Time-History Statics of Soot Formation in A Model Gas Turbine Combustor

Kenji Miki[1], Francisco j Guzman[1], and Kumud Ajmani[2]

[1]NASA Glenn Research Center, Cleveland, OH

[2]HX5 LLC, Brook Park, OH

ASME Turbo Expo 2026

Turbomachinery Technical Conference and Exposition

GT2026-176156, June 15-19, 2026

Outline

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- Problem Setup
  - In-house CFD code, OpenNCC
  - Soot Modeling, two-equation model
  - Test Case: DLR Aero-Combustor
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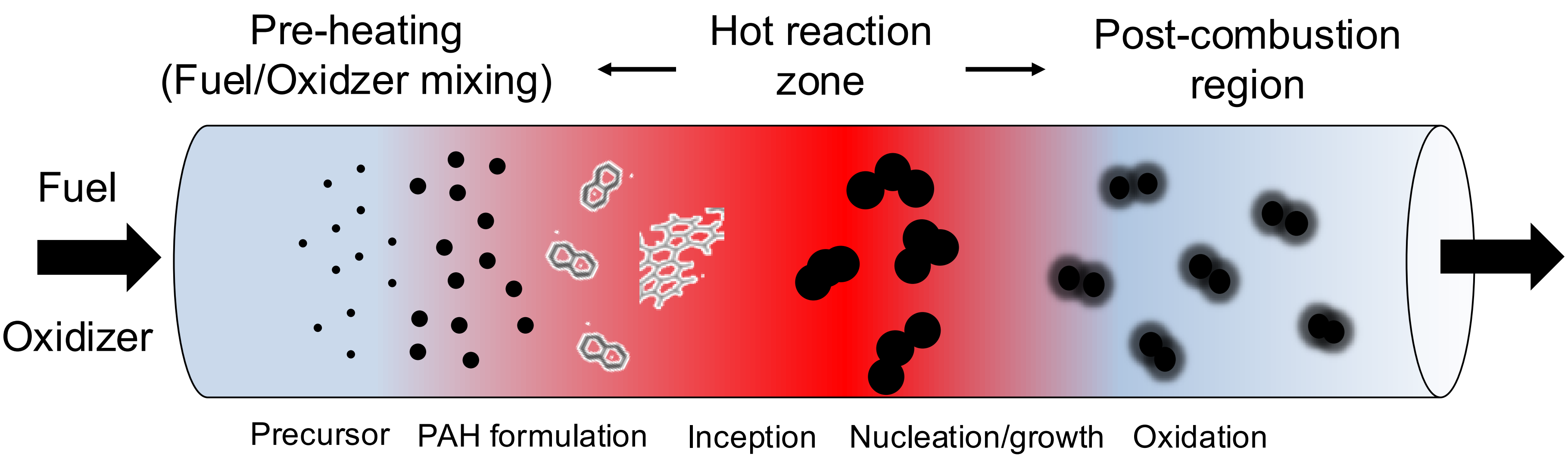
  - Time-History Statistic of Soot Formation
- Results
  - Particle-based Statistic vs. LES results
  - Identification of Key Soot Formation Region (temperature, equivalence ratio, and species)
  - Discussion of Model Deficiency and Possible Model Improvement
- Conclusion

[1] Ajmani, K., Guzman, F. J., and Miki, K., 2025,," Proceedings of the ASME Turbo Expo Memphis, Tennessee.

Introduction: Motivation and Background

- Soot formation is a complex dynamic and intermittent process. Although the major steps in soot formation, **formation of precursors**, **inception**, **growth** and **evolution**) are similar for a variety of carbonaceous fuels, applications, and operating conditions, it remains unclear when the temporal transition between these steps occurs.



An engineering prediction tool coupled with computational fluid physics (CFD), therefore needs to accurately model all these complex steps of soot formation.

Introduction: Soot Model

- There are two types of soot models: semi-empirical precursor models and detailed models solving for the particle size distribution function and number density function.

Detailed models:

- ❖ It solves for the distribution functions via an approximation of the population balance equation (PBE)
- ❖ There are closure modes for PBE equations: variants of the method of moments (*e.g*., MOMIC[1], DQMOM[2] , CQMOM[3], HMOM[4]) and the sectional methods (e.g., BMMSM[5]).
- ❖ Computationally expensive, but better representation of the characteristic complex soot formations (*e.g*., bimodal soot size distribution, *etc.)*

Semi-empirical precursor models:

- ❖ It solves for the soot mass fraction and soot number density scalars, but do not solve for the distribution functions.
- ❖ Computationally inexpensive, but modeling uncertainty in the empirical kinetics coupled with chemistry including fuel decomposition steps, oxidation, and aromatic carbon species formation.

[1] Frenklach, M., 2002, Chemical Engineering Science, 57, pp. 2229 – 2239. ,[2] Marchisio, D. L., and Fox, R. O., 2005, Journal of Aerosol Science, 36(1), pp. 43-73., [3] Yuan, C., and Fox, R. O., 2011, Journal of Computational Physics, 230(22), pp. 8216-8246.[4] Mueller, M. E., Blanquart, G., and Pitsch, H., 2009, Combustion and Flame, 156(6), pp. 1143-1155.[5] Maldonado Colmán, H., Attili, A., and Mueller, M. E., 2024, Combustion and Flame, 265, p. 113496.

Our Numerical Approach for Soot Prediction [X]

- **Solver**: In-house CFD code, OpenNCC, with 2nd order upwind differencing, explicit time-stepping, LES solver (two-equation, non-linear k-ε model with sub-filtering).

- **Chemistry**: Multiple Time-Scale Flamelet Progress Variable (MTSFPV[1]) with the flamelet table generated using Flamelet Generation Manifold (FGM) method. 75-species Skeletal Kinetics [2] for Ethylene fuel was used.

- **Soot Model [**Fairweather, *et al.*1992]**:**
  - Source terms for soot mass fraction and soot number density computed with semi-empirical, two-equation model

$$\frac{\partial}{\partial t}\left(\bar{\rho}\,\overline{Y}_{p,j}\right) + \frac{\partial}{\partial x_i}\left(\bar{\rho} u_i \overline{Y}_{p,j}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}(D + D_T)\frac{\partial \overline{Y}_{p,j}}{\partial x_i}\right) = \overline{\dot{S}_{p,j}}$$

$$\overline{\dot{S}_{p,j}} = S_1 + S_2 - S_3$$

S_1: soot nucleation, S_2: surface-growth and S_3: oxidation source

Acetylene is the only soot nucleation and growth species, and O_2 and OH are used for oxidation.

[1] Ajmani, K., Guzman, F. J., and Miki, K., 2025,," Proceedings of the ASME Turbo Expo Memphis, Tennessee. [2]Wang, H., and Frenklach, M., 1997, Combustion and Flame, 110, pp. 173-221.

Open National Combustion Code (OpenNCC)

OpenNCC is the releasable version of the National Combustion Code (NCC), which has been continuously updated for more than two decades at NASA Glenn Research Center (GRC)

Main Features

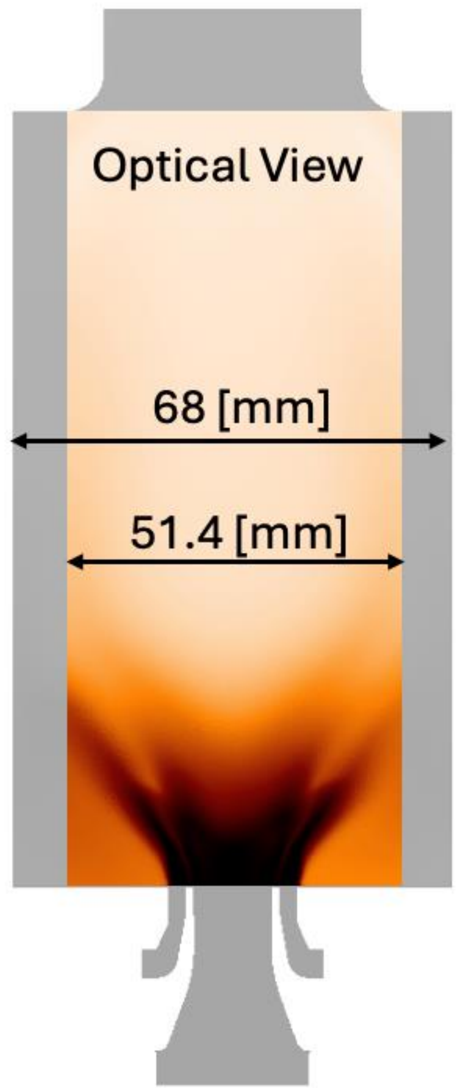
- ✓ Numerics: Central scheme + Jameson-Schmidt-Turkel (**CD-JST**) scheme, upwind scheme + Roe/**AUSM**
- ✓ Turbulence: **Cubic non-linear k-ε model with the wall function**, Low-Re model, local dynamic k-model (LDKM)
- ✓ Combustion: Finite Rate Chemistry, eddy-breakup model (EBU) , PDF , Linear Eddy Model (LEM), Dynamic Thickened Flame Model (DTF), **Table-Lookup (MTSFPV)**
- ✓ Spray: Lagrangian liquid phase model
- ✓ Soot Model: sectional method and **semi-empirical 2-equation model model**[1]
- ✓ Other features: Low-Mach preconditioning, transition model, unstructured mesh, adaptive mesh refinement (AMR), sliding mesh, radiation, massively parallel computing

[1] Fairweather, M., Jones, W. P., and Lindstedt, R. P., 1992, Combustion and Flame, 89, pp. 45-63.

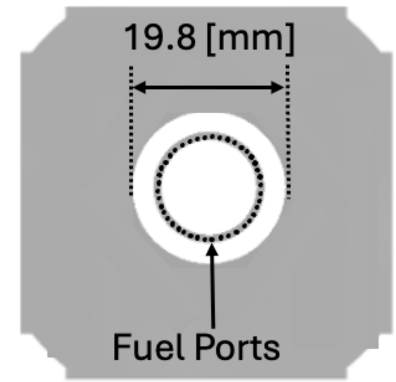
DRL Aero-Combustor [1]

