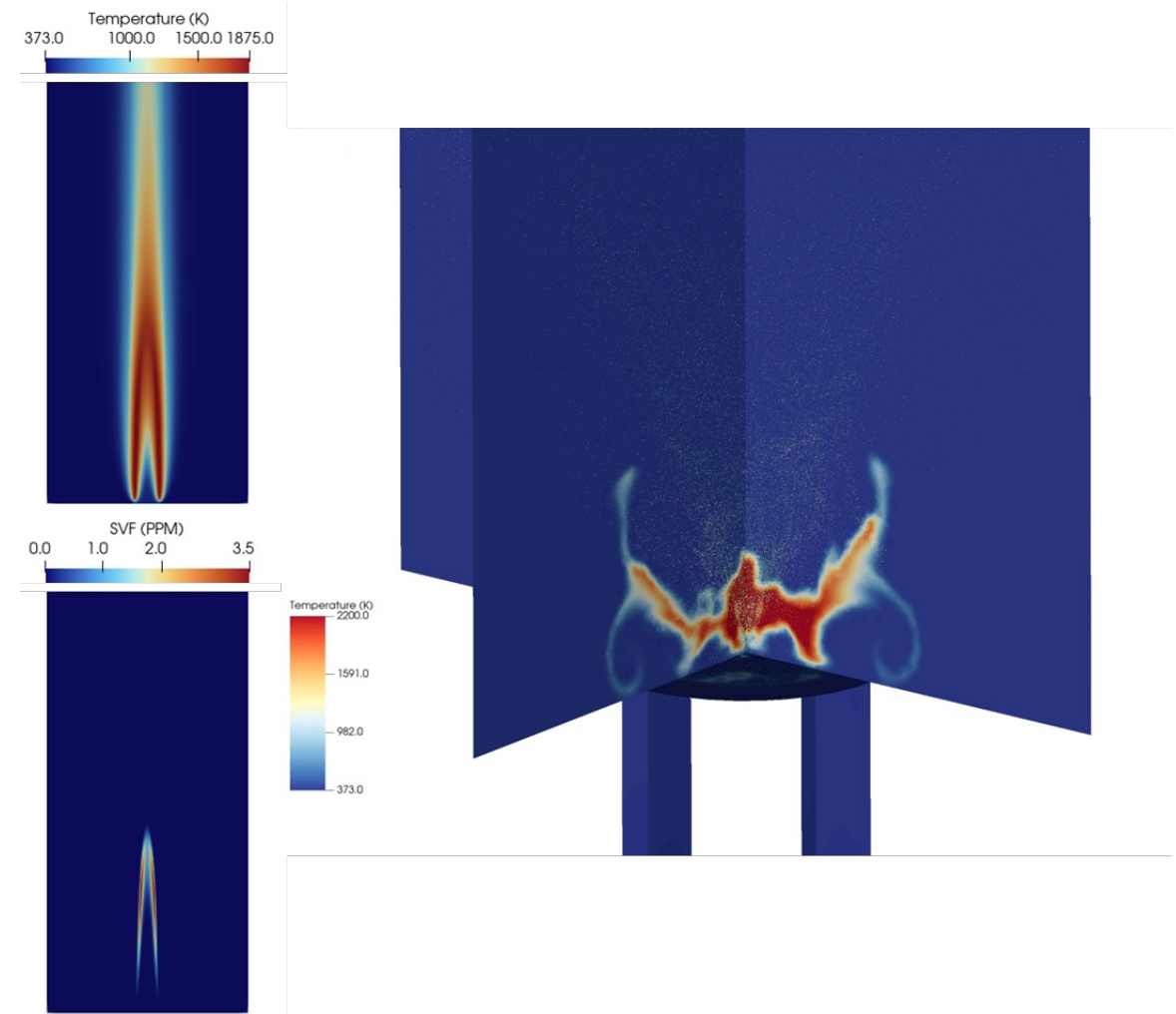
Unimodal distributions driven by
condensation dominance

Discussion and Conclusions

1. Skeletal mechanism retaining key PAH chemistry
 2. Validation of 308 species mechanism on laminar burning speed and IDT
 3. General agreement on number and mass emission indices in comparison with detailed and experimental results in reactor network
 4. Counterflow diffusion results show reasonable agreement to experimental results in small aromatics, accountable differences in soot, reasonable trends
- Need additional experimental Jet-A validation data, especially particle size distribution
 - Mechanism is still too large for finite rate chemistry in CFD simulations

Future Work

1. Improvements to the skeletal mechanism, e.g. rate value optimizations, further reductions in species counts
2. Improvements to the soot model chemistry, e.g. nucleation
3. Exercise reaction mechanism and soot model in CFD studies
 - Flamelet generated manifold chemistry closure for reaction mechanism





Analysis of a Surrogate Jet Fuel Skeletal
Mechanism With PAH Chemistry

Thank you for your attention. Any questions?

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