# Assessment of a sectional model for soot formation in laminar flames:

## Sensitivity to model parameters, and application to practical fuels

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# Contents

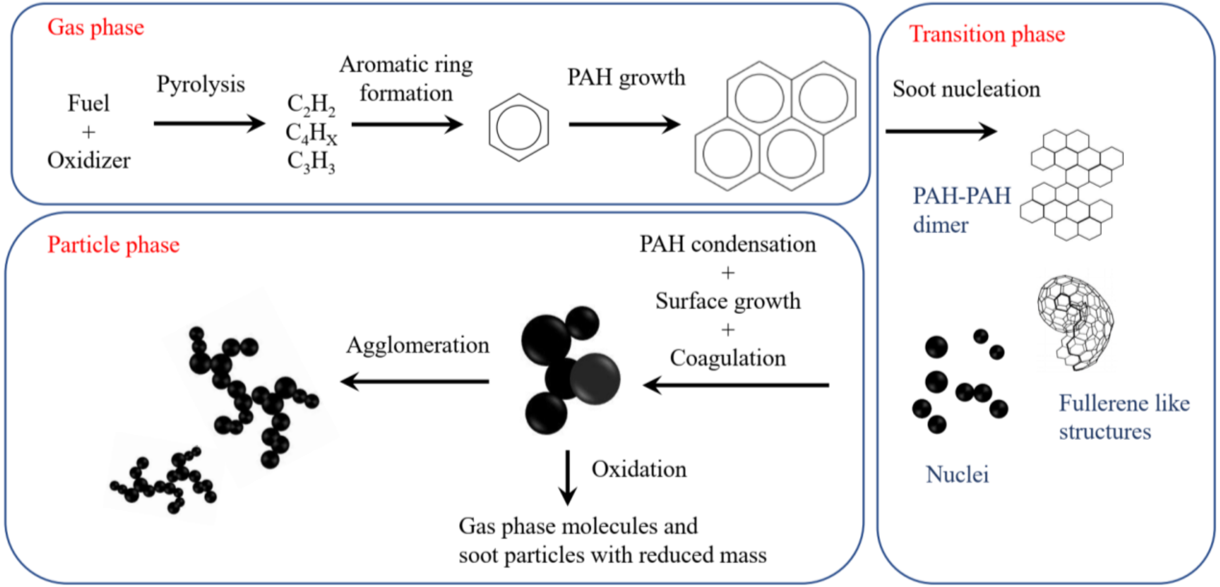
# Introduction

## Motivation for Soot Research

- Soot from combustion systems
- Environmental implications
- Consequences to human health
- Gaps in understanding of soot
- Challenges in numerical modeling