(a) 3D view

(b) Cross section and Optical View



(c) Endwall



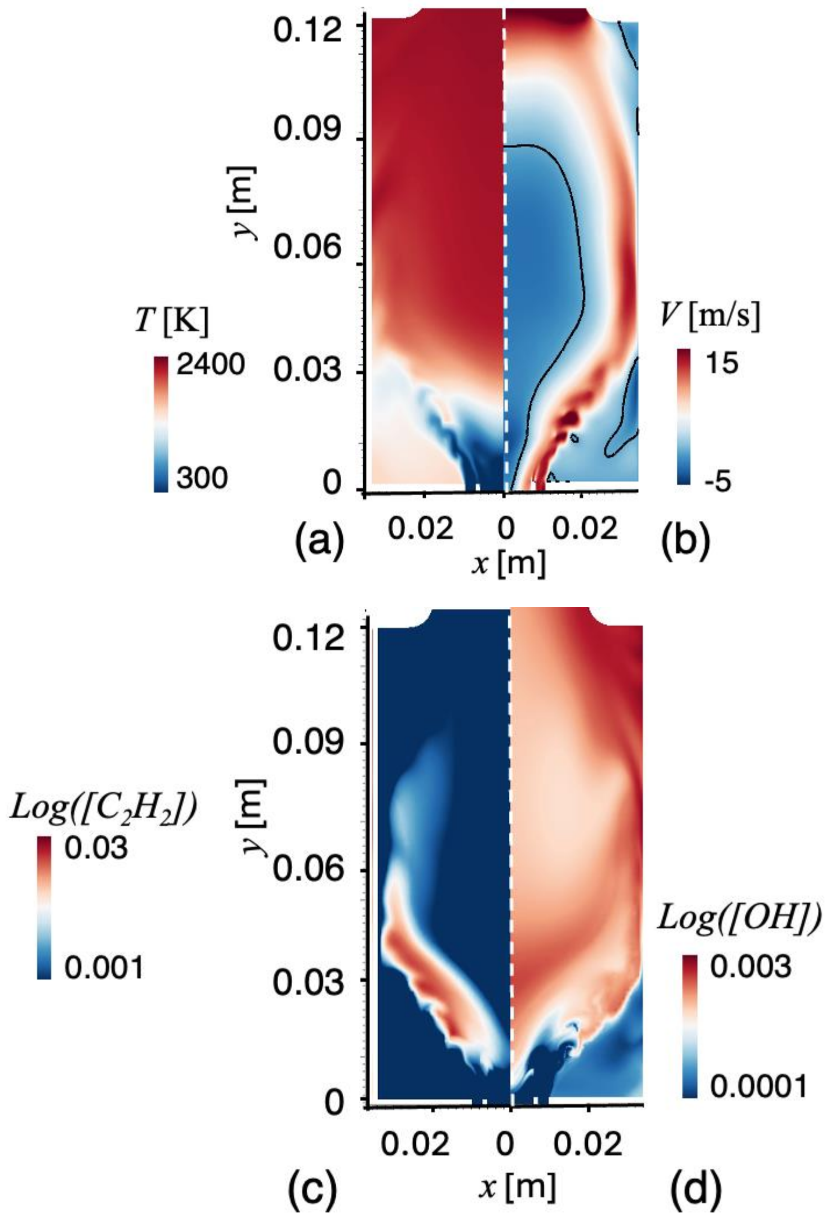
Operating condition

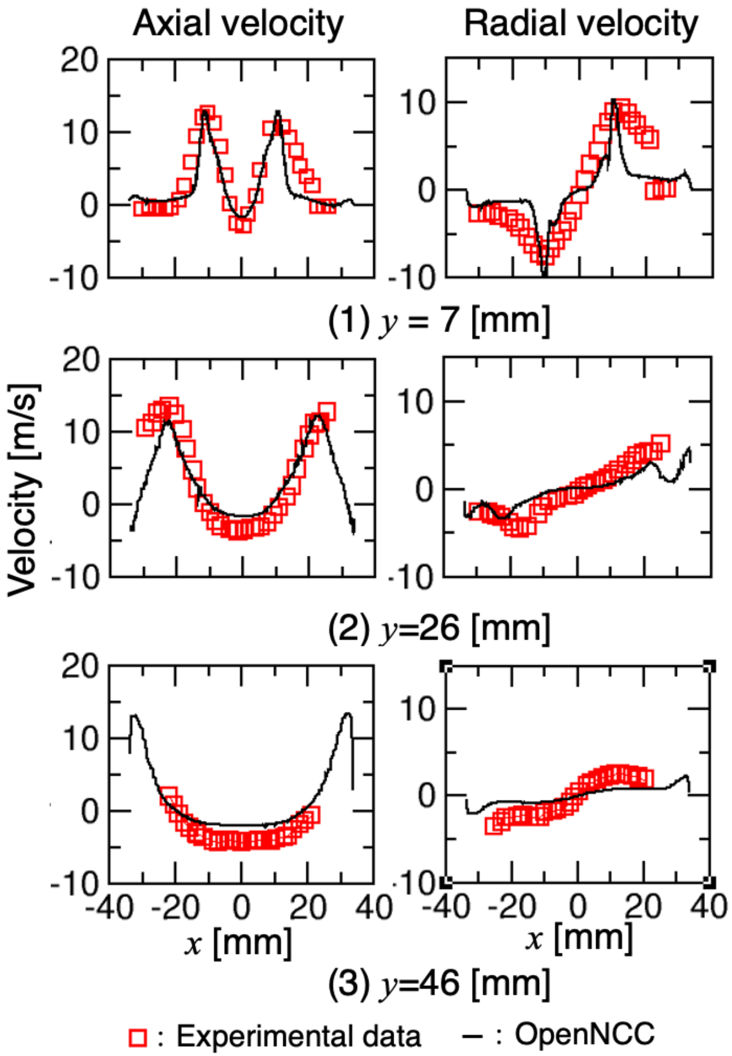
	Ring air	Central air	Fuel (C_2H_4)
MFR [g/s]	7.08	3.03	0.83
T [K]	297	297	293

- The detailed measurements of the soot, temperature and velocity fields were acquired by DLR [1]
- The gaseous fuel (ethylene) is injected in the gap between the two air streams.

[1] Geigle, K. Pel al., Journal of Engineering for Gas Turbines and Power, 136(2)

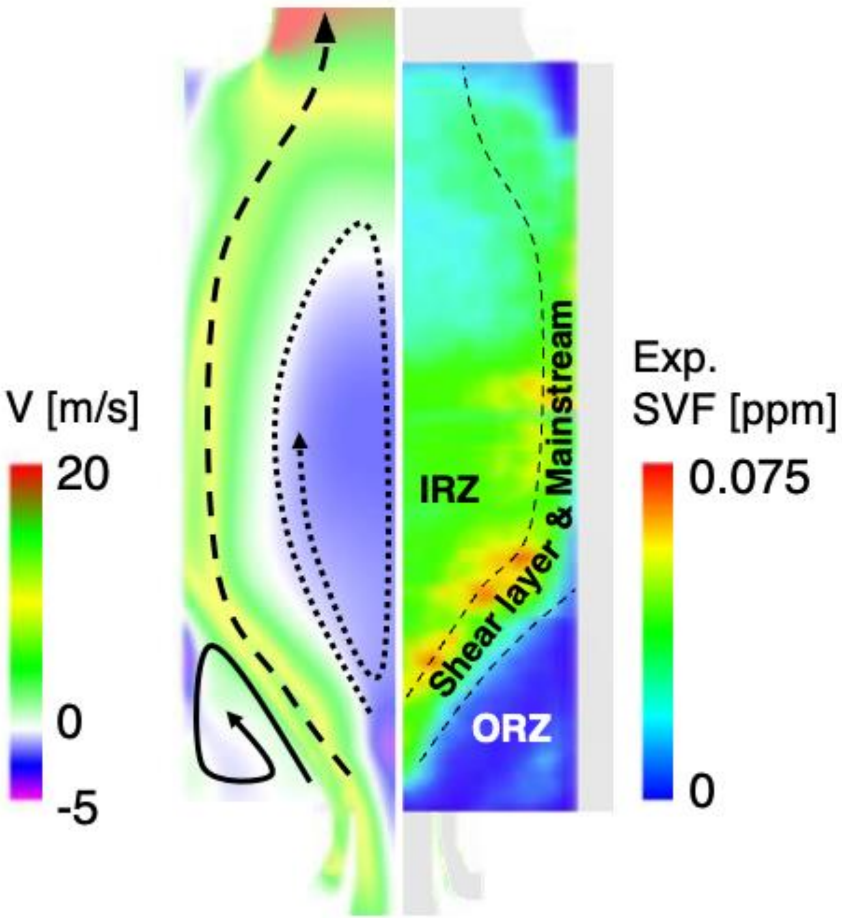
Instantaneous/Time Averaged Flow Fields





MTSFPV predicted the flow fields reasonably well.

Soot Formation and Particle Trajectory



(Left) Schematic Particle Paths

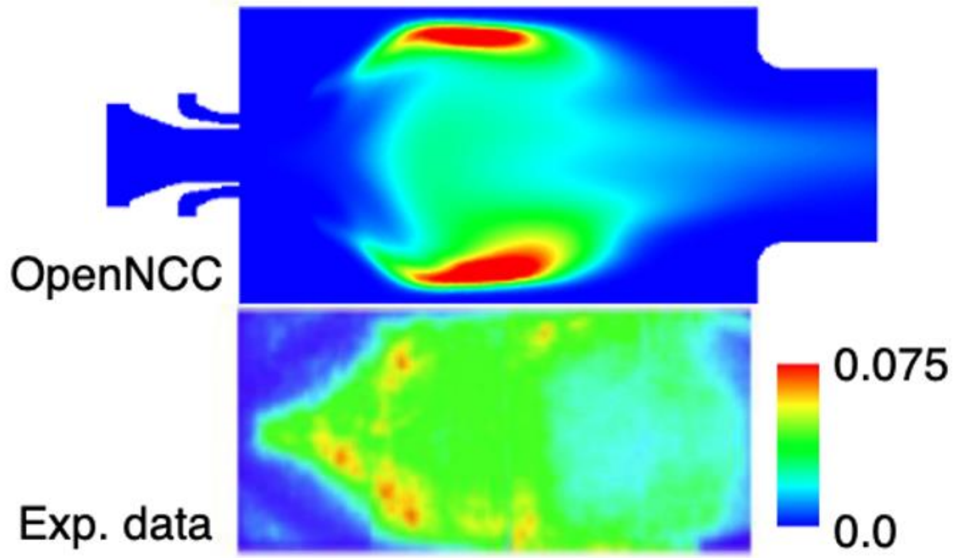
(Right) Three Soot Formation Regions

<u>Key Observation</u>

- There are 3 primary flow regions:
  1. outer recirculation zone (ORZ)
  2. inner recirculation zone (IRZ)
  3. the shear layer / mainstream region
- Primary areas of soot formation are the shear layer/mainstream region and IRZ.
- The soot formation takes place in the pockets of rich burned gas, and soot quickly oxidizes in the *OH*-rich lean burned gas regions (downstream)

We consider only soot formation along the shear layer / mainstream region.

Predicted Soot Volume Fraction (SVF)



- This model uses only acetylene as the soot precursor and ignores the PAH species and other gaseous soot precursors (*e.g.*, benzene, pyrene, *etc.*).
- The sub-filter scale turbulence-chemistry-soot interactions are not explicitly modeled.
- The soot formation and evolution are known to occur by a very specific range of gas-phase compositions [1] → Any sharp local variations in species concentration that favor soot-formation cannot be explicitly resolved.

Our objective is to address the weaknesses of the semi-empirical soot model by proposing modifications based on **time-history effect.**

[1]Han, W., Raman, V., Mueller, M. E., and Chen, Z., 2019, Proceedings of the Combustion Institute, 37(1), pp. 985-992.

Time-History Effect

Japan Cheery Blossom Forecast

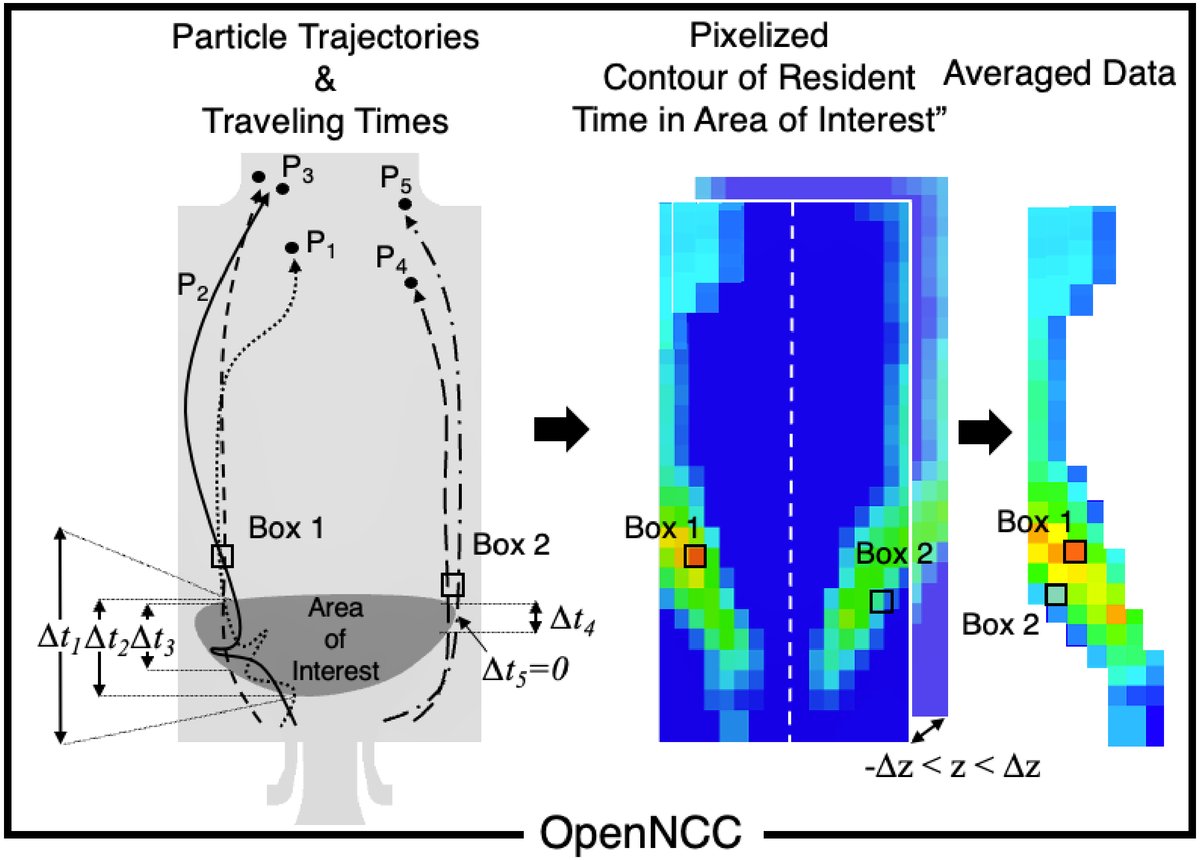
Rule of Cherry Blossom Blooming

According to the **"600°C rule"**, you add up each day's maximum temperature (in °C) starting from February 1st, and when the total reaches 600°C, the cherry blossoms bloom!

