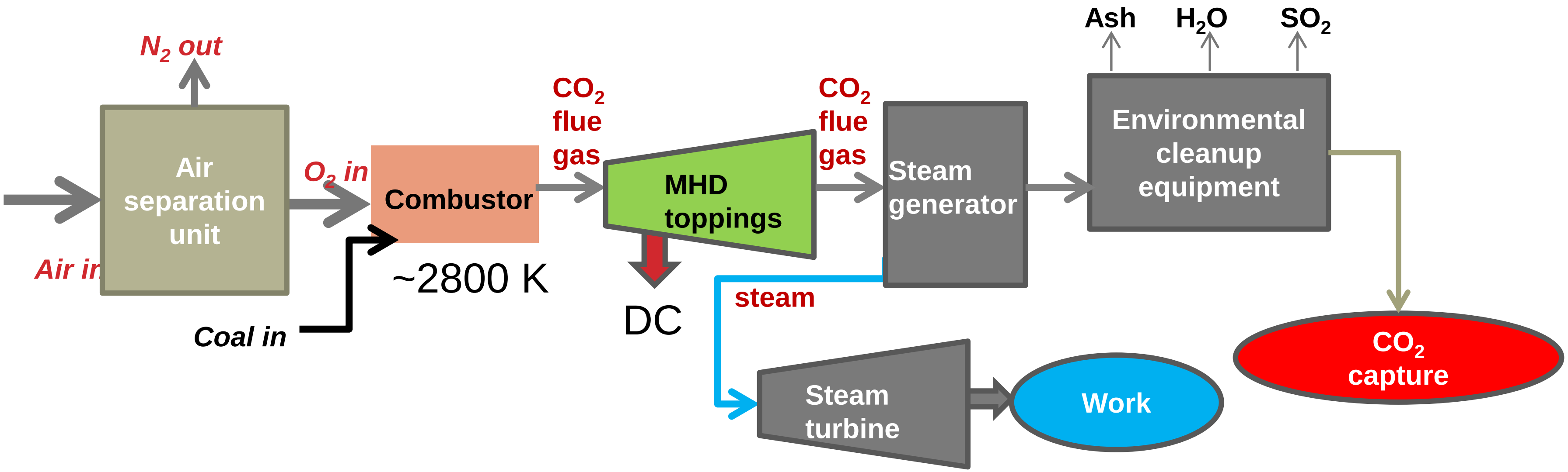
HIGH-FIDELITY MODELS FOR COAL COMBUSTION: TOWARD HIGH-TEMPERATURE OXY-COAL FOR DIRECT POWER EXTRACTION

XINYU ZHAO
UNIVERSITY OF CONNECTICUT
DANIEL C. HAWORTH[1], MICHAEL F. MODEST[2], JIAN CAI[3]
[1]THE PENNSYLVANIA STATE UNIVERSITY
[2]UNIVERSITY OF CALIFORNIA, MERCED
[3]UNIVERSITY OF WYOMING

SPONSORED BY NATIONAL ENERGY TECHNOLOGY LABORATORY

HIGH-TEMPERATURE OXY-COAL COMBUSTION



Challenging factors:

- Highly-concentrated chemically-reactive and radiatively-participative species
- Shift of heat transfer patterns
- Change of modeling priority (devolatilization versus surface-reaction)

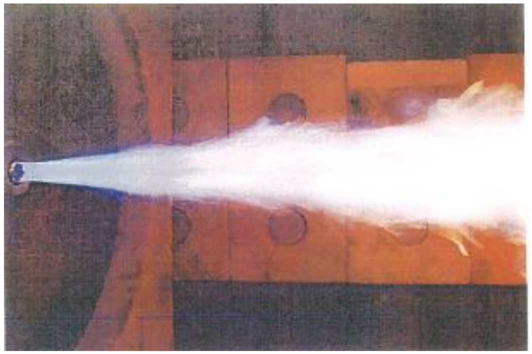
OBJECTIVES

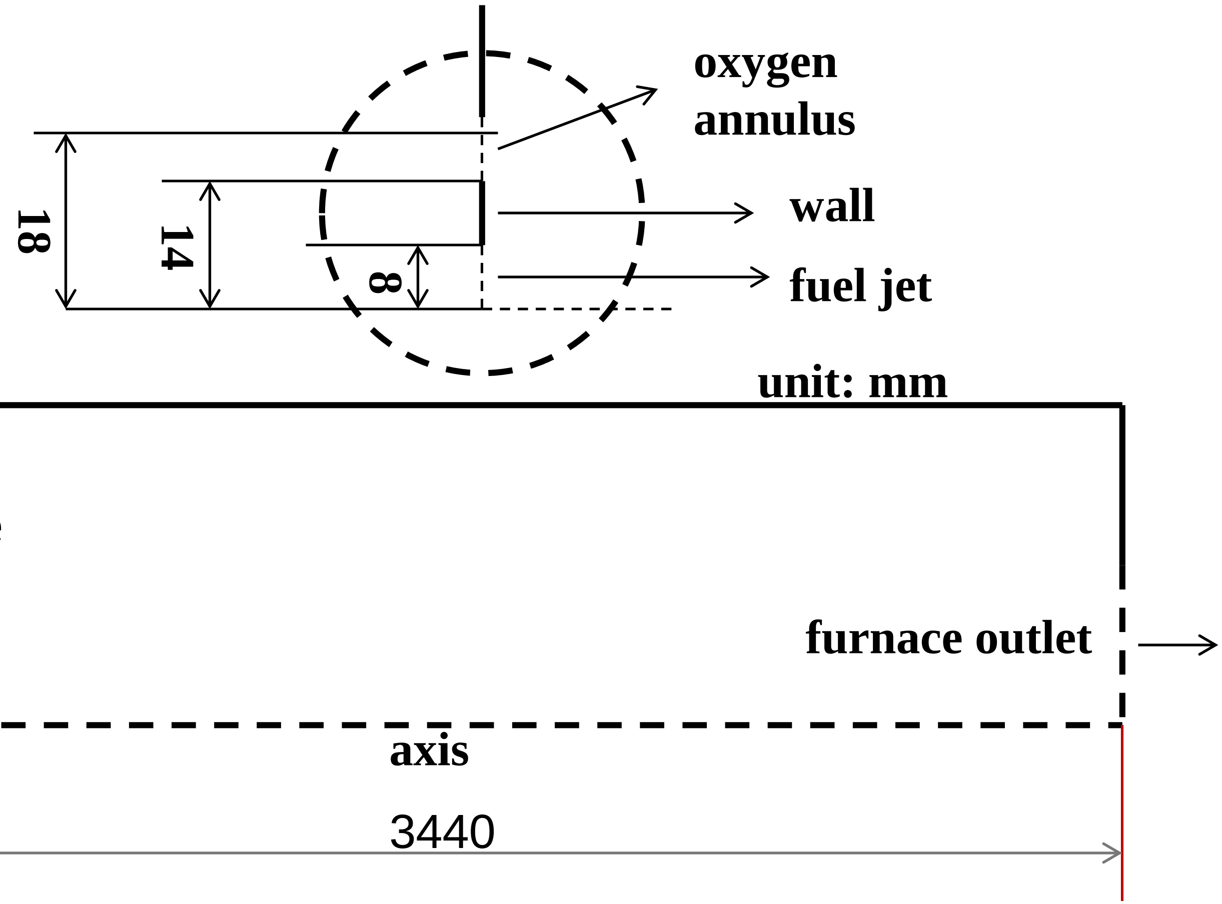
Explore the flow, chemistry, and heat transfer, and their interactions through high-fidelity models.