# Introduction

## Pathways of Soot Formation

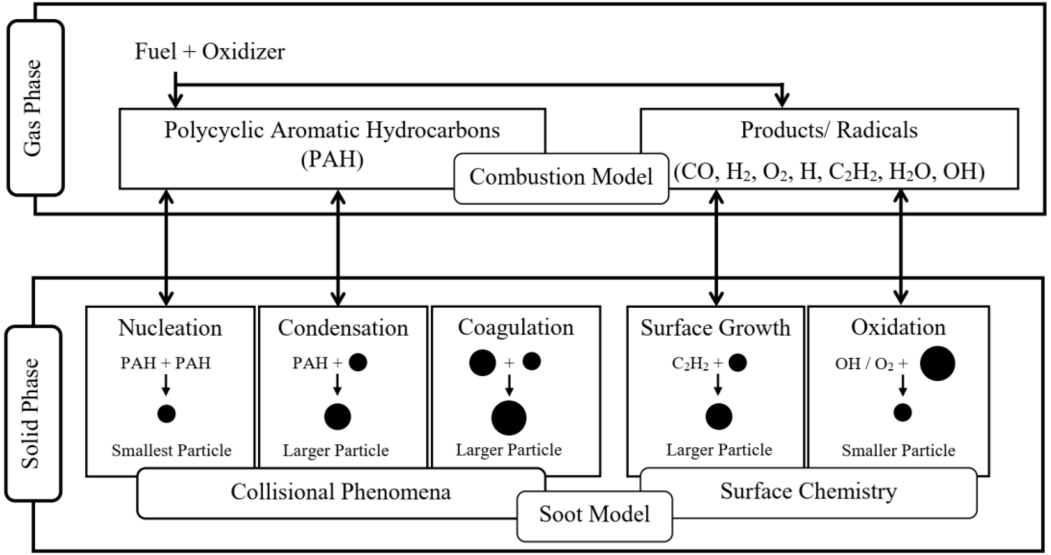





Wang, Y. and Chung, S.H., *Prog. Energy Combust. Sci., 74*:152-238, 2019

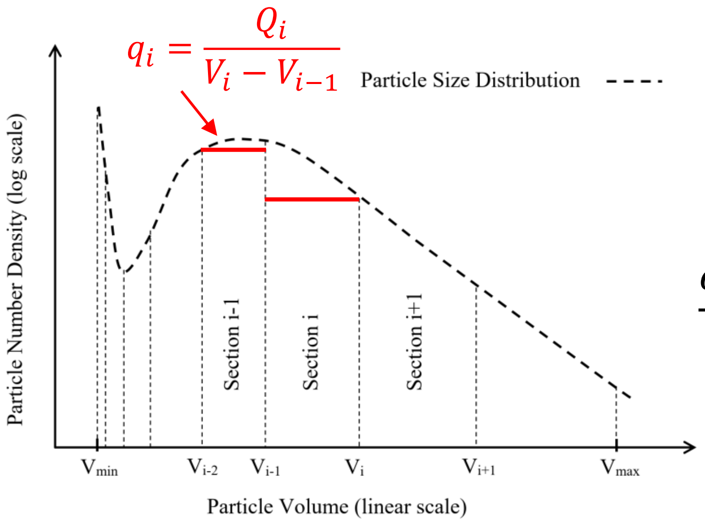
# Sectional Soot Model

## Modeling Methodology



# Sectional Soot Model

## Model Formulation




$$q_i = \frac{Q_i}{V_i - V_{i-1}}$$

$$V_i = V_{min} \left( \frac{V_{max}}{V_{min}} \right)^{\frac{i}{n_{sec}}}$$

$$\frac{\partial(\rho Y_{s,i})}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_{s,i}) = -\nabla \cdot (\rho Y_{s,i} \mathbf{V_T}) + \nabla \cdot (\rho D_{s,i} \nabla Y_{s,i}) + \rho_s (\dot{Q}_{nuc,i} + \dot{Q}_{cond,i} + \dot{Q}_{coag,i} + \dot{Q}_{sg,i} + \dot{Q}_{ox,i})$$

$$(i = 1,..,n_{sec})$$



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# Sectional Soot Model

## Soot Source Terms

### Nucleation

$$PAH + PAH \rightarrow Soot\ particle + Gas\ phase\ products$$

$$\dot{Q}_{nuc,1} = 2 v_{PAH} \beta_{PAH,PAH} N_{PAH}^{2}$$

$$\mathrm{A4 + A4} \rightarrow \text{Soot particle} + 10\mathrm{H_2}$$

Gas phase coupling

$$\frac{d[\mathrm{A4}]}{dt} = -\frac{\dot{Q}_{nuc,1}}{v_{\mathrm{A4}} n_{avo}} \qquad \frac{d[\mathrm{H_2}]}{dt} = -5\frac{d[\mathrm{A4}]}{dt}$$

A4 = Pyrene ($C_{16}H_{10}$)



M. Frenklach and H. Wang. *Symp. (Int.) Combust.*, 23(1):1559–1566, 1991

# Sectional Soot Model

## Soot Source Terms

### PAH Condensation

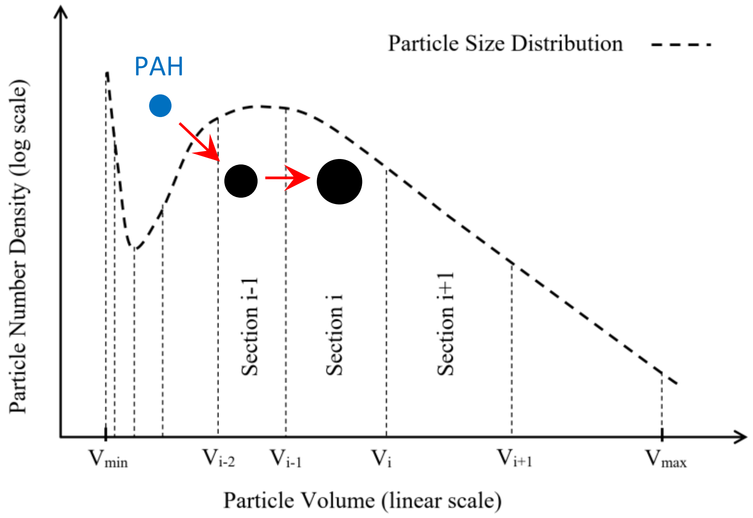
$$PAH + Soot \rightarrow Larger\ Soot\ particle$$
$$+Gas\ phase\ products$$

$$\Delta\dot{Q}_{cond,i} = v_{PAH}\beta_{i,PAH}\ N_{PAH}\frac{Q_i}{V_i - V_{i-1}}\ln\left(\frac{V_i}{V_{i-1}}\right)$$

$$\boxed{\mathrm{A4}} + \text{Soot particle} \rightarrow \text{Larger Soot particle} + \boxed{5\mathrm{H}_2}$$

Gas phase coupling

$$\frac{d[\mathrm{A4}]}{dt} = -\frac{\Delta\dot{Q}_{cond,i}}{v_{\mathrm{A4}}n_{avo}} \qquad \frac{d[\mathrm{H}_2]}{dt} = -5\frac{d[\mathrm{A4}]}{dt}$$




$$\Delta\dot{Q}_{cond,i} = \Delta\dot{Q}^{in}_{cond,i} + \Delta\dot{Q}^{out}_{cond,i}$$
$$\dot{Q}_{cond,i} = \Delta\dot{Q}^{out}_{cond,i-1} + \Delta\dot{Q}^{in}_{cond,i}$$



S.P. Roy. PhD thesis, 2014

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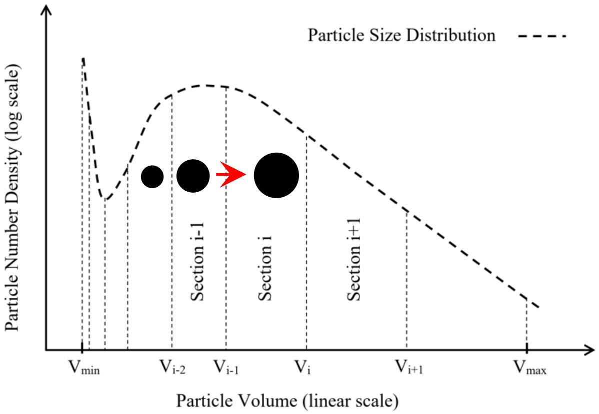
# Sectional Soot Model