This simple formula is so accurate that Japan Meteorological Agency has used it for years.

Some of physical phenomena are greatly influenced by "time-history effect".

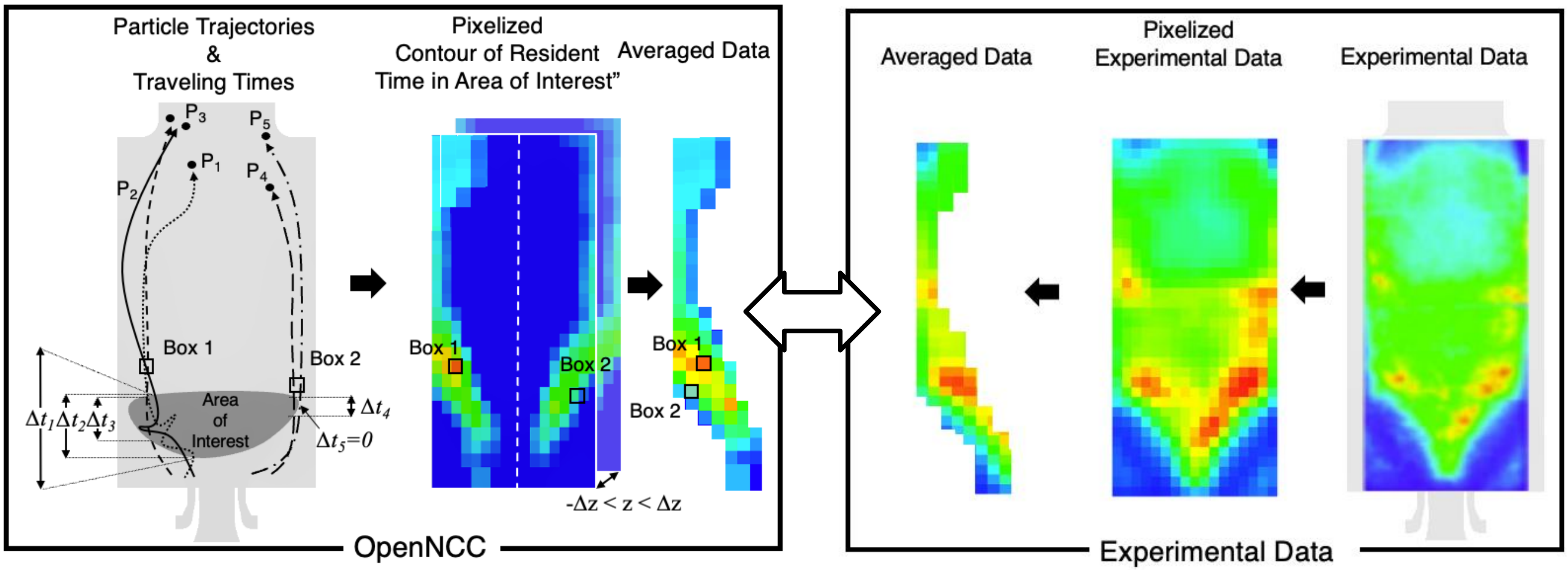
Schematic of Particle Based Statistical Approach -1-



Step 1: The area of interest (AoI) (e.g., 1200 [K] < T < 1300 [K], *etc.*) is defined.
Step 2: The 10,000 massless particles are randomly injected and records residence time (τ) of each particle in the AoI.
Step3: Post-processing: At the end of particle data collection, particle statistics (e.g., τ) within spatial bins or boxes are calculated.
Step 4: The pixelized contour plots of residence time (τ) are constructed and the contour is folded for averaging.

Schematic of Particle Based Statistical Approach -2-

From OpenNCC | From experimental data [1]



Step 5: Similar to **Step 4**, the experimental profile of the soot volume fraction is pixelized and folded for averaging.

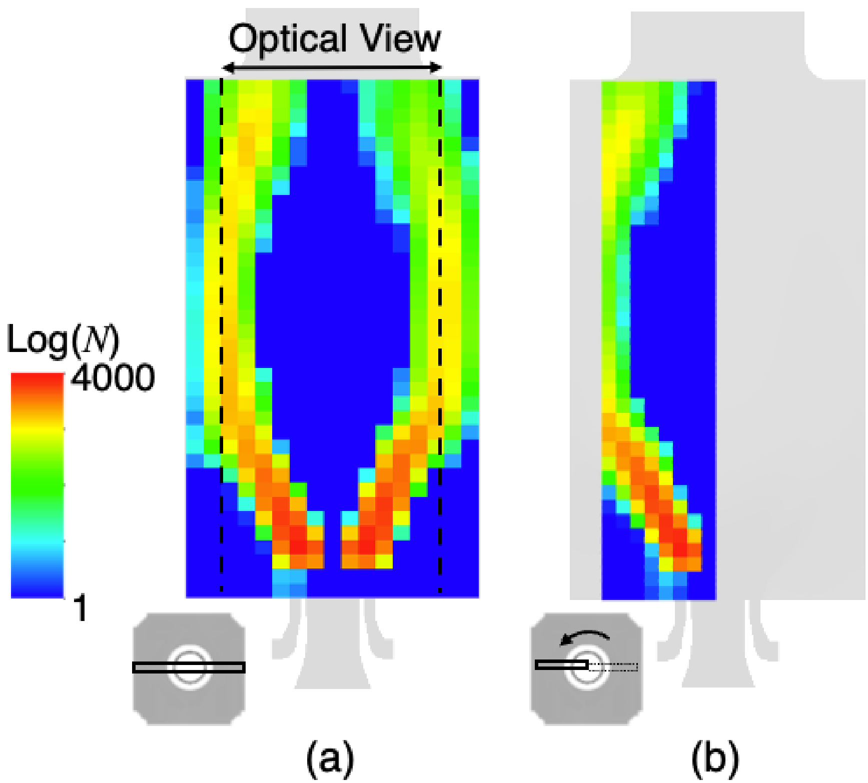
Step 7: The correlation coefficient, which refers to "**time-history correlation coefficient**" (THCC), between the two pixelized profiles (CFD particle data and experimental data) is calculated.

THCC answers "*if a reactive pocket of gas stays in a fuel rich region for a long time at a specific temperature, then how does such a time-history of the fluid in that region produce soot at a later time or location?*"

[1] Geigle, K. Pel al., Journal of Engineering for Gas Turbines and Power, 136(2)

Sanity Check: Statistical Convergence

Particle number density



Sanity Check: Statistical Convergence

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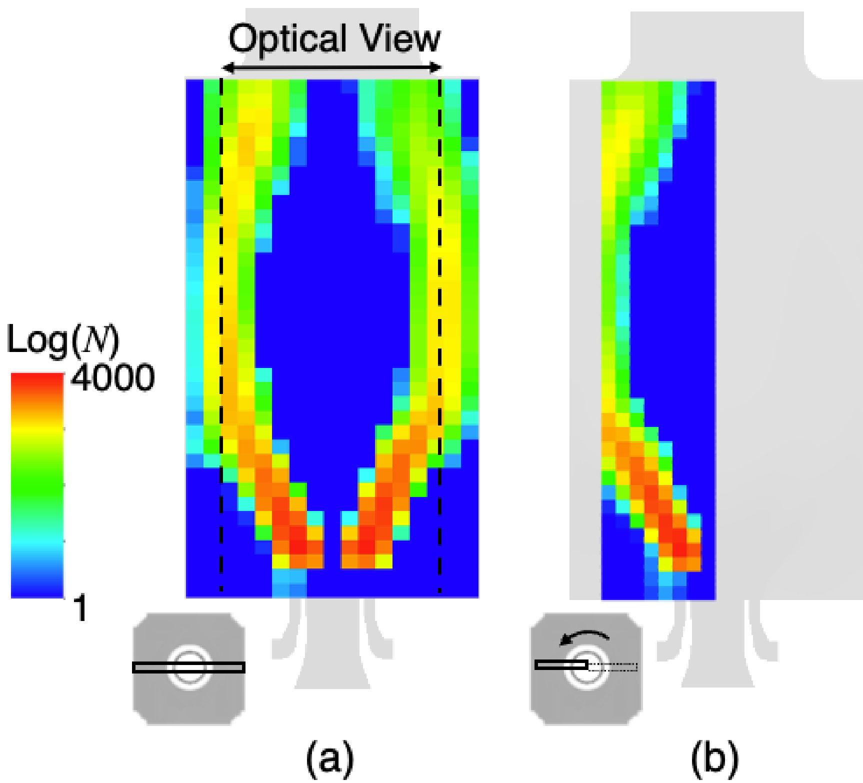
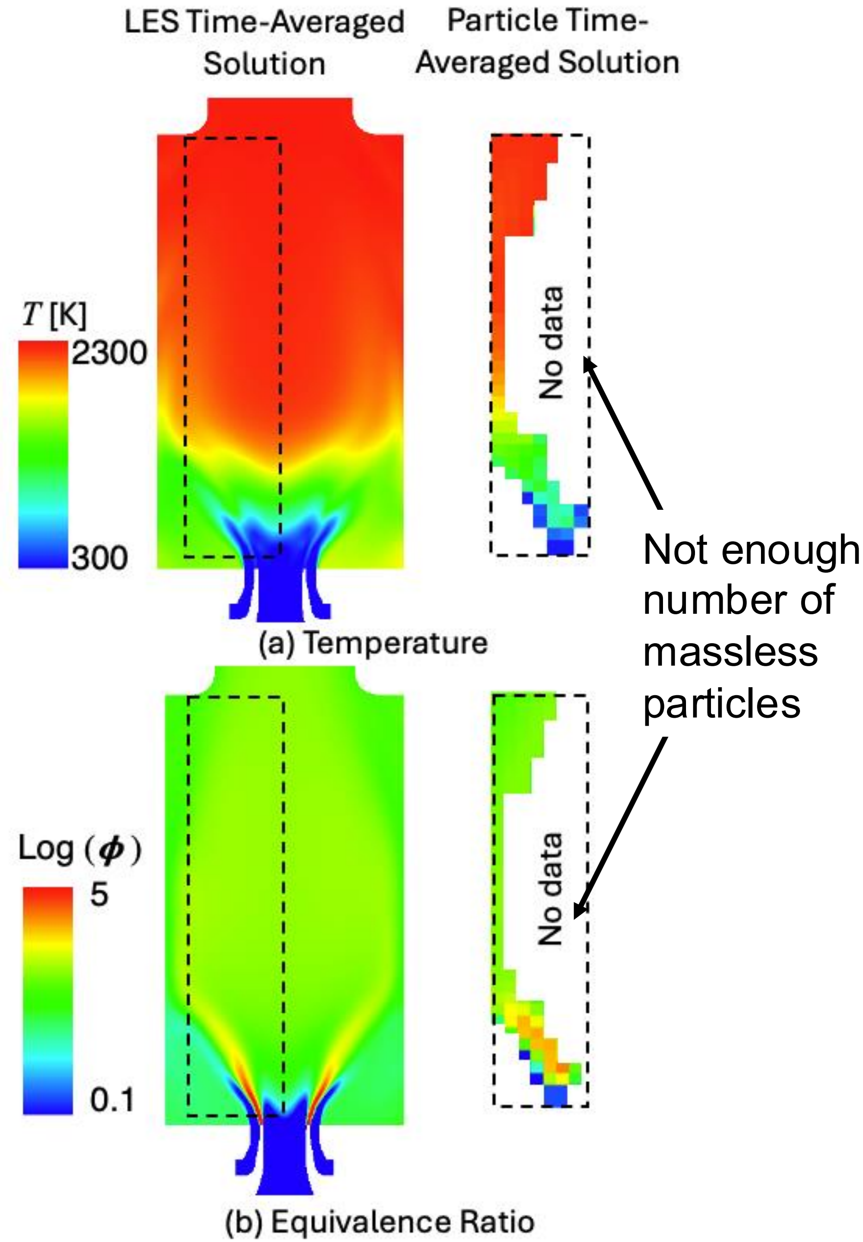
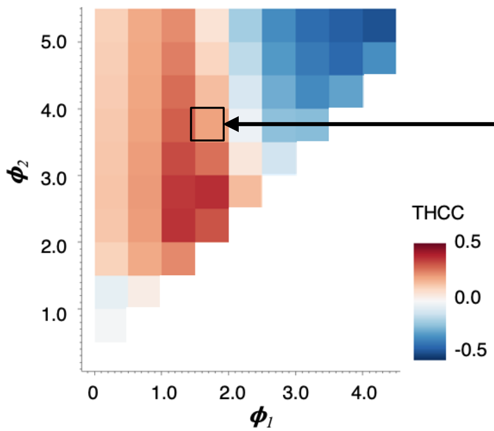




- It is confirmed that there are enough number of particles reaching each “box” so that the predicted flow fields are consistent with time-averaged LES result.