Physics	Proposed models
Turbulent flow field	RANS-based model (LES)
Gas-phase chemistry	Detailed chemistry models
Turbulence-chemistry-radiation interactions	Transported PDF models
Radiative heat transfer	P1 model (Photon Monte Carlo)
Spectral properties of gas/particle	k-distribution considering CO_2, H_2O, CO, and particles.
Char surface reaction model	CBK model with CO_2, H_2O, O_2
Devolatilization model	CPD model/ Two-rates model with fitted parameter

A SYSTEMATIC APPROACH HAS BEEN ADOPTED

IMPLEMENT AND VALIDATE PMC-LBL FOR HIGH-T OXY-CH_4

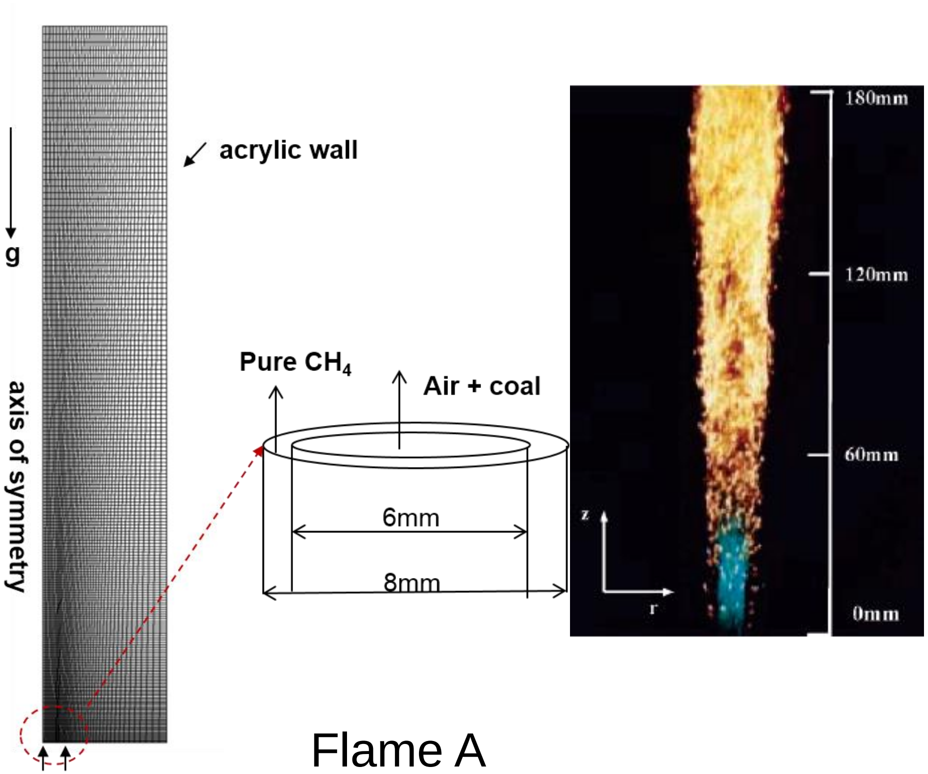




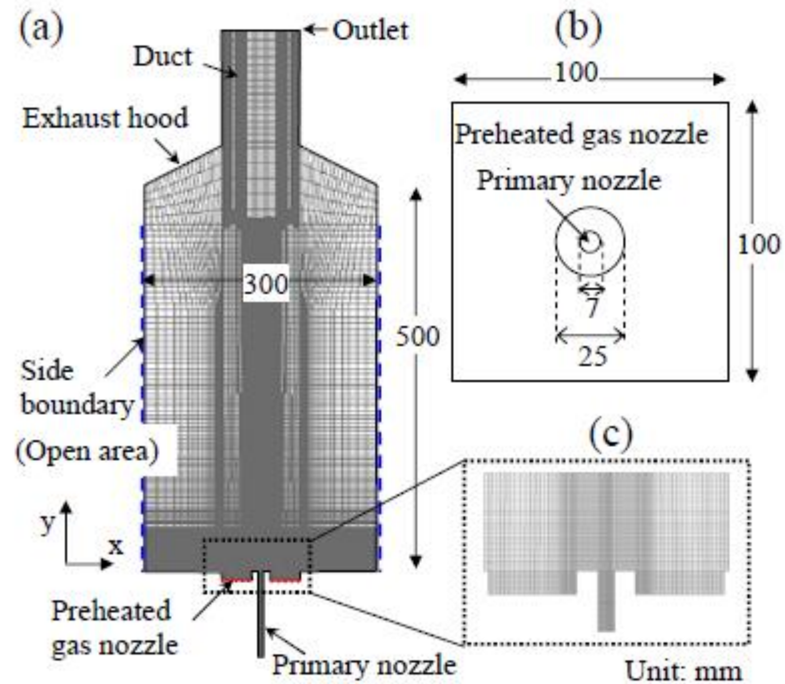
N. Lallemant, F. Breussin, R. Weber, T. Ekman, J. Dugue, J. M. Samaniego, O. Charon, A. J. Van Den Hoogen, J. Van Der Bemt, W. Fujisaki, T. Imanari, T. Nakamura and K. IINO. Flame Structure, heat transfer and pollutant emissions characteristics of oxy-natural gas flames in the 0.7-1 MW thermal input range. Journal of Institute of Energy, 73, pp. 169-182