Soot Source Terms

## Soot Coagulation

$$Soot + Soot \rightarrow Larger\ Soot\ particle$$




Kumar and Ramkrishna Model (KR96)

$$\dot{Q}_{coag,i} = \frac{dN_i}{dt} \frac{(V_i - V_{i-1})}{\ln\left(\frac{V_i}{V_{i-1}}\right)}$$

Gelbard et al. Model (GS00)

$$\dot{Q}_{coag,i} = \sum_{r=1}^{i-1} \sum_{p=1}^{i-1} \beta^1_{r,p,i} Q_r Q_p - Q_i \sum_{r=1}^{i-1} \beta^2_{r,i} Q_r - \frac{1}{2} \beta^3_{i,i} Q_i^2 - Q_i \sum_{r=i+1}^{n_{sec}} \beta^4_{r,i} Q_r$$




S. Kumar and D. Ramkrishna. *Chem. Engg. Sci.*, 51(8):1311–1332, 1996.
F. Gelbard, Y. Tambour, and J. H. Seinfeld. *J. Colloid Interface Sci.*,76(2):541–556, 1980

# Sectional Soot Model

## Soot Source Terms

### Surface Growth

$$Soot + C_2H_2 \rightarrow Larger\ Soot\ particle + Gas\ phase\ products$$

$$\Delta\dot{Q}_{sg,i} = 2 v_C k_4 [C_2H_2][C^*_{s,n}]_i n_{avo}$$

$$[C^*_{s,n}]_i = \frac{\alpha k_{ss} \chi_{C_{s,n}} S_i}{n_{avo}}$$

$\alpha$ = Steric factor → Unity; $f(T, v_i)$ (ABF00)

Depletion of surface radicals $\xi_{dc} = 0$ ← SR4a

Conservation of surface radicals $\xi_{dc} = 1$ ← SR4b

#### Hydrogen-Abstraction-$C_2H_2$-Addition (HACA)

| | |
|---|---|
| SR1 | $C_{s,n} + H \leftrightarrow C^*_{s,n} + H_2$ |
| SR2 | $C_{s,n} + OH \leftrightarrow C^*_{s,n} + H_2O$ |
| SR3 | $C^*_{s,n} + H \rightarrow C_{s,n}$ |
| SR4a | $C^*_{s,n} + C_2H_2 \rightarrow C_{s,n+2} + H$ |
| SR4b | $C^*_{s,n} + C_2H_2 \rightarrow C^*_{s,n+2} + H_2$ |

#### Extended HACA (Ext-HACA)

| | |
|---|---|
| SR7 | $C_{s,n} + CH_3 \leftrightarrow C^*_{s,n} + CH_4$ |
| SR8 | $C_{s,n} + C_3H_3 \leftrightarrow C^*_{s,n} + C_3H_4$ |
| SR9 | $C_{s,n} + C_2H \leftrightarrow C^*_{s,n} + C_2H_2$ |



M. Frenklach and H. Wang. *Symp. (Int.) Combust.*, 23(1):1559–1566,1991.
J. Y. Hwang and S. H. Chung. *Combust. Flame*, 125(1-2):752–762, 2001.
J. Appel, H. Bockhorn, and M. Frenklach. *Combust. Flame*, 121(1-2):122–136, 2000

# Sectional Soot Model

## Soot Source Terms

### Soot Oxidation

$$Soot + \mathrm{OH}/\mathrm{O_2} \rightarrow Smaller\ Soot\ particle + Gas\ phase\ products$$

SR5 $\mathrm{C}_{s,n} + \mathrm{O_2} \leftrightarrow \mathrm{C}^*_{s,n-2} + 2\mathrm{CO}$

SR6 $\mathrm{C}_{s,n} + \mathrm{OH} \leftrightarrow \mathrm{C}^*_{s,n-1} + \mathrm{CO}$

$$\Delta\dot{Q}_{ox,i,O_2} = -2 v_C k_5 [\mathrm{O_2}][\mathrm{C}^*_{s,n}]_i n_{avo}$$

$$\Delta\dot{Q}_{ox,i,OH} = -\gamma v_C \beta_{i,OH} n_{avo} [\mathrm{OH}] \frac{Q_i}{V_i - V_{i-1}} \ln\left(\frac{V_i}{V_{i-1}}\right)$$



M. Frenklach and H. Wang. *Symp. (Int.) Combust.*, 23(1):1559–1566,1991.

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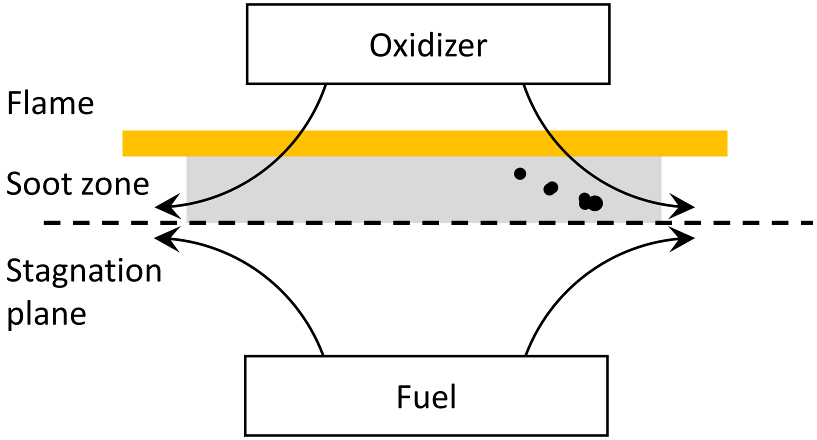
# Model Validation