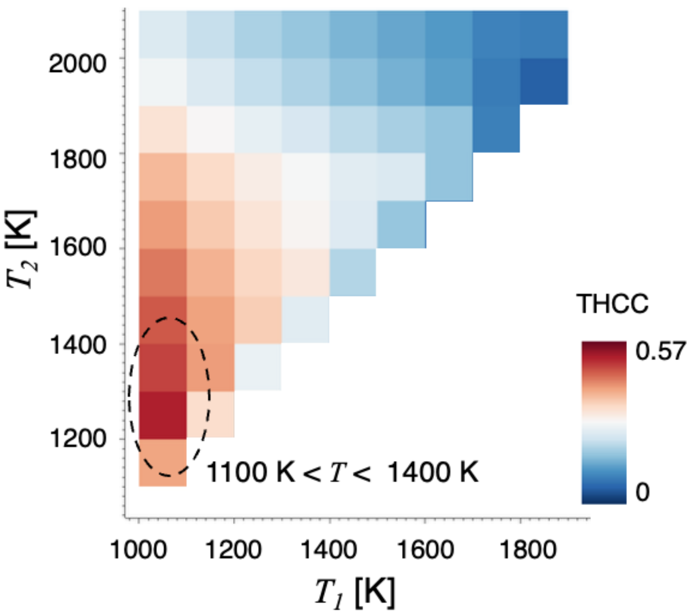
Time-History Correlation Coefficient (THCC) Results

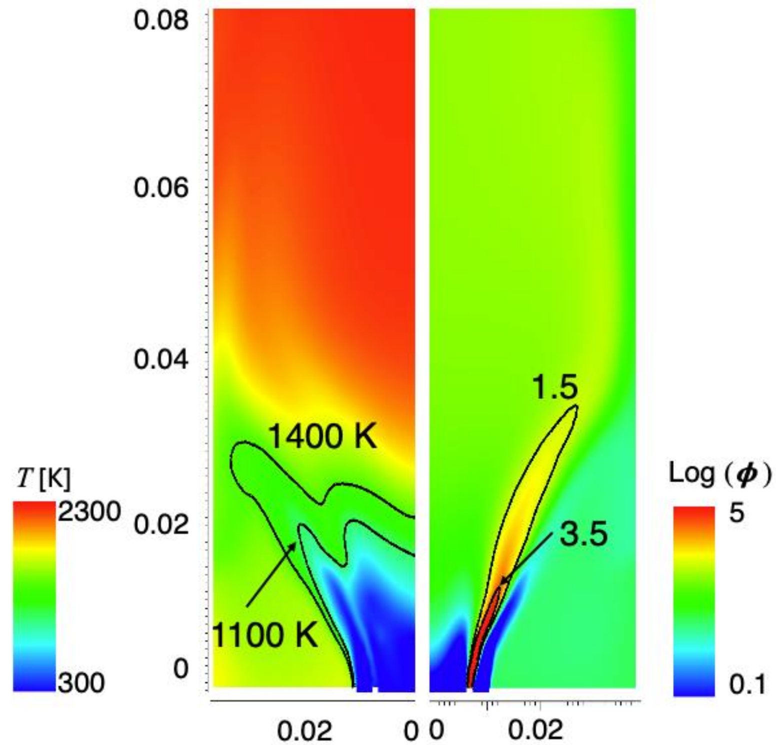


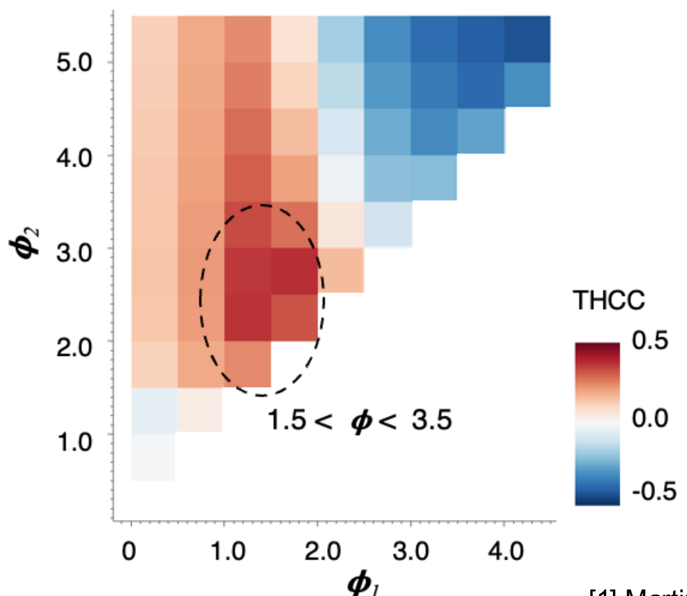
Calculate the THCC for each "box" specified by the AoI, say *1.5 < ϕ < 4.0*

Dark blue/red says "the particles staying in the AoI longer/shorter in the past correlate the soot formation later"

THCC Matrix: Temperature and Equivalence ratio





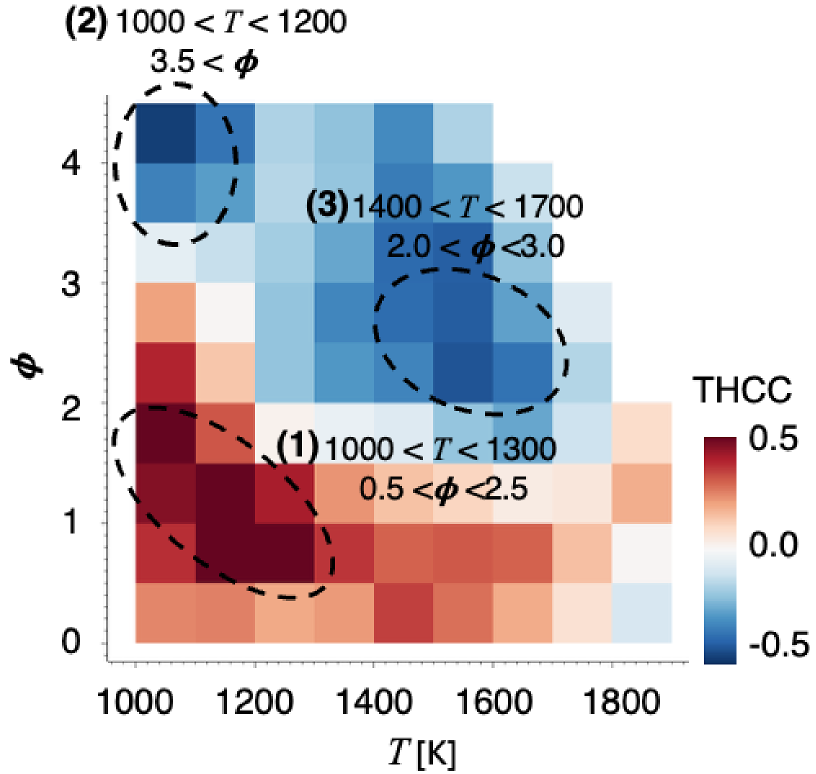


- The soot formation is favored in a fuel-rich region, and the soot oxidizes in the hot region in the presence of hydroxyl radicals, OH, O2 and O.
- These results are consistent with the "**soot bell curve**" or "**soot island**" formation threshold, where the soot concentration peaks within a specific range of conditions[1].

[1] Martin, J. W., Salamanca, M., and Kraft, M., 2022, Progress in Energy and Combustion Science, 88

Key Regions of Temperature + Equivalence Ratio

We can combine two parameters, T, and ϕ to specify the AoI.



Region (1) : 1000 [K] < T < 1300 [K] and 0.5 < ϕ < 2.5

Region (2) : 1000 [K] < T < 1200 [K] and 3.5 < ϕ

Region (3) : 1400 [K] < T < 1700 [K] and 2.5 < ϕ < 3.0

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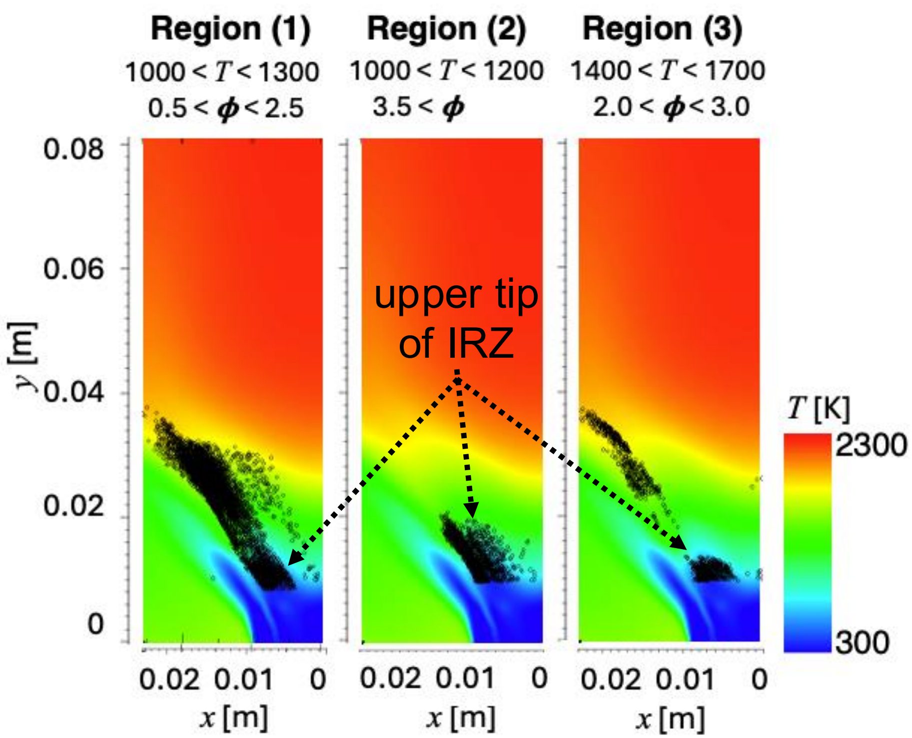


It is experimentally observed that the upper tip of IRZ is full of intermittent mixing of pockets of rich burned gas, OH-rich lean and cold air *[1]*

Region (1) : 1000 [K] < T < 1300 [K] and 0.5 < ϕ < 2.5

- The inner side of the shear layer, the moderately fuel-rich region where the fuel and oxidizer rapidly mix together.

Region (2) : 1000 [K] < T < 1200 [K] and 3.5 < ϕ

- The very fuel-rich cold region, which is near the upper tip of the IRZ.

Region (3) : 1400 [K] < T < 1700 [K] and 2.5 < ϕ < 3.0

- A combination of **Region (1)** and **Region (2)**

[1] Litvinov, I., Yoon, J., Noren, C., Stöhr, M., Boxx, I., and Geigle, K. P., 2021, Combustion and Flame, 231.

Investigation of Critical Species

Using the correlation between species profiles, experimental SVF and THCC, we could identify the key species out of 75 species (ethylene combustion, developed by Wang *et al.* [1])

Species	Max concentration	CC with Exp. Data (soot)	Max. THCC. with Exp. Data (soot)
O	2.10E-04	0.07	0.45
O_2	1.60E-01	-0.17	0.73
H_2	4.00E-03	0.018	0.43
OH	2.00E-03	0.17	0.65
CO	7.30E-02	0.37	0.21
HCO	1.60E-06	-0.4	0.74
CH_2*	1.20E-07	-0.24	0.76
C_2H_2	2.70E-02	-0.27	0.73
C_2H_4	2.60E-01	-0.48	0.75
C_3H_3	2.40E-05	0.08	0.57
C_4H	6.00E-08	-0.15	0.45
C_5H_5	2.80E-06	0.2	0.4
C_6H_5	5.60E-07	0.19	0.63
C_6H_6	2.20E-04	-0.15	0.36

(shaded rows) : Max. Corr. Coeff. Time-His. with Exp. Data > 0.6

[1] Wang, H., and Frenklach, M., 1997, Combustion and Flame, 110, pp. 173-221

Investigation of Critical Species

Using the correlation between species profiles, experimental SVF and THCC, we could identify the key species out of 75 species (ethylene combustion, developed by Wang *et al.* [1])

1. **Fuel and small hydrocarbons** (C_2H_2, C_2H_4, C_3H_3)

2. **Oxidation species** (OH, O, O_2, H_2).
Although H_2 is not a direct oxidant, it was evaluated because it is a by-product indicating a spontaneous process relevant to soot formation has occurred [2].