A SYSTEMATIC APPROACH HAS BEEN ADOPTED

IMPLEMENT AND VALIDATE TRANSPORTED PDF – COAL SOLVER



Flame A



Flame B

Flame A: S. M. Hwang, R. kurose, F. Akamatsu, H. Tsuji, H. Makino and M. Katsuki. Application of optical diagnostics techniques to a laboratory-scale turbulent pulverized coal flame. Energy Fuels (2005), 19, 382-392

FlameB: M. Taniguchi, H. Okazaki, H. Kobayashi, S. Azuhata, H. Miyadera, H. Muto, T. Tsumura. Pyrolysis and ignition characteristics of pulverized coal particles. ASME. Vol. 123. pp. 32-38.

OUTLINE

Methods

Chemistry and turbulence-chemistry interactions

Radiative heat transfer

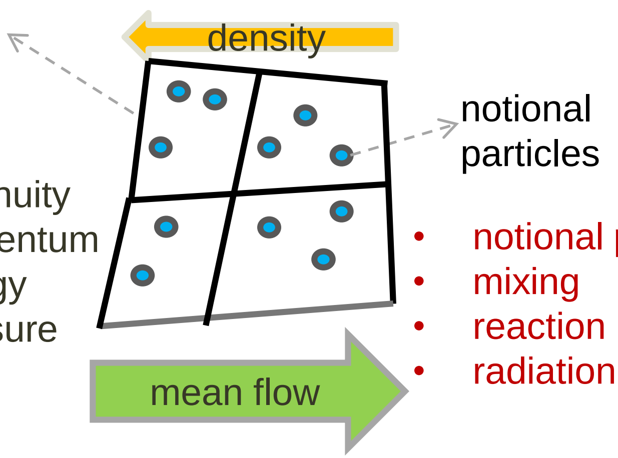
High-fidelity models in coal combustion

Conclusions

METHOD

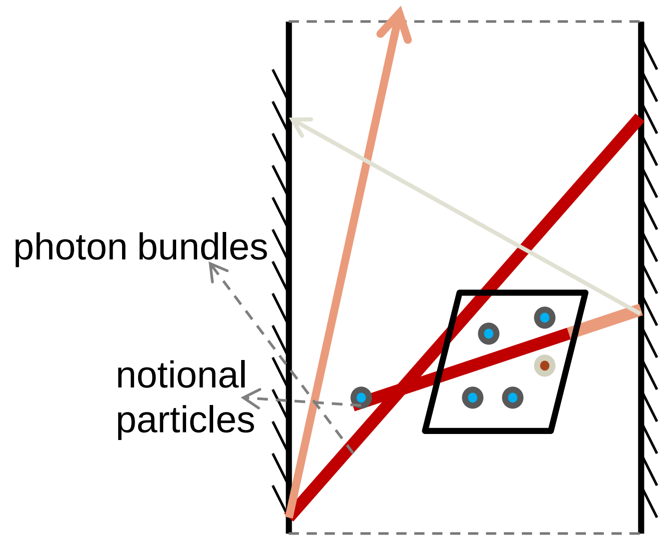
Transported composition PDF method

Photon Monte Carlo method + LBL



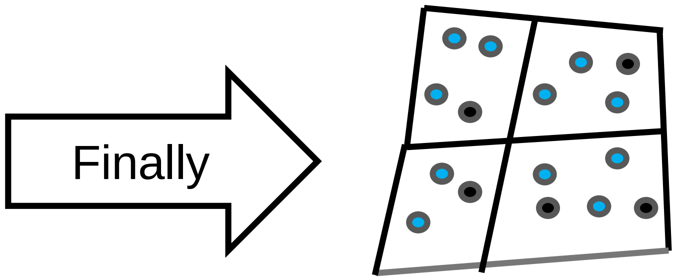
- continuity
- momentum
- energy
- pressure
- k, ε

- notional particle tracking
- mixing
- reaction
- radiation



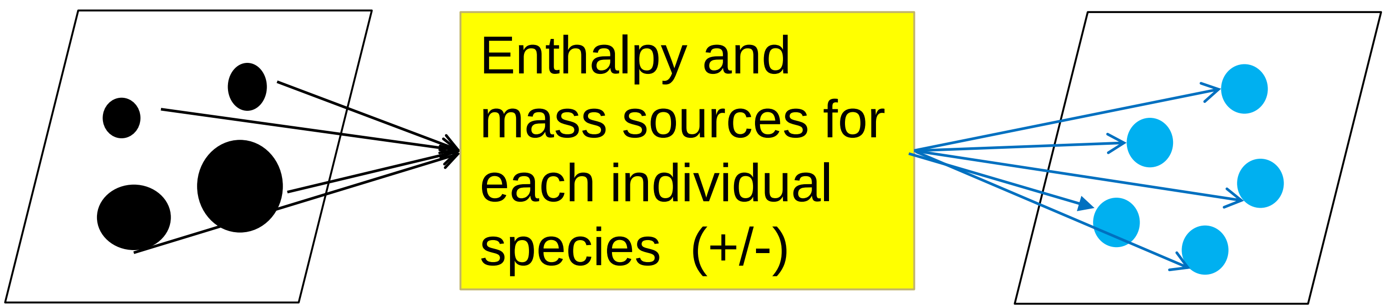
$\langle S_c \rangle \neq S_c(\tilde{T})$ Turbulence-chemistry-radiation interactions $\langle I_{b\eta} \rangle \neq I_{b\eta}(\tilde{T})$

METHOD



Transported PDF/PMC/coal solver

The coupling model is a challenging aspect.