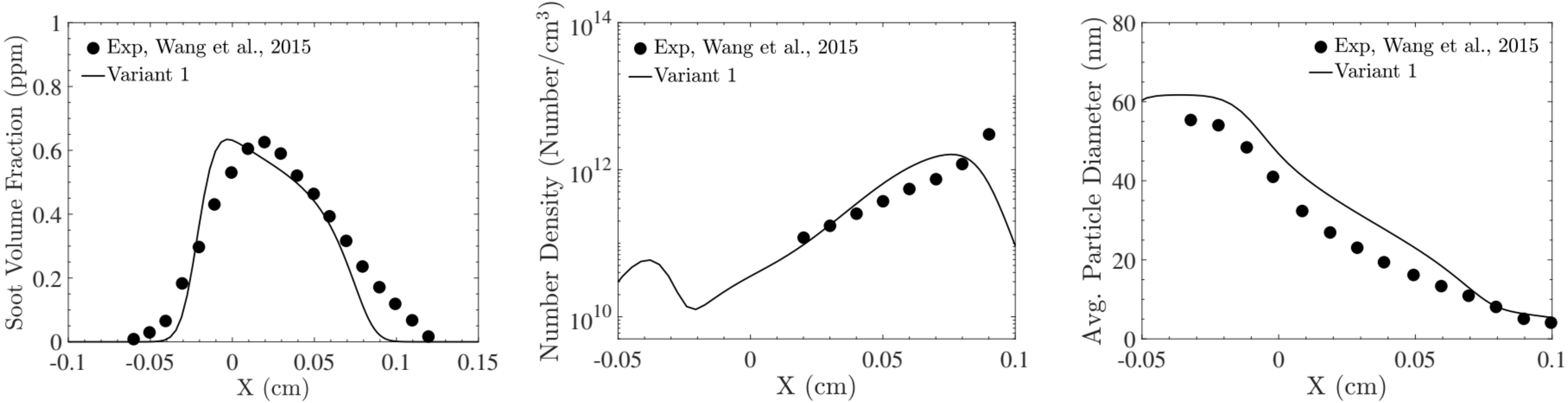
## Flame Configuration




| Parameter | Fuel | Oxidizer |
|---|---|---|
| Composition (by volume) | $C_2H_4$ | $O_2$ = 0.25%<br>$N_2$ = 0.75% |
| Temperature (K) | 300 | 300 |

# Model Validation

## Results




| | Gas Chem. | Surf. Chem. | Steric Fac. | $\xi_{dc}$ | Coagulation |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |

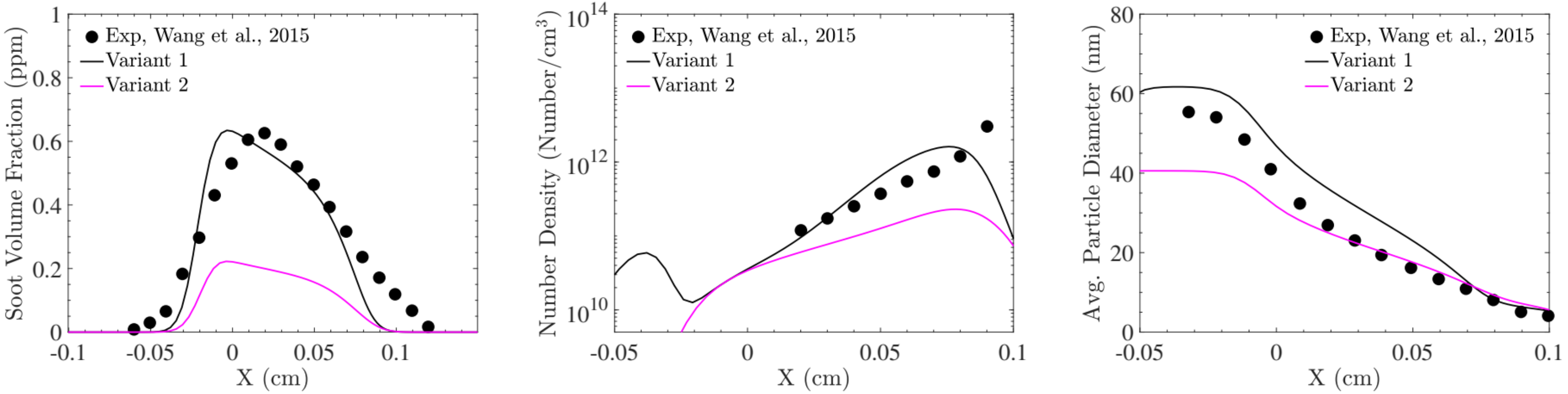
# Model Validation

## Sensitivity to model parameters

| Variant | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| Gas chemistry | KM2 | ABF | KM2 | KM2 | KM2 | KM2 | KM2 |
| Surface chemistry | HACA | HACA | HACA | HACA | HACA | Ext-HACA | HACA |
| Steric factor | ABF00 | ABF00 | ABF00 | ABF00 | ABF00 | ABF00 | 1 |
| Radical treatment $\xi_{dc}$ | 0.85 | 0.85 | 0 | 1 | 0.85 | 0.85 | 0.85 |
| Coagulation model | KR96 | KR96 | KR96 | KR96 | GS80 | KR96 | KR96 |