3. **Species that can be measured** (CH*, *etc.,* CH_2* was initially selected as a CH* representative)

4. **Aromatic Species** (C_6H_6, C_6H_5). **Benzene**, C_6H_6,[1,3] and **phenyl** ,C_6H_5, [4-6] were evaluated as they both are key species involved in the formation of higher order

Many species such as O_2, OH, *and* C_6H_5, show very strong THCC, but very weak correlation with respect to experimental data.

→ **Different species have a different way to contribute to soot formation**.

[1] Wang, H., and Frenklach, M., 1997, Combustion and Flame, 110, pp. 173-221
[2] Wang, H., 2011, Proceedings of the Combustion Institute, 33(1), pp. 41-67
[3] Hansen, N., Yang, B., Braun-Unkhoff, M., Ramirez, A., and Kukkadapu, G., 2022, Combustion and Flame, 243.
[4] Chu, T. C., Buras, Z. J., Smith, M. C., Uwagwu, A. B., and Green, W. H., 2019, Phys Chem Chem Phys, 21(40), 22248-22258.
[5] Couch, D. E., Zhang, A. J., Taatjes, C. A., and Hansen, N., 2021, Angew Chem Int Ed Engl, 60(52), pp. 27230-27235.
[6] Johansson, K. O., Head-Gordon, M. P., Schrader, P. E., Wilson, K. R., and Michelsen, H. A., 2018, Science, 361(6406), pp. 997-1000.

Further Reduction of Key Species

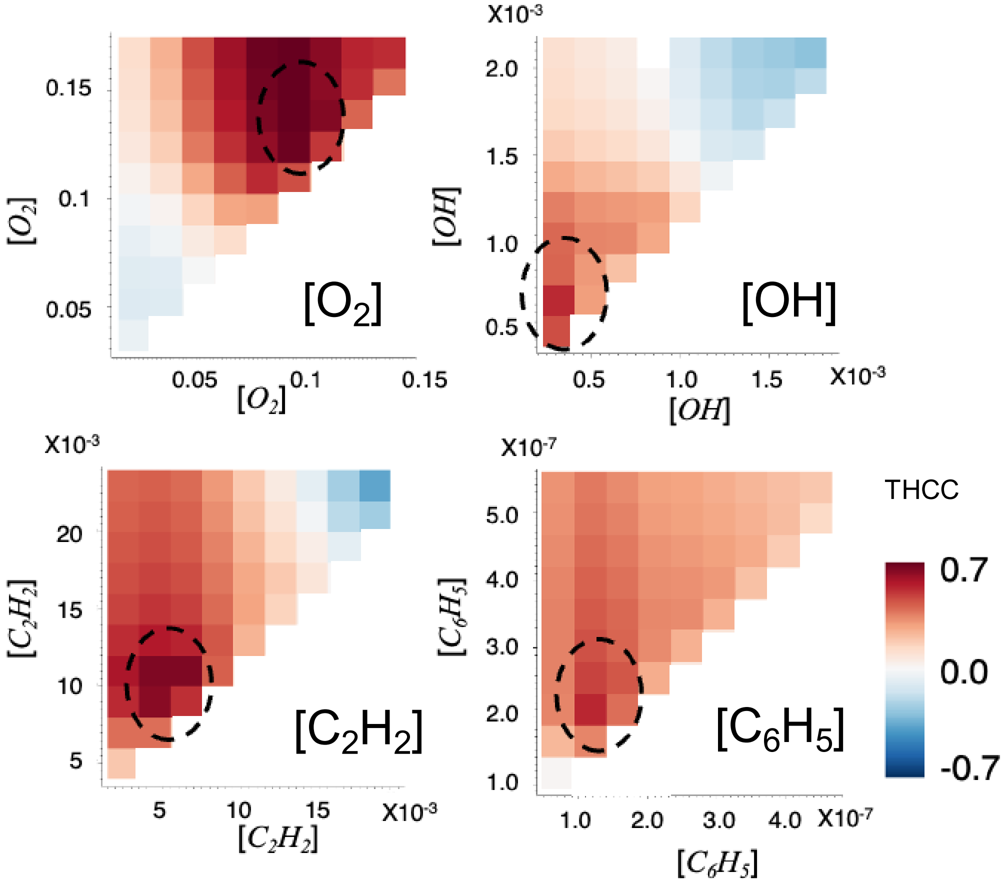
Utilizing the THCC with the experimental measurement of soot enables us to down-select critical species (*i.e*., ***O_2, OH, HCO, CH_2*, C_2H_2, C_2H_4,*** and ***C_6H_5***) that could be used to improve the soot model by considering the time-history effect.

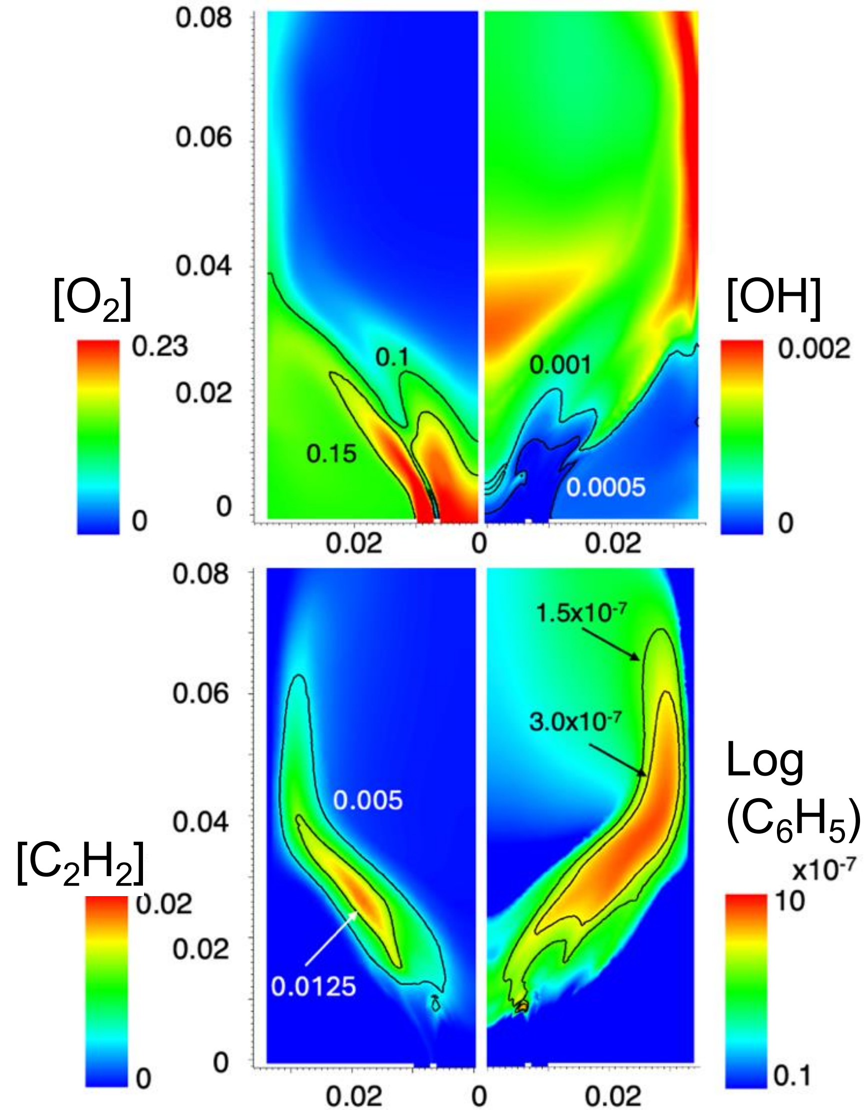
We can eliminate some species if some additional species which are strongly correlated to each other, and hence do not provide the necessary orthogonality for model improvement.

1. HCO, which is a good marker of the heat release, is strongly correlated with the temperature.
2. CH_2* and C_2H_4 are also strongly correlated with the C_2H_2 and ϕ,
3. Considering the structure of the soot model and the relatively strong correlations of HCO, CH_2*, and C_2H_4 with respect to OH.

THCC selects the species: **O_2, OH, C_2H_2,** and **C_6H_5** *to improve the current soot model by considering time-history effect.*

THCC Matrices and Critical Regions





- The region inside the dashed circle indicates the range of species concentration where the time-history effect is tightly correlated with the soot formation.

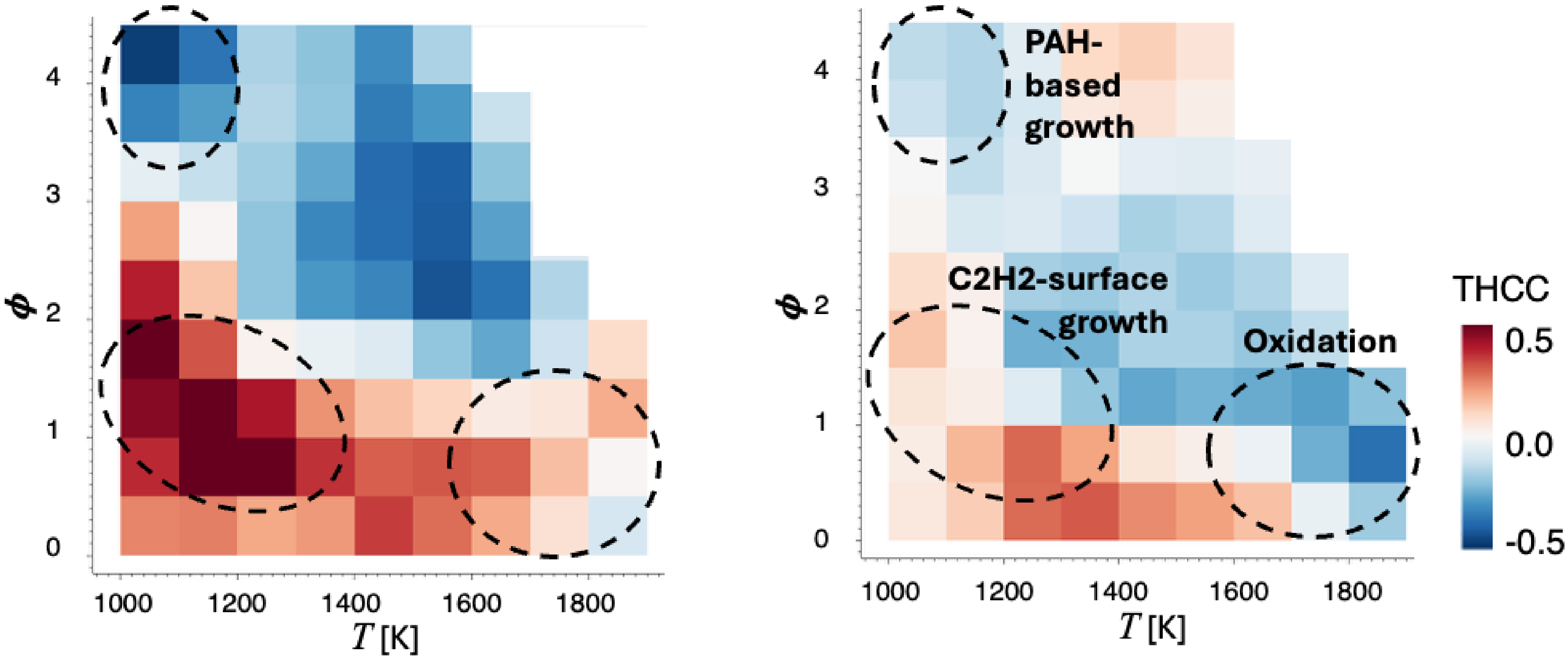
Model Inadequacy and Modifications

How can we utilize the THCC results in terms of possible improvements made for the current empirical two-equation soot model

⬇

Comparing THCC metrices with the experimental SVF and with the CFD predicted SVF, it tells the region(s) of the parameter space where the current soot model (in)accurately takes into account the time-history effect.

Where Does Current 2-Eq. Model Fails?