Coal parcels in one cell (solid phase)

PDF notional particles in one cell (gas phase)

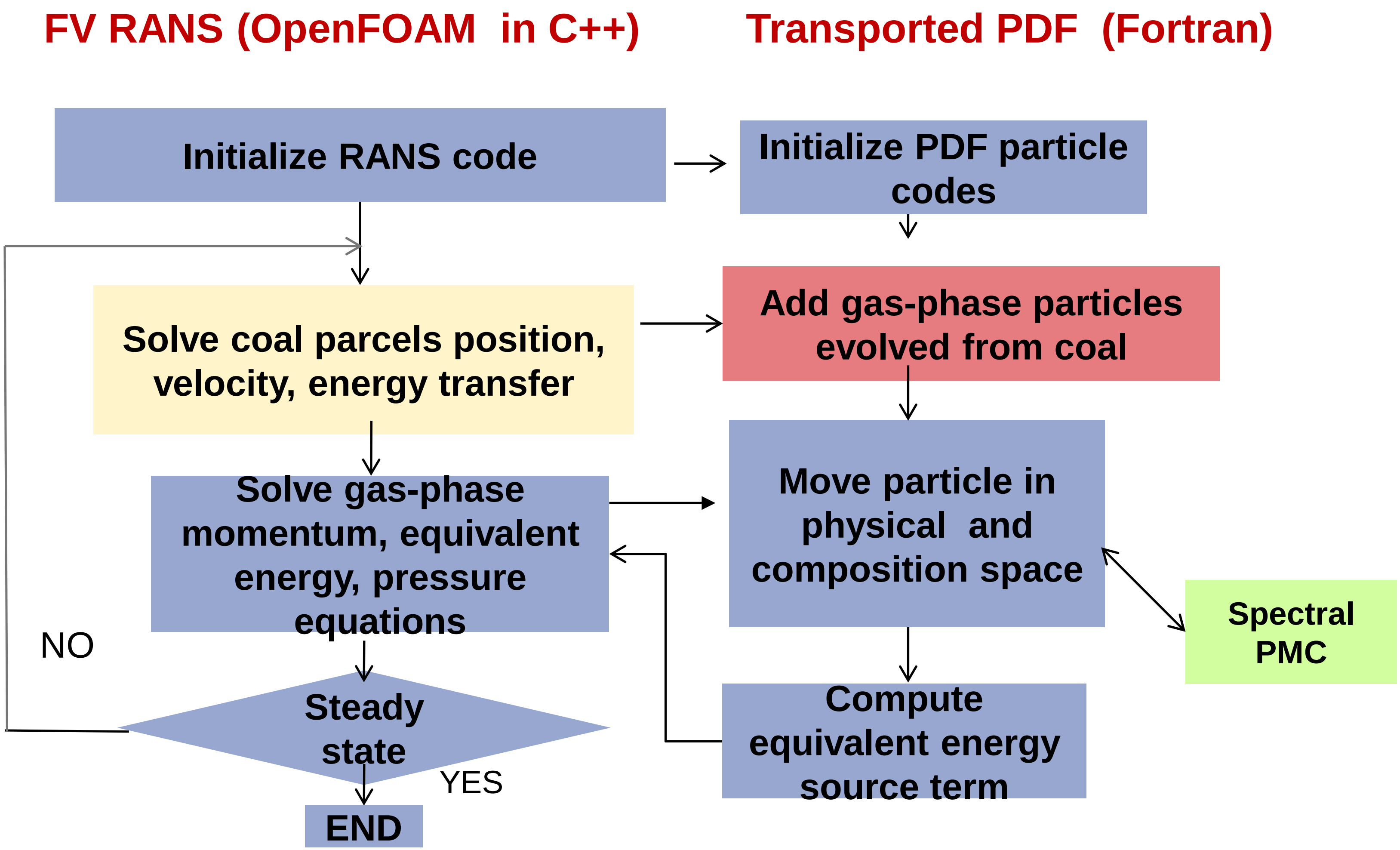
TYPICAL SUB-MODELS

- **Turbulence:** standard k-epsilon model with adjusted $C_{\varepsilon 1}$
- **Chemical mechanisms**
    - GRI-Mech 2.11
- **Radiative heat transfer**
    - P1 radiation with gray gas and particles
    - P1 with k-distribution (Cai et al.)
- **Mixing models**
    - Euclidean minimum spanning tree model (EMST)
    - Variable C_{Φ}
- **Chemical acceleration**
    - In situ adaptive tabulation (ISAT) (parallel)
- **Devolatilization**
    - two-rates model
    - single-rate model
    - modified single-rate model
- **Surface reaction**
    - diffusion-kinetic-control model
    - oxy-char combustion model **

*Mehta, R. S., Haworth, D. C., Modest, M. F. An assessment of gas-phase reaction mechanisms and soot models for laminar atmospheric-pressure ethylene-air flames. Proc. Combust. Inst. 32, 2009, 1327-1337.

** Murphy, J. J., and Shaddix, C. R. Combustion kinetics of coal chars in oxygen-enriched environments. Combust. Flame. 144 ,2006, 710-729

SOLUTION ALGORITHM



OUTLINE

Methods

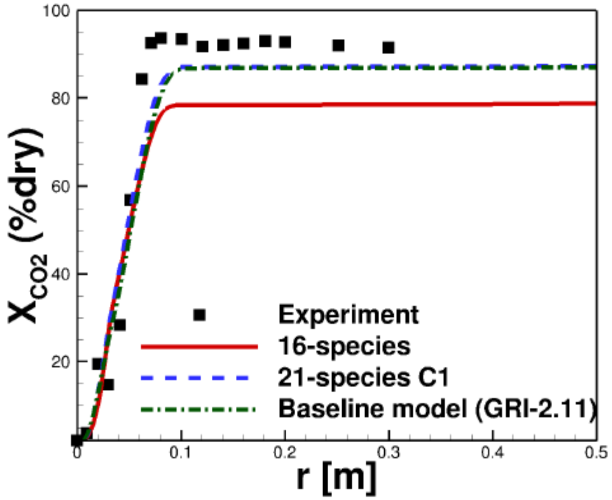
Chemistry and turbulence-chemistry interactions