# Model Validation

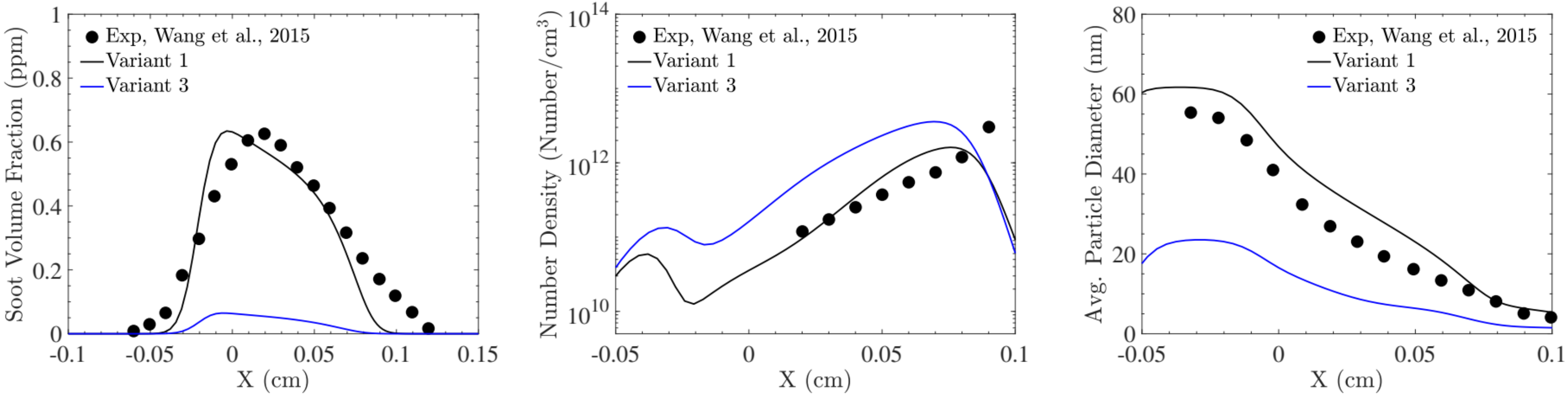
## Sensitivity to model parameters




| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 2 | ABF | HACA | ABF00 | 0.85 | KR96 |

# Model Validation

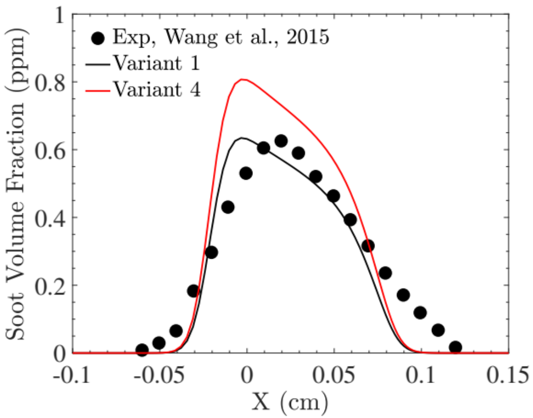
## Sensitivity to model parameters

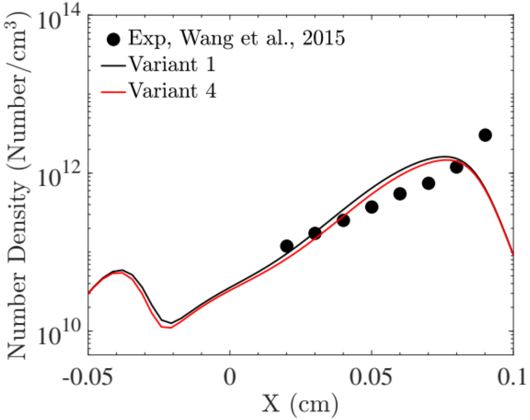


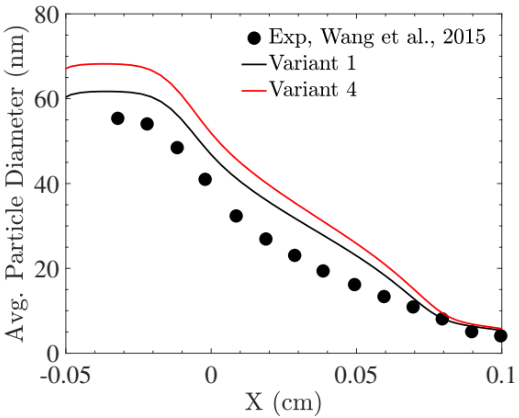

| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 3 | KM2 | HACA | ABF00 | 0 | KR96 |