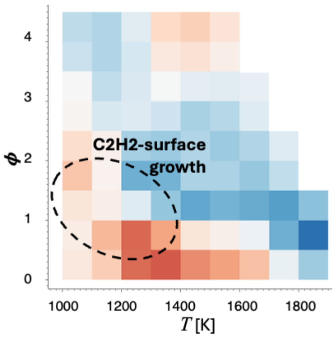


(a) With Exp. SVF

(b) With CFD SVF

- There are three different regions showing noticeably different THCC between the two plots:
  1. **C2H2-surface growth** (1000 [K] < T < 1300 [K] and 0.5 < ϕ < 2.0)
  2. **PAH-based growth** (1000 [K] < T < 1200 [K] and 3.5 < ϕ)
  3. **Oxidation** (1600 [K] < T and ϕ < 1.5)

Region 1: 1000 [K] < T < 1300 [K] and 0.5 < ϕ < 2.0



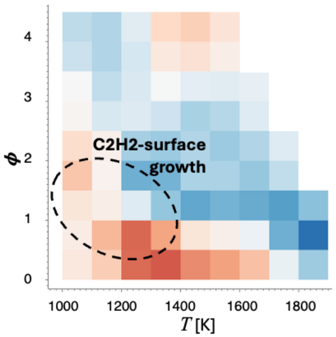
The authors speculate that this moderately rich mixture fractions region is mainly related to the ***acetylene-based surface growth*** [1]

$$\overline{\dot{S}_{p,j}} = S_1 + S_2 - S_3$$

S_1: soot nucleation, $\boldsymbol{S_2}$**: surface-growth** and S_3: oxidation source

[1] Chong, S. T., Hassanaly, M., Koo, H., Mueller, M. E., Raman, V., and Geigle, K.-P., 2018, Combustion and Flame,192, 452-472.

Region 1: 1000 [K] < T < 1300 [K] and 0.5 < ϕ < 2.0



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- *The reasonable choice of parameters are like* S_2*([C_2H_2], T, τ) or S_2*([C_2H_2], ϕ, τ). where τ *is the resident time in the AoI.*
- However, the correlation between the contours of [C_2H_2] and T is very high, so S_2*([C_2H_2], ϕ, τ) is preferable.

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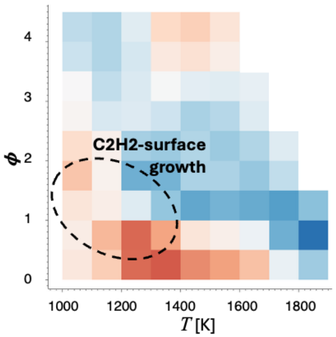

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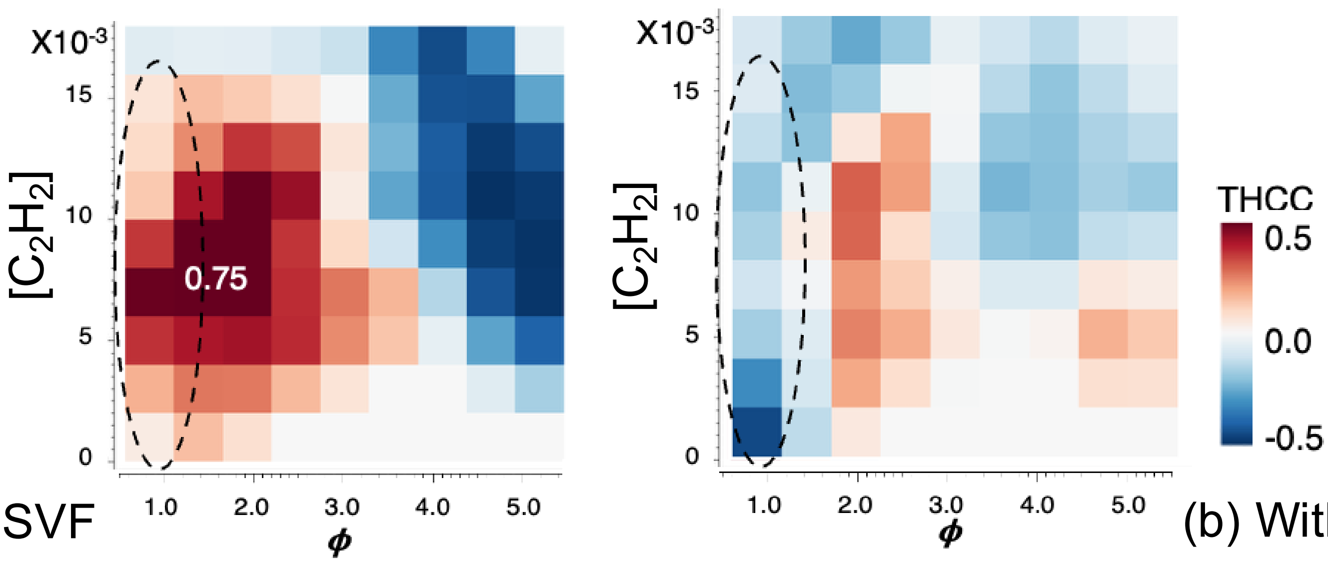
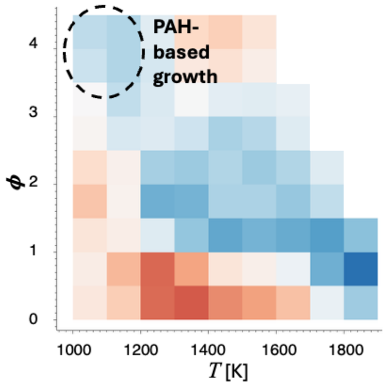


(a) With Exp. SVF

(b) With CFD SVF

[1] Chong, S. T., Hassanaly, M., Koo, H., Mueller, M. E., Raman, V., and Geigle, K.-P., 2018, Combustion and Flame,192, 452-472.

Region 2: 1000 [K] < T < 1200 [K] and 3.5 < ϕ

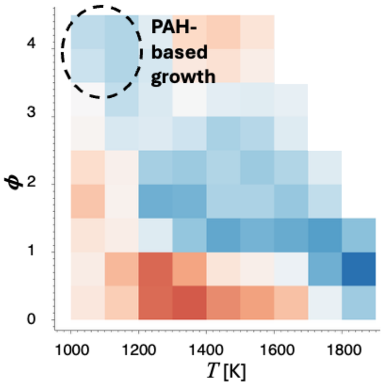


This very fuel rich region seems to be associated with the PAH-based growth

$$\overline{\dot{S}_{p,j}} = S_1 + S_2 - S_3 + S_{PAH}$$

To mimic the PAH-based growth for this region, $[C_6H_5]$, which is **a precursor for the growth of PAH species.**

Region 2: 1000 [K] < T < 1200 [K] and 3.5 < ϕ



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- To determine which combination is the best, we calculates THCC matrices with CFD/Exp SVF and found the choice of $[C_6H_5]$ and $[C_2H_2]$ was found to be the more favorable option.

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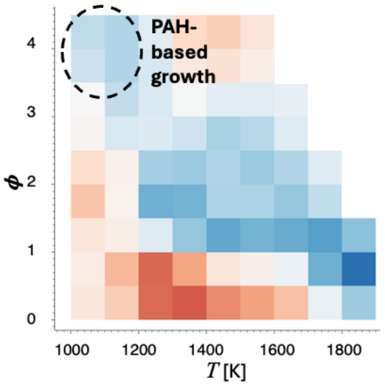

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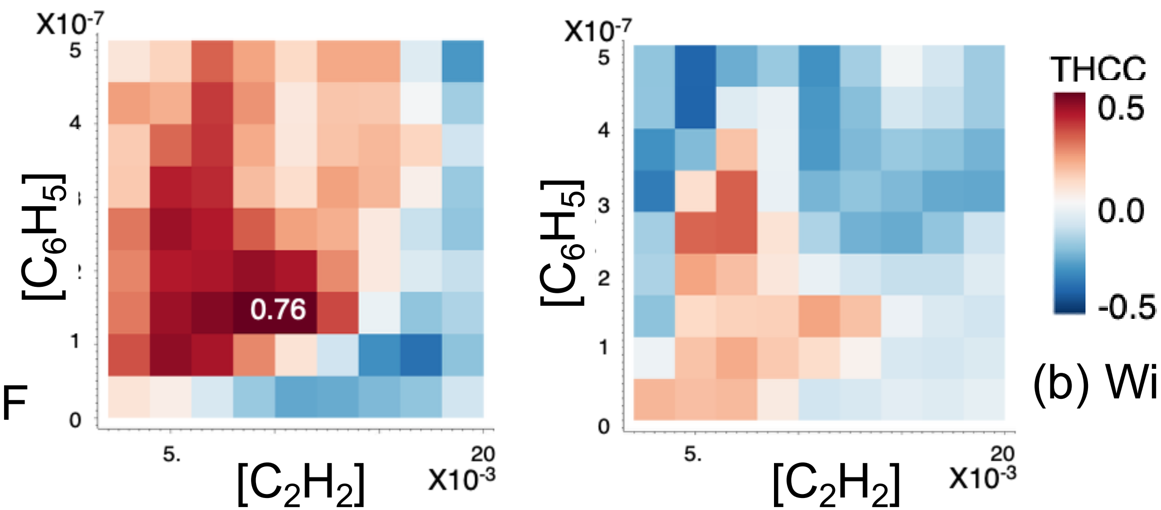
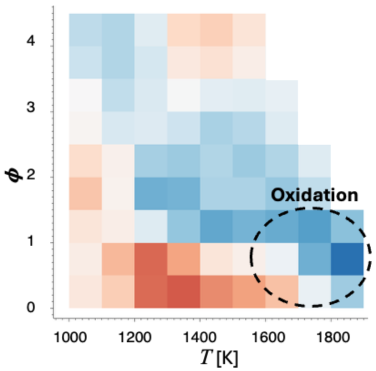


(a) With Exp. SVF

(b) With CFD SVF

Region 3: 1600 [K] < *T* and ϕ < *1.5*

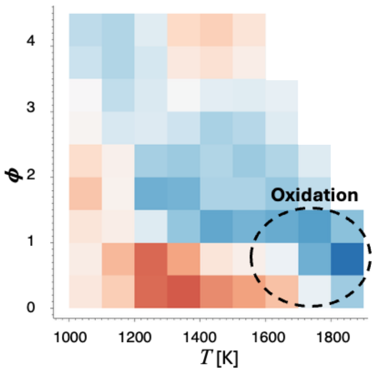


The discrepancy seen in the hot fuel-lean region could be associated with the current oxidation term, S_3, which does not include any time-history effect.

$$\overline{\dot{S}_{p,j}} = S_1 + S_2 - S_3$$

S_1: soot nucleation, S_2: surface-growth and $\boldsymbol{S_3}$**: oxidation source**

Region 3: 1600 [K] < T and $\phi < 1.5$



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- The reasonable choice of parameters for S_3 are:

$S_3^*([O_2], T, \tau)$ or $S_3^*([O_2], \phi, \tau)$ or $S_3^*([OH], T, \tau)$ or $S_3^*([OH], \phi, \tau)$

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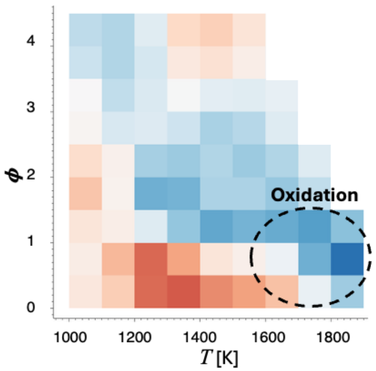

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S_3*([O_2], T, τ) or S_3*([O_2], ϕ, τ) or S_3*([OH], T, τ) or S_3*([OH], ϕ, τ)

- The correlation between [O_2] and T, *and* that between [OH] and T is strong. Due to the weak orthogonality, the combinations of [O_2]+T and [OH]+T are ruled out.