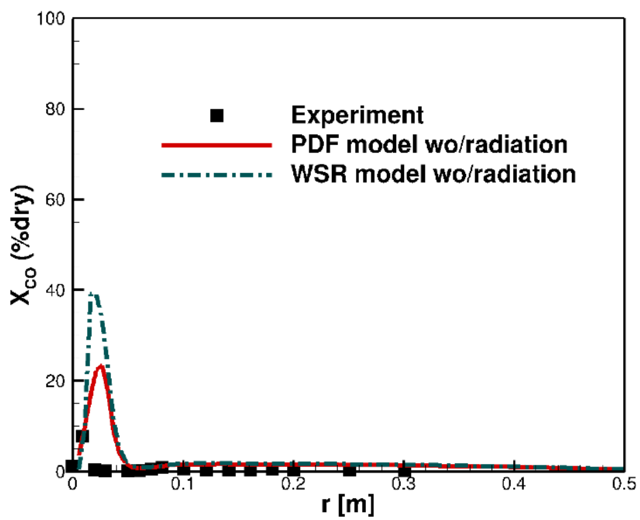
Radiative heat transfer

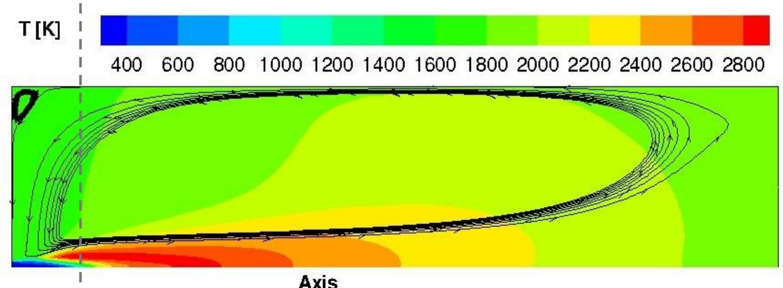
High-fidelity models in coal combustion

Conclusions

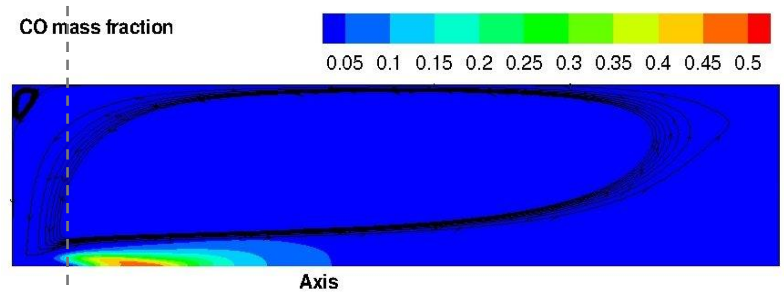
TCI IN HIGH-TEMPERATURE OXY-CH_4 COMBUSTION







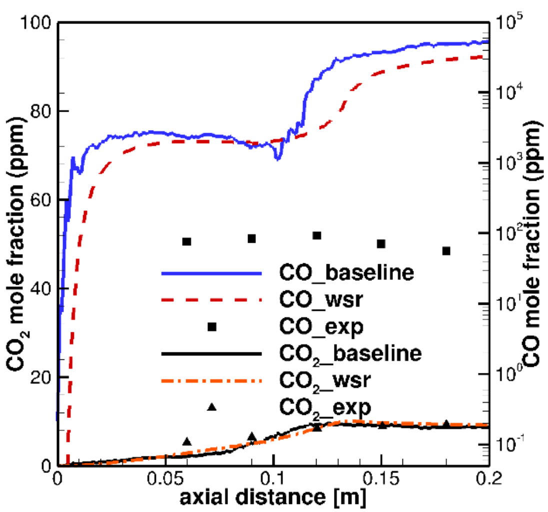
mean temperature

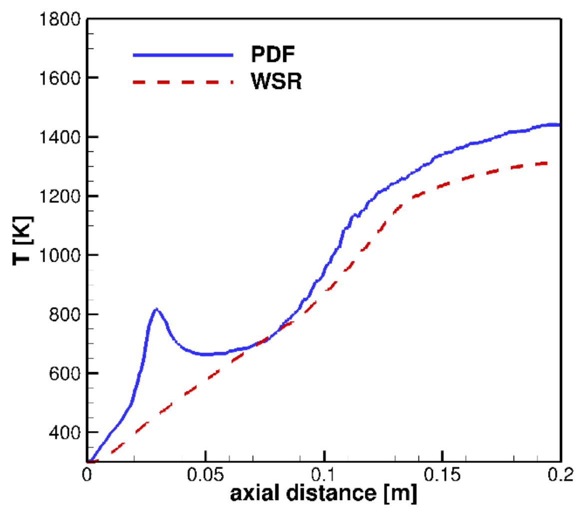


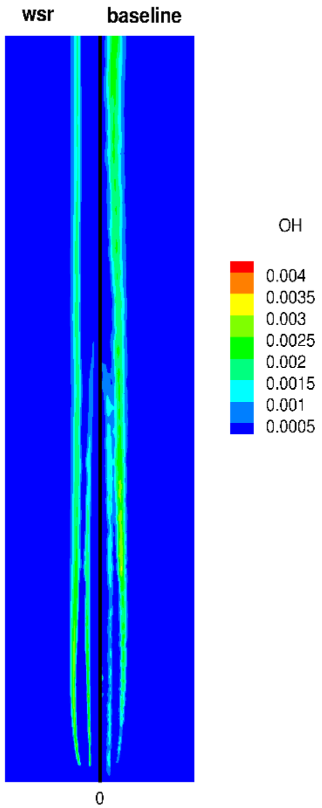
mean CO mass fraction

TCI IN TURBULENT COAL COMBUSTION

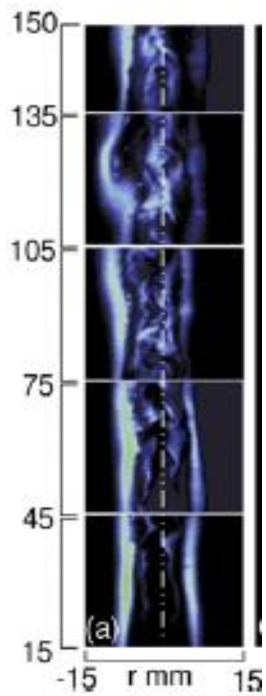
The effect of turbulence-chemistry interactions is reflected in the flame structure.







Computed Y_{OH}



OH PLIF

OUTLINE

Methods

Chemistry and turbulence-chemistry interactions

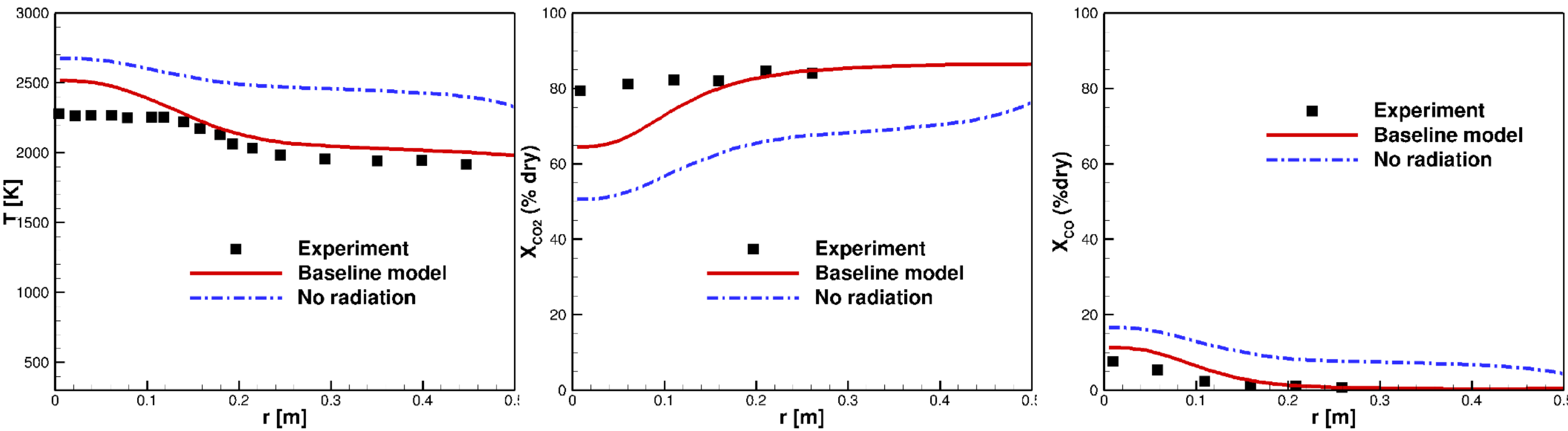
Radiative heat transfer

Advantage and difficulties of using high-fidelity models

Conclusions

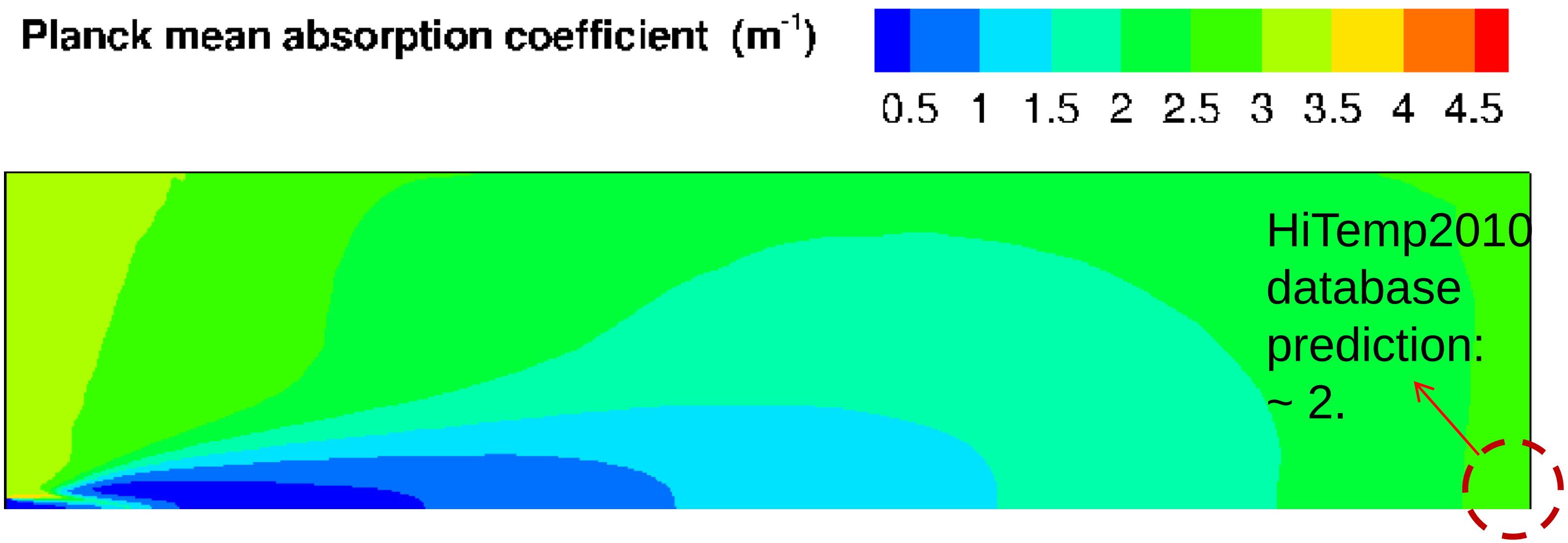
RADIATION IS DOMINANT IN THE HIGH-T OXY-CH_4 FLAME

mean temperature | mean X_{CO2} | mean X_{CO}



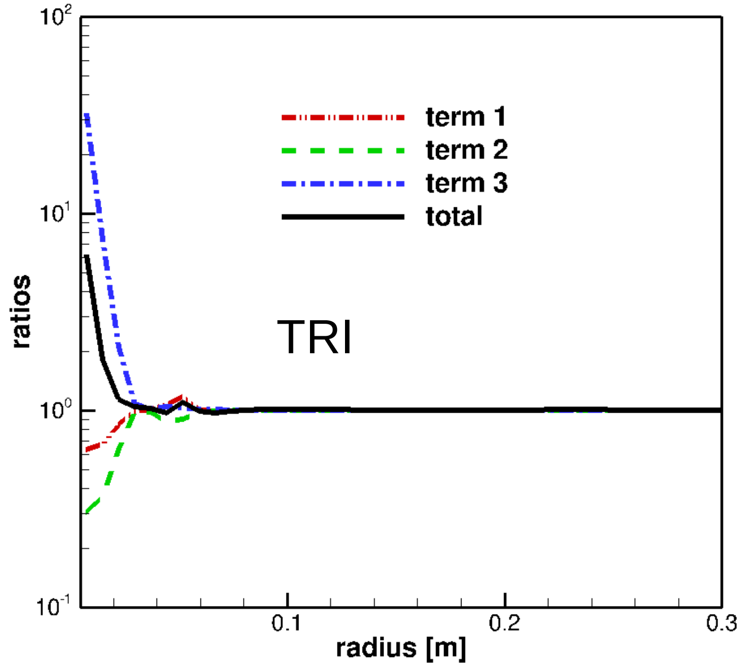
x= 1.42m

SPECTRAL PMC MODEL CAN PREDICT ABSORPTION COEFFICIENTS IN THE HIGHLY PARTICIPATIVE ENVIRONMENT.



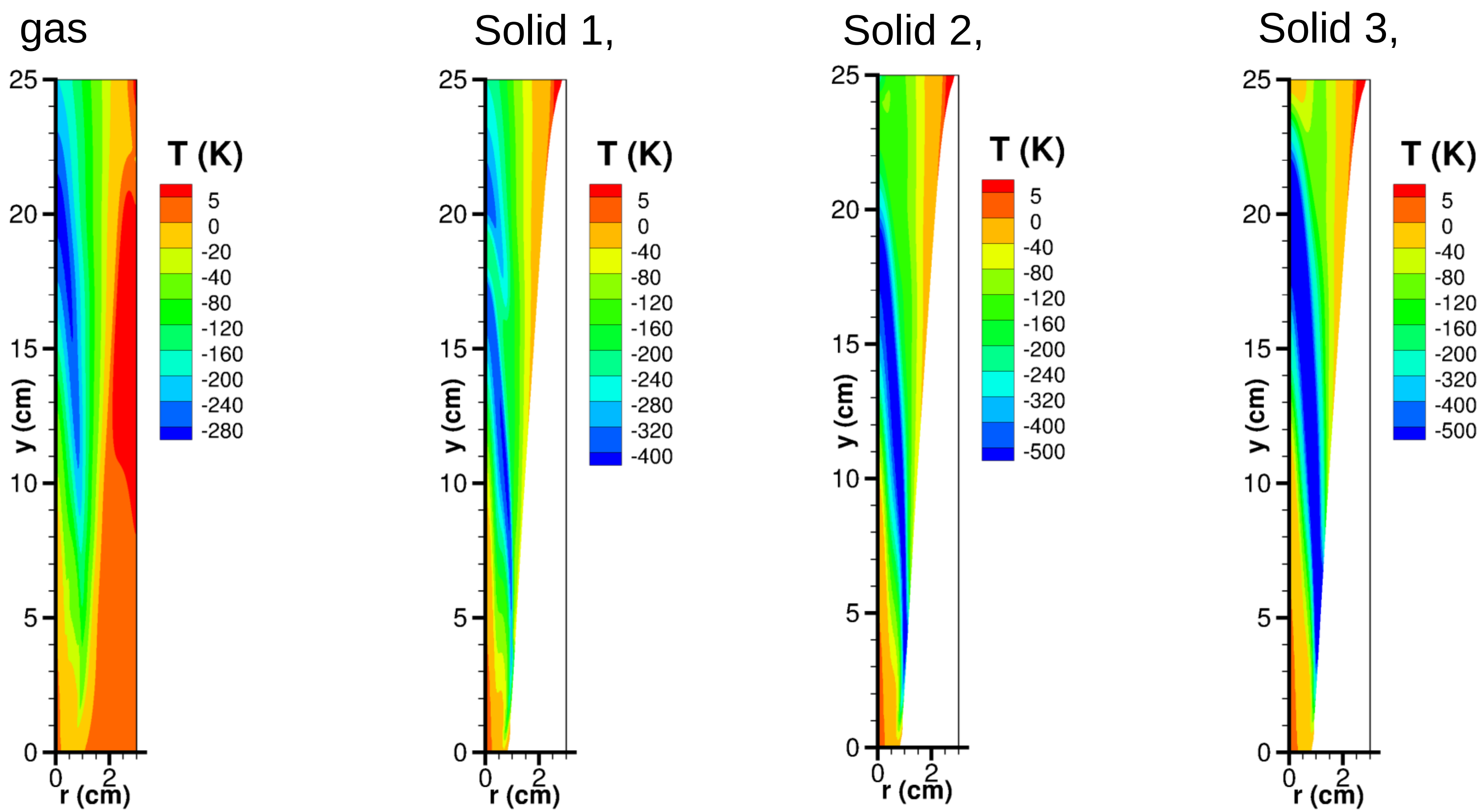
C. Yin, L. A. Rosendahl, S. K. Kær. Chemistry and radiation in oxy-fuel combustion: a computational fluid dynamics modeling study. Fuel. 90(7), pp. 2519-2529.

TURBULENCE-CHEMISTRY-RADIATION INTERACTIONS ARE INTENSE ONLY IN THE FLAME CORE, NEAR THE NOZZLE.



$$\frac{\langle \kappa_P(T,\underline{Y})T^4\rangle}{\kappa(\langle T\rangle,\langle \underline{Y}\rangle)\langle T\rangle^4} = \underbrace{\frac{\langle \kappa_P(T,\underline{Y})T^4\rangle}{\langle \kappa(T,\underline{Y})\rangle\langle T^4\rangle}}_{\text{term 1}} \times \underbrace{\frac{\langle \kappa(T,\underline{Y})\rangle}{\kappa(\langle T\rangle,\langle \underline{Y}\rangle)}}_{\text{term 2}} \times \underbrace{\frac{\langle T^4\rangle}{\langle T\rangle^4}}_{\text{term 3}}$$

THE LABORATORY-SCALE FLAME IS OPTICALLY-THIN. RADIATION HAS HIGHER INFLUENCE TO LARGER PARTICLES.

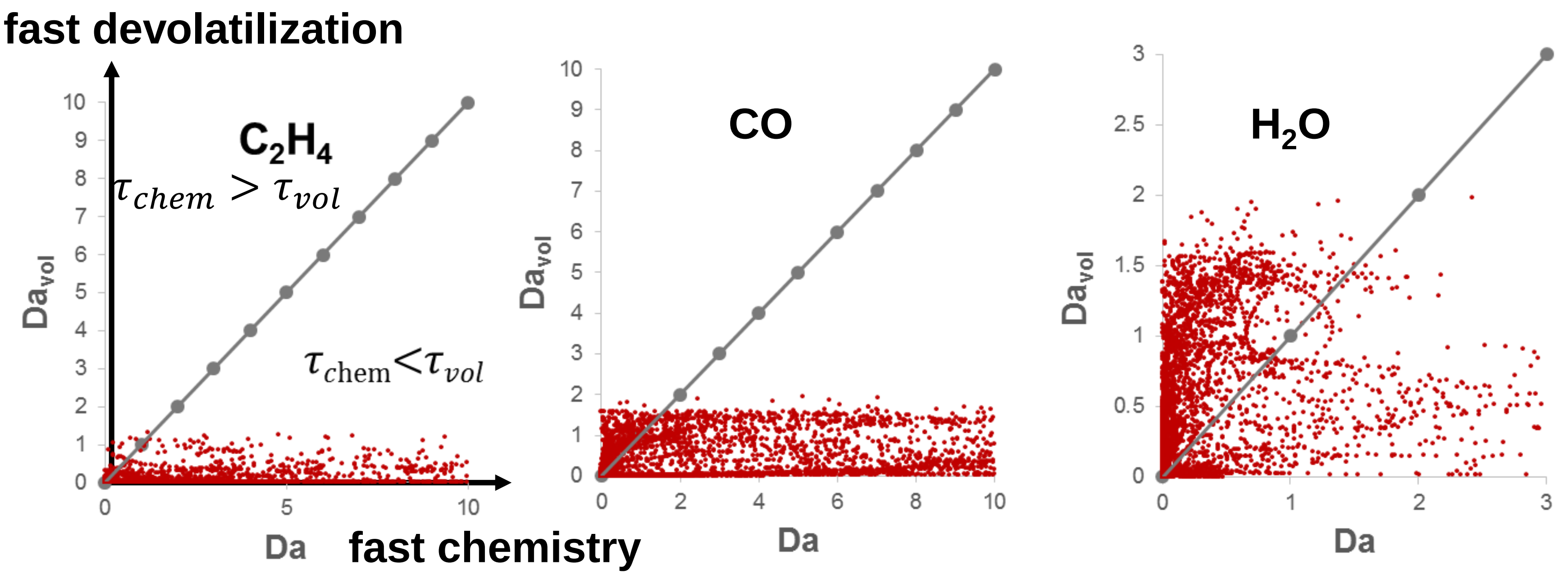


Courtesy of Jian Cai

OUTLINE

- Methods
- Chemistry and turbulence-chemistry interactions
- Radiative heat transfer
- **High-fidelity models in coal combustion**
- Conclusions

THE ASSUMPTION OF EQUILIBRIUM CHEMISTRY CAN BE EXAMINED BY THE FINITE-RATE MODEL.

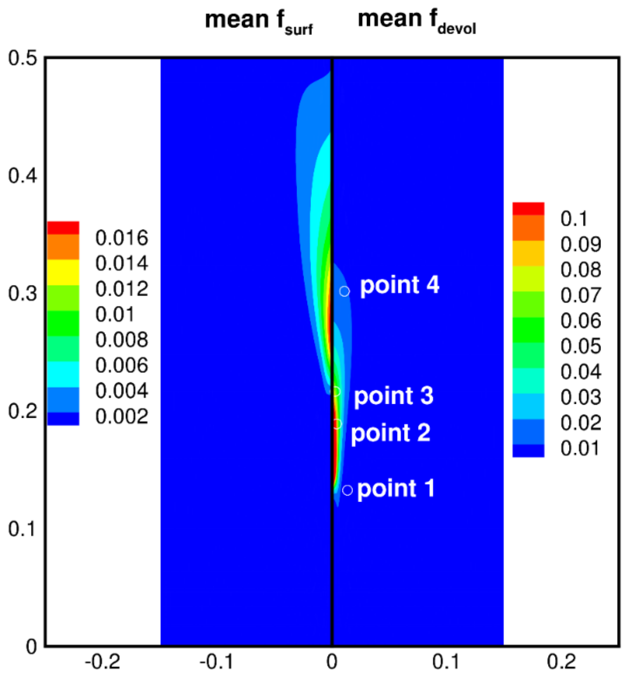


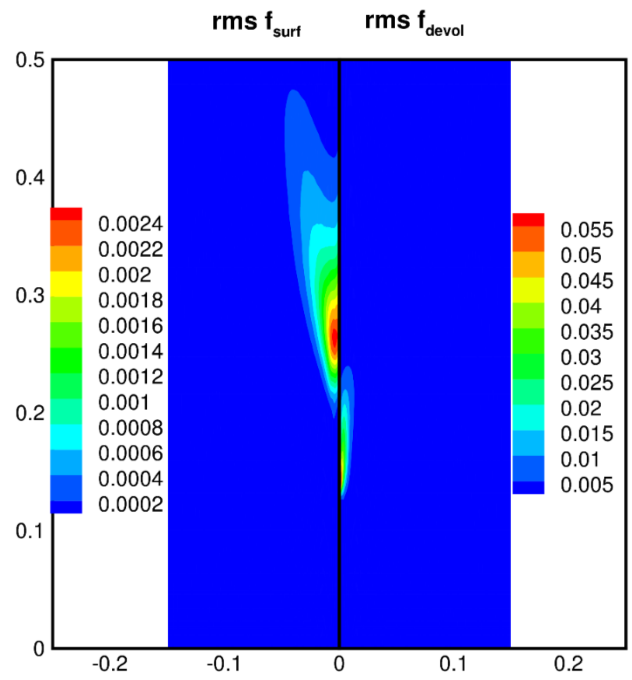
$$Da = \frac{\tau_f}{\tau_c} \quad Da_{vol} = \frac{\tau_f}{\tau_{vol}}$$

THE MIXTURE FRACTIONS OF DEVOLATILIZATION AND SURFACE REACTION CAN BE RECONSTRUCTED FROM THE RESULTS.