# Model Validation

## Sensitivity to model parameters



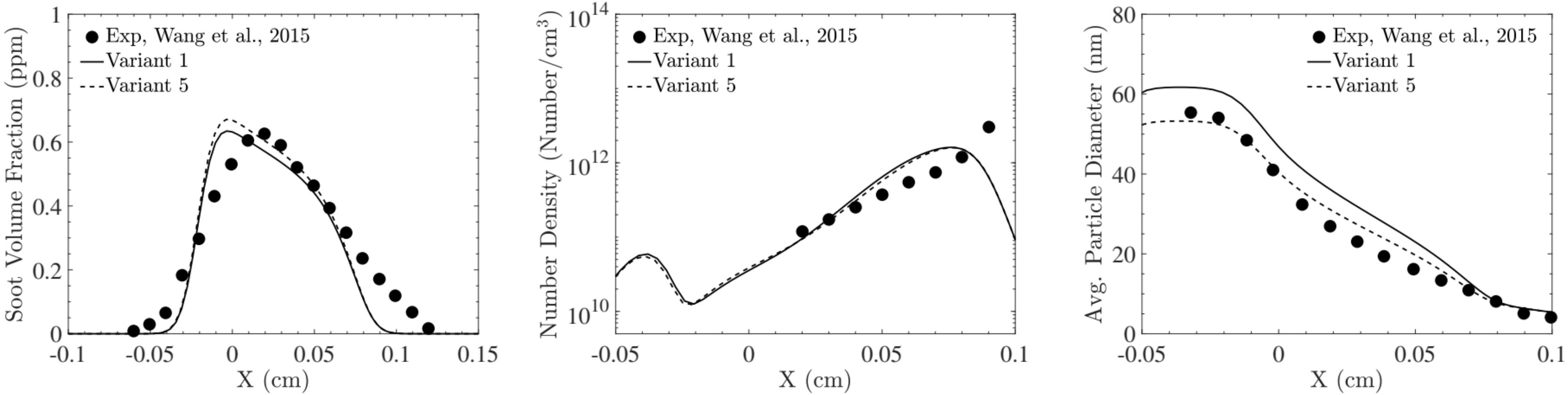




| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 4 | KM2 | HACA | ABF00 | 1 | KR96 |

# Model Validation

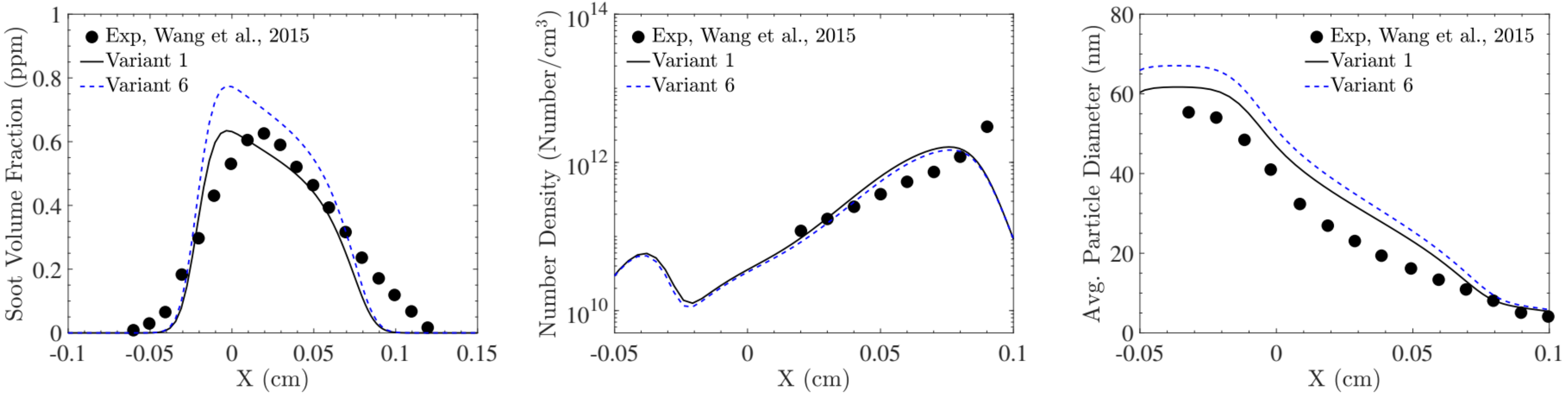
## Sensitivity to model parameters




| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 5 | KM2 | HACA | ABF00 | 0.85 | GS80 |

# Model Validation

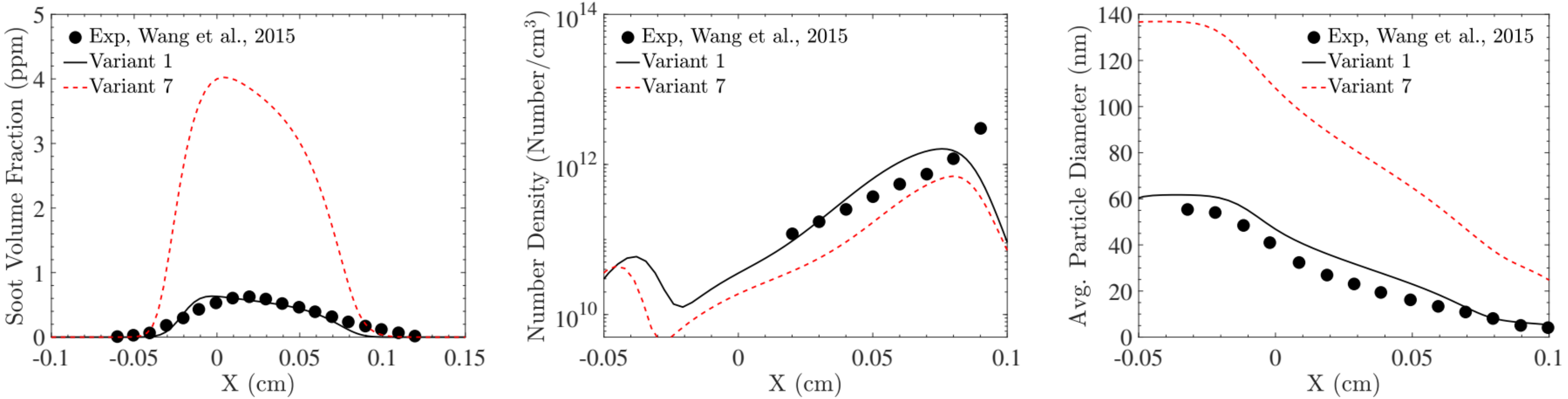
## Sensitivity to model parameters




| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 6 | KM2 | Ext-HACA | ABF00 | 0.85 | KR96 |

# Model Validation

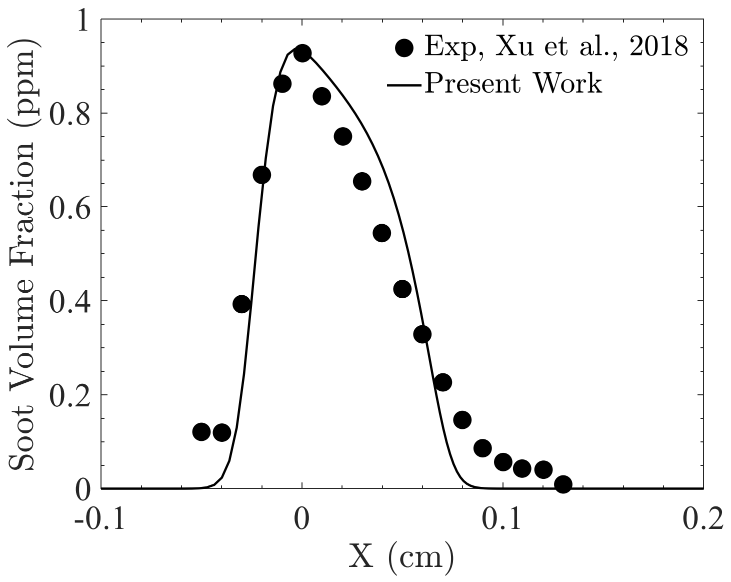
## Sensitivity to model parameters




| | | | | | |
|---|---|---|---|---|---|
| Variant 1 | KM2 | HACA | ABF00 | 0.85 | KR96 |
| Variant 7 | KM2 | HACA | 1 | 0.85 | KR96 |

# Model Validation

## Target flames: Non-premixed flames




| Parameter | Fuel | Oxidizer |
|---|---|---|
| Composition (by volume) | $C_2H_4$ | $O_2$ = 0.30%<br>$N_2$ = 0.70% |
| Temperature (K) | 300 | 300 |

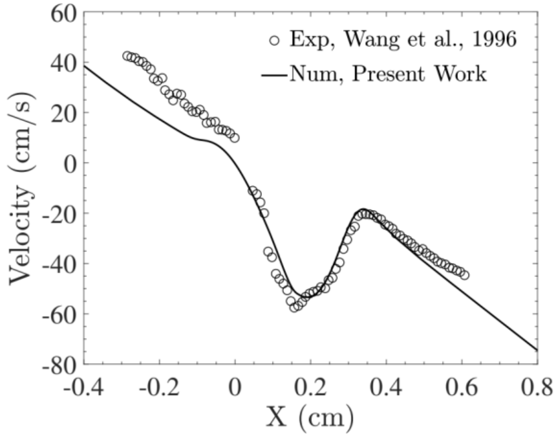
Variant-1, $\xi_{dc} = 0.8$

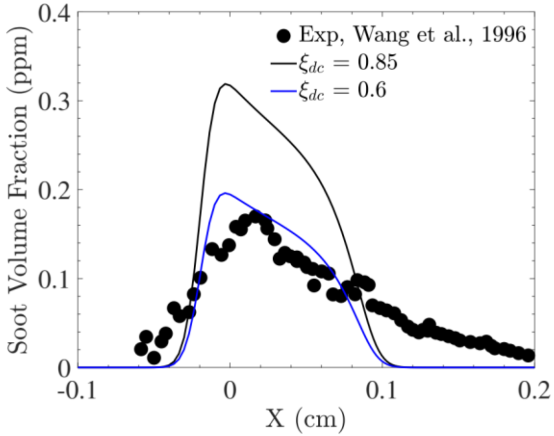


Xu, L., Yan, F., Zhou, M., Wang, Y. and Chung, S.H., *Combust. Flame*, *197*:304-318, 2018

# Model Validation

Target flames: Non-premixed flames




| Parameter | Fuel | Oxidizer |
|---|---|---|
| Composition (by volume) | $C_2H_4$ | $O_2$ = 0.21%<br>$N_2$ = 0.79% |
| Temperature (K) | 300 | 300 |

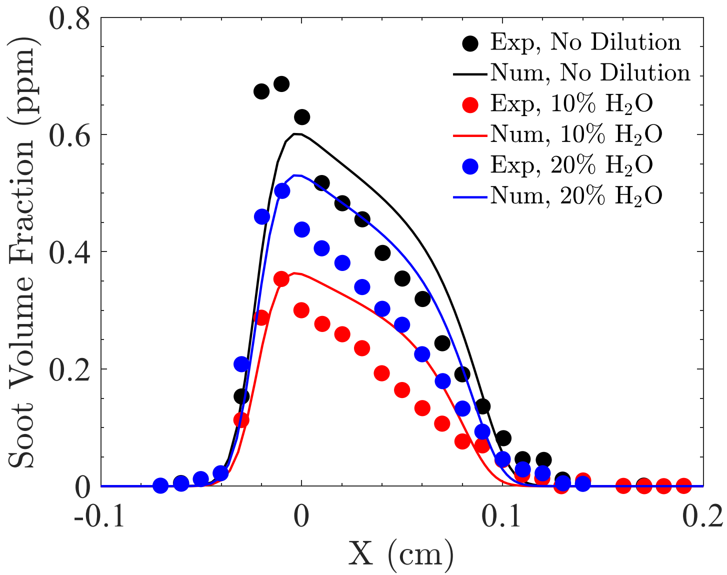
Variant-1, $\xi_{dc} = 0.6$



H. Wang, D.X. Du, C.J. Sung, and C.K. Law. *Symp. (Int.) Combust.*, 26(2):2359–2368, 1996.

# Model Validation

## Target flames: Non-premixed flames




| Parameter | Fuel | Oxidizer |
|---|---|---|
| Composition (by volume) | $C_2H_4$<br>$H_2O$ | $O_2$ = 0.25%<br>$N_2$ = 0.75% |
| Temperature (K) | 393 | 300 |

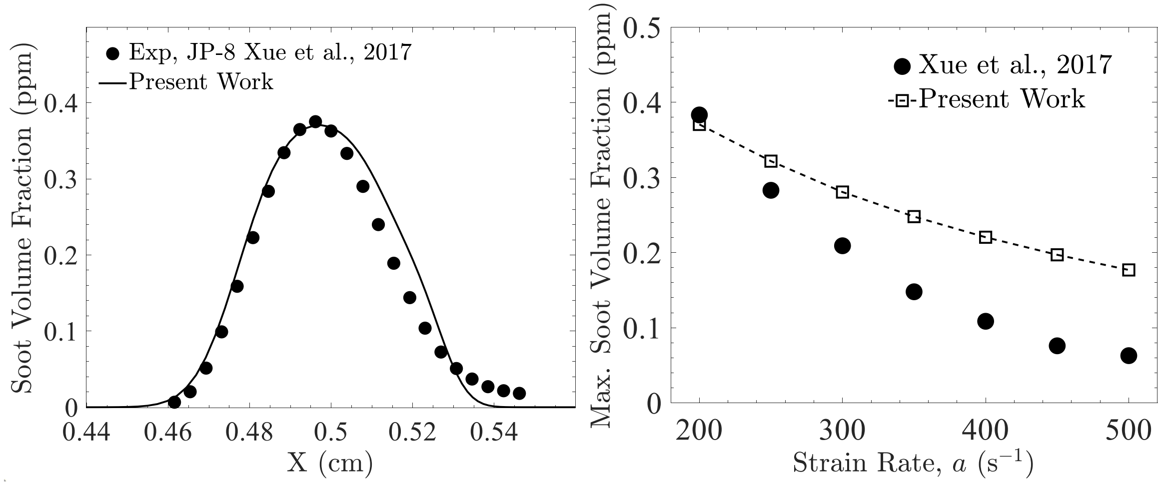
Variant-1, $\xi_{dc} = 0.6$



Mahmoud, N., Yan, F., Zhou, M., Xu, L. and Wang, Y., *Energy & Fuels,* 33:5582-5596, 2019

# Model Validation

## Application to practical fuels: JP-8




| Parameter | Fuel | Oxidizer |
|---|---|---|
| Composition (by volume) | JP-8 = 10%<br>$O_2$ = 90% | $O_2$ = 0.40%<br>$N_2$ = 0.60% |
| Temperature (K) | 473 | 473 |

JP-8 Surrogate = n-decane (80%), 1,2,4-trimethylbenzene (20%) (by mass)

Variant-1, $\xi_{dc} = 0.8$



X. Xue, X. Hui, P. Singh, and C-J. Sung. *Fuel*, 210:343–351, 2017

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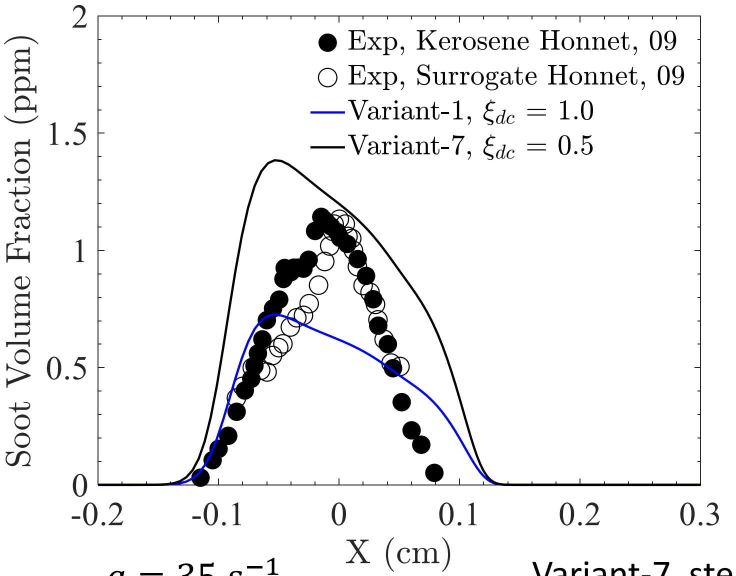
# Model Validation

## Application to practical fuels: Kerosene




$a = 35\ s^{-1}$

| Parameter | Fuel | Oxidizer |
| --- | --- | --- |
| Composition (by mass) | Surr = 42%<br>$O_2$ = 58% | $O_2$ = 0.23%<br>$N_2$ = 0.77% |
| Temperature (K) | 450 | 293 |

Kerosene Surrogate =
n-decane (80%),
1,2,4-trimethylbenzene (20%)
(by mass)

Variant-7, steric factor = 1



S. Honnet, K. Seshadri, U. Niemann, and N. Peters. *Proc. Combust. Inst.*, 32(1):485–492, 2009.

# Summary and Future Scope

## Summary

- Sensitive to radical treatment
- Sensitive to chemical kinetic mechanism
- Good qualitative and quantitative soot prediction
- Applicable to practical fuels

## Future Scope

- Accuracy of model for varied flame conditions (strain rate, pressure etc.)
- Functional relationship of radical treatment parameter
- Modeling for complex physics of soot formation processes

**Thank you..**

**Questions ?**