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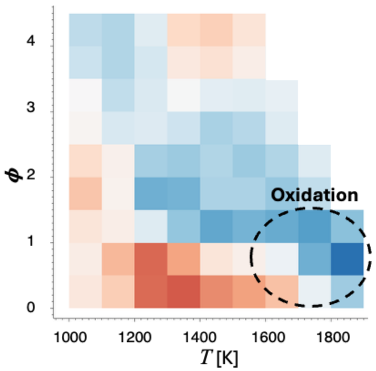

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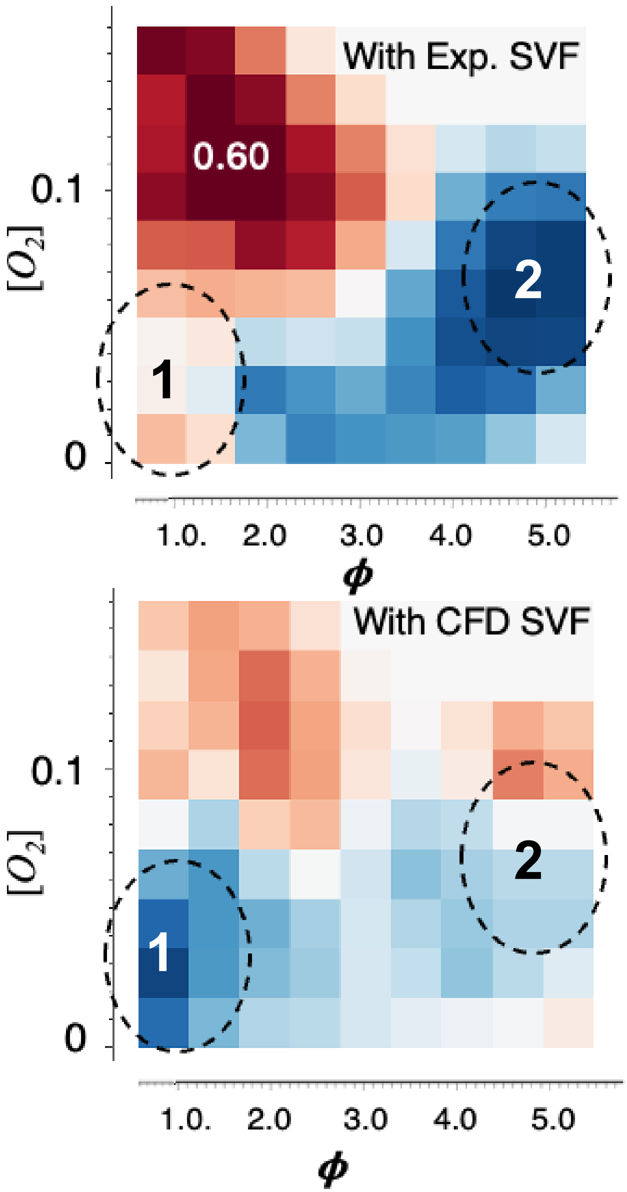
- The correlation between [O_2] and T, *and* that between [OH] and T is strong. Due to the weak orthogonality, the combinations of [O_2]+T and [OH]+T are ruled out.

- Comparison of the THCC matrices with the experimental SVF and the CFD predicted SVF for the two remaining combinations of [O_2]+ϕ and [OH]+ϕ was performed

THCC Matrices of $[O_2]$ and ϕ for Oxidation



About $[O_2]+\phi$, it is found that the current model fails to predict the time-history effect, especially in two regions:

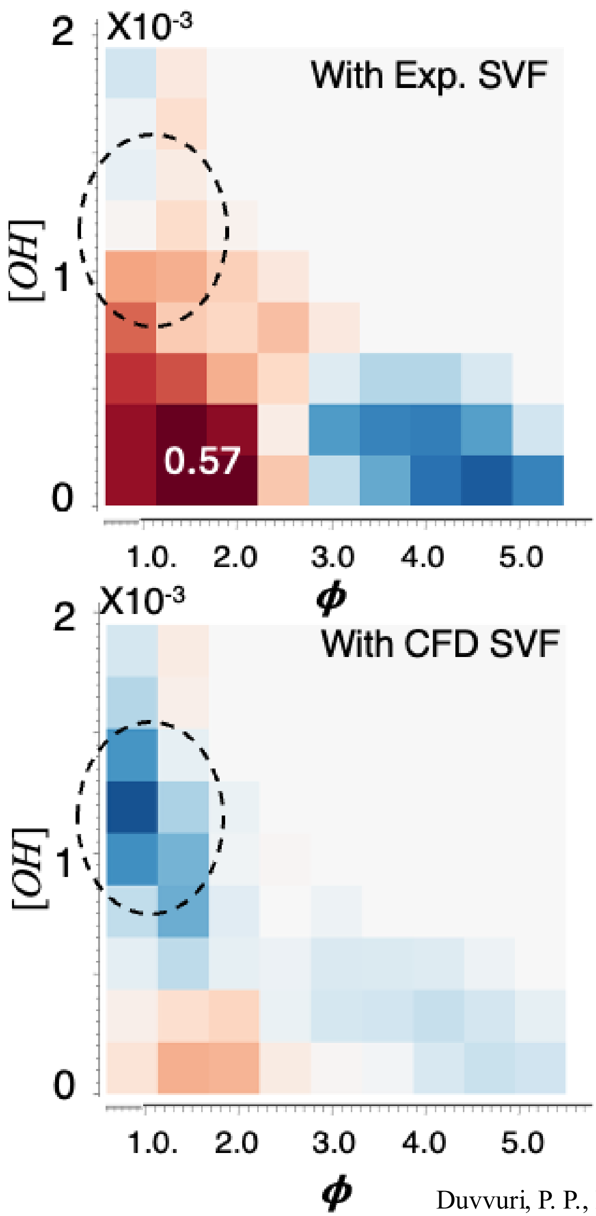
1. **$[O_2] < 0.07$ and $\phi < 1.5$**

- This corresponds to the downstream region of the V-shape soot formation along the shear layer

2. **$[O_2] < 0.1$ and $\phi > 4.5$.**

- This is the very fuel rich upstream region.

THCC Matrices of [OH]+ϕ for Oxidation

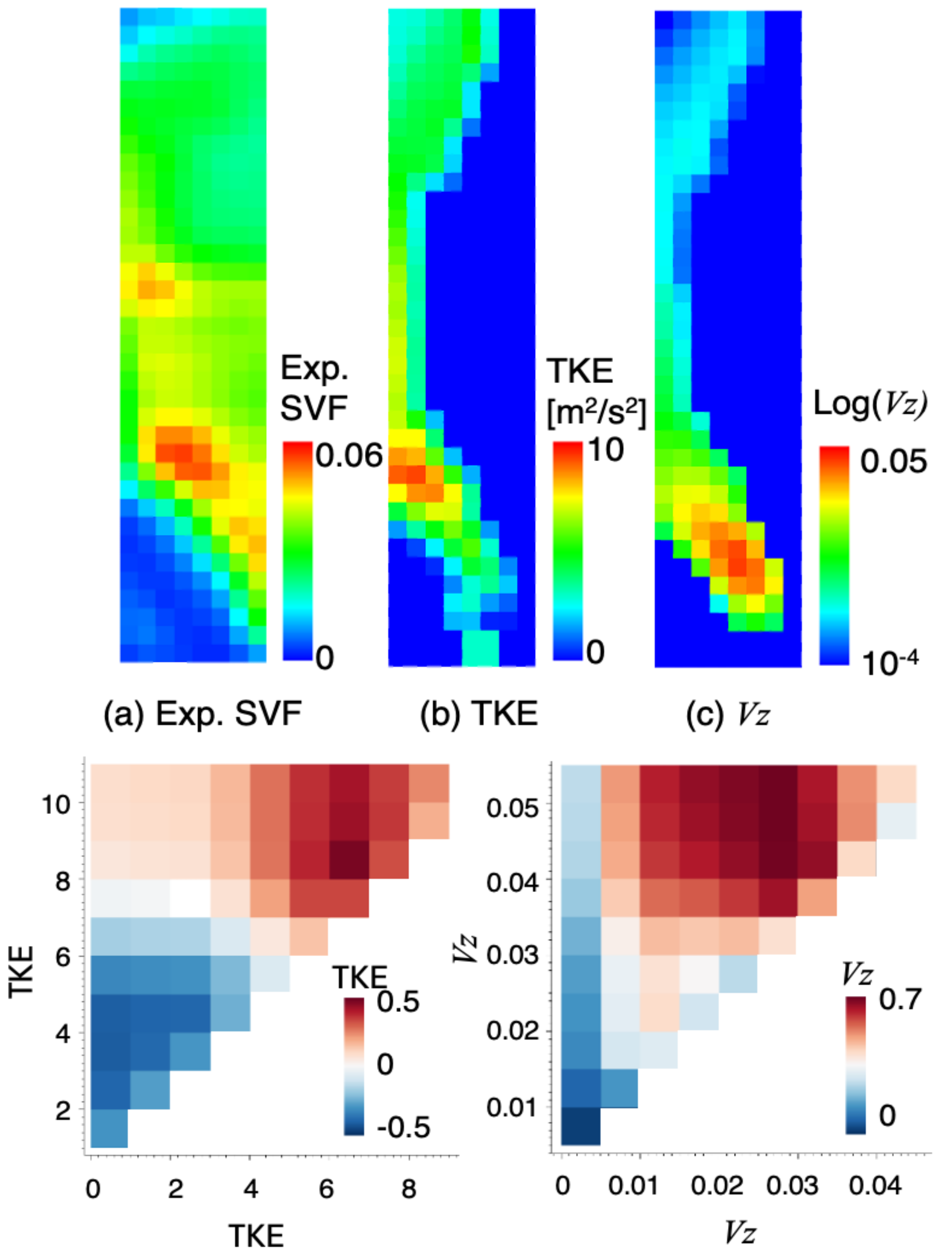


- The model also fails in the region:
  $[OH] < 1\times10^{-3}$ and $\phi < 1.5$,
  which is close to the region of $[O_2] < 0.07$ and $\phi < 1.5$
- Since [OH] and $[O_2]$ are strongly correlated, it is expected to see overlap in regions where the current semi-empirical model fails to predict the correct oxidation trend.
- Duvvuri, *et al* [1] reported that the soot disappears in the lean mixture region due to "spurious oxidation" and emphasized the important of model accuracy of the oxidation process in the lean region.

Our analysis confirms that $S_3^*([O_2], \phi, \tau)$ and $S_3^{**}([OH], \phi, \tau)$ should be added.

Duvvuri, P. P., Maldonado Colmán, H., and Mueller, M. E., 2022 Proceedings of the Combustion Institute, 39(1), pp. 959-967

Discussion: Turbulent Effect on Soot Prediction



- There has been active research about turbulence-chemistry-soot interactions (TCSI) in the context of LES (*e.g.*, [1,2]).
- THCC approach can identify the importance of the time-history effect on the soot formation in terms of TCSI.

[1] Duvvuri, P. P., Maldonado Colmán, H., and Mueller, M. E., 2022, Proceedings of the Combustion Institute, 39(1), pp. 959-967.
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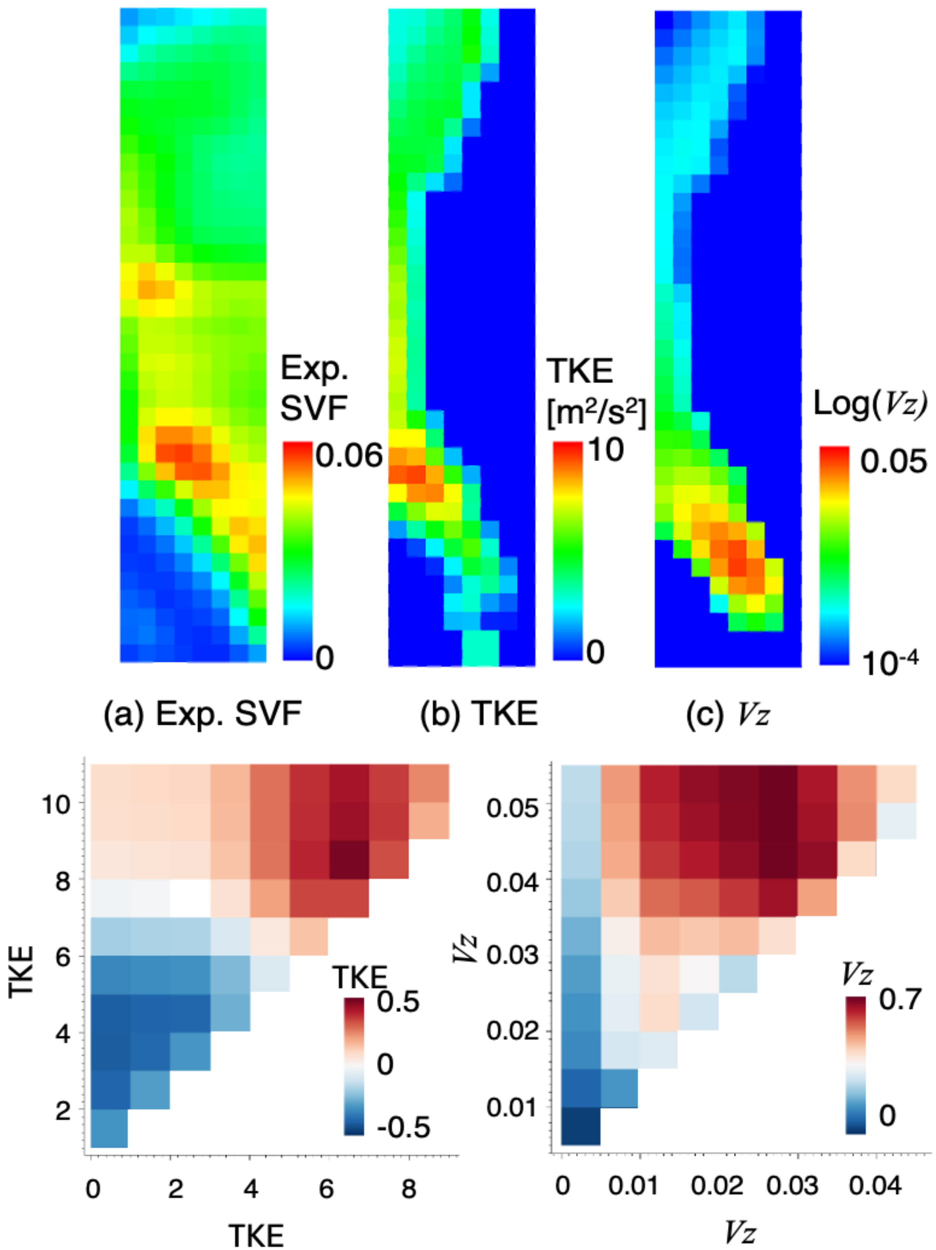

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From the THCC matrices (TKE and Vz), there is a favorable condition of turbulent intensity for the TCSIs through the time-history effect.

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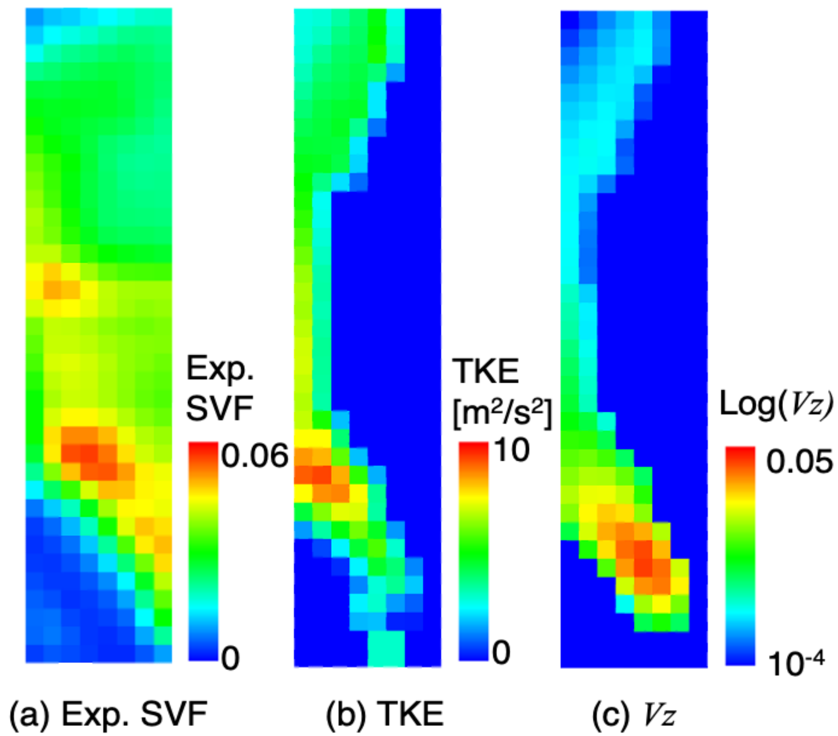

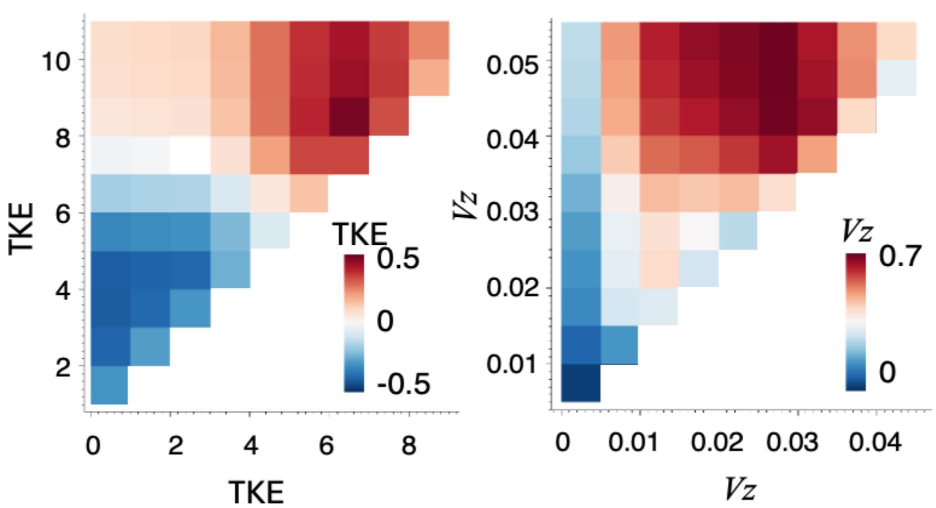

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From the THCC matrices (TKE and Vz), there is a favorable condition of turbulent intensity for the TCSIs through the time-history effect.

Out of many combinations, we show some key results the THCC matrices:

1. $[C_6H_5]$+TKE,
2. $[C_6H_5]$+Vz
3. $[C_2H_2]$+TKE

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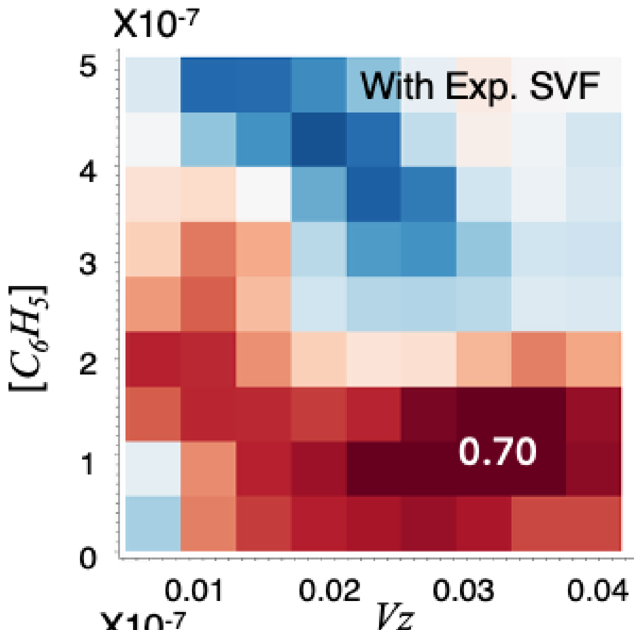
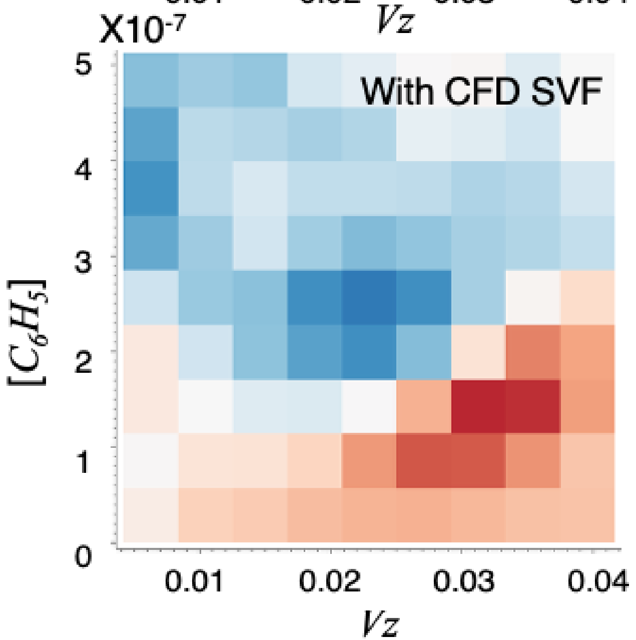
THCC matrices of Key Turbulent Quantities

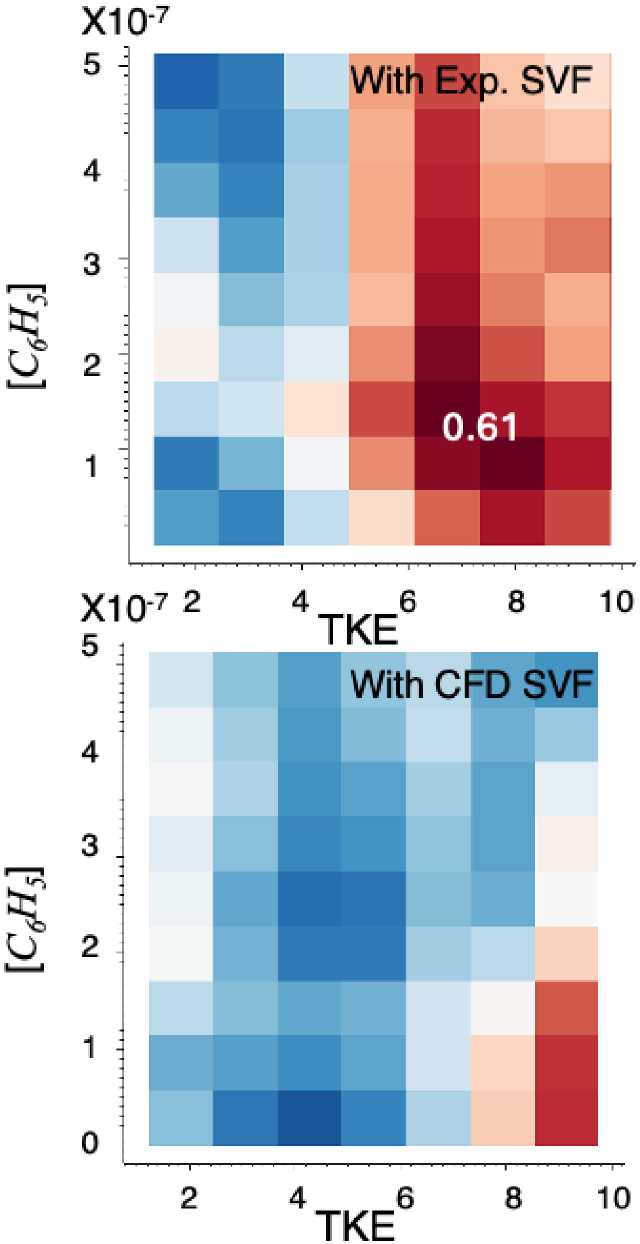




- Comparing two THCC matrices with exp/CFD SVF, it is found that current model roughly captures the [C_6H_5] and Vz correlation.
- [C_6H_5] and VZ is not a good combination for the model modification.

$$S_{PAH}*([C_6H\ \ ],\ [C\ \ H_2],\ Vz,\ \tau)$$

THCC matrices of Key Turbulent Quantities



- Comparing two THCC matrices with exp/CFD SVF, it is found that current model cannot capture the time-history effect of [C_6H_5] and TKE.

- Adding TKE as an additional variable could further improve the soot predictions in fuel-rich, high-nucleation regions of the combustor.

$$S_{PAH}^*([C_6H_5], [C_2H_2], \text{TKE}, \tau)$$

Conclusion

- The time-history effect in the context of soot formation was investigated with a particle-based statistical approach using the DLR aero-combustor.
- Time-history statistics (*e.g.,* time-history correlation coefficient or THCC) were then calculated with respect to the experimental SVF.
- Time-history effects of certain flow variables, including turbulent quantities, and multiple species are indeed important for soot formation.
- We could identify certain key species (O_2, OH, C_2H_2, and C_6H_5) that could have significant impact on improving the current acetylene-based semi-empirical model of Fairweather *et al*.
- Comparing the THCC matrices with exp/CFD SVF, we identify the model inadequacy and propose:

  - C_6H_5-based nucleation in fuel-rich regions,
  - acetylene-based surface growth
  - oxidation source terms related to OH and O_2 species.

Time-history based modifications can provide a feasible path towards improving the accuracy of current engineering tools for CFD prediction of soot formation in gas-turbine combustors.

Thank you!

Questions?

Acknowledgement

- This work was supported by the HyTEC (Hybrid Thermally Efficient Core) project managed by Ms. Laura Evans.
- Simulations conducted on NASA Advanced Supercomputing (NAS) Pleiades computers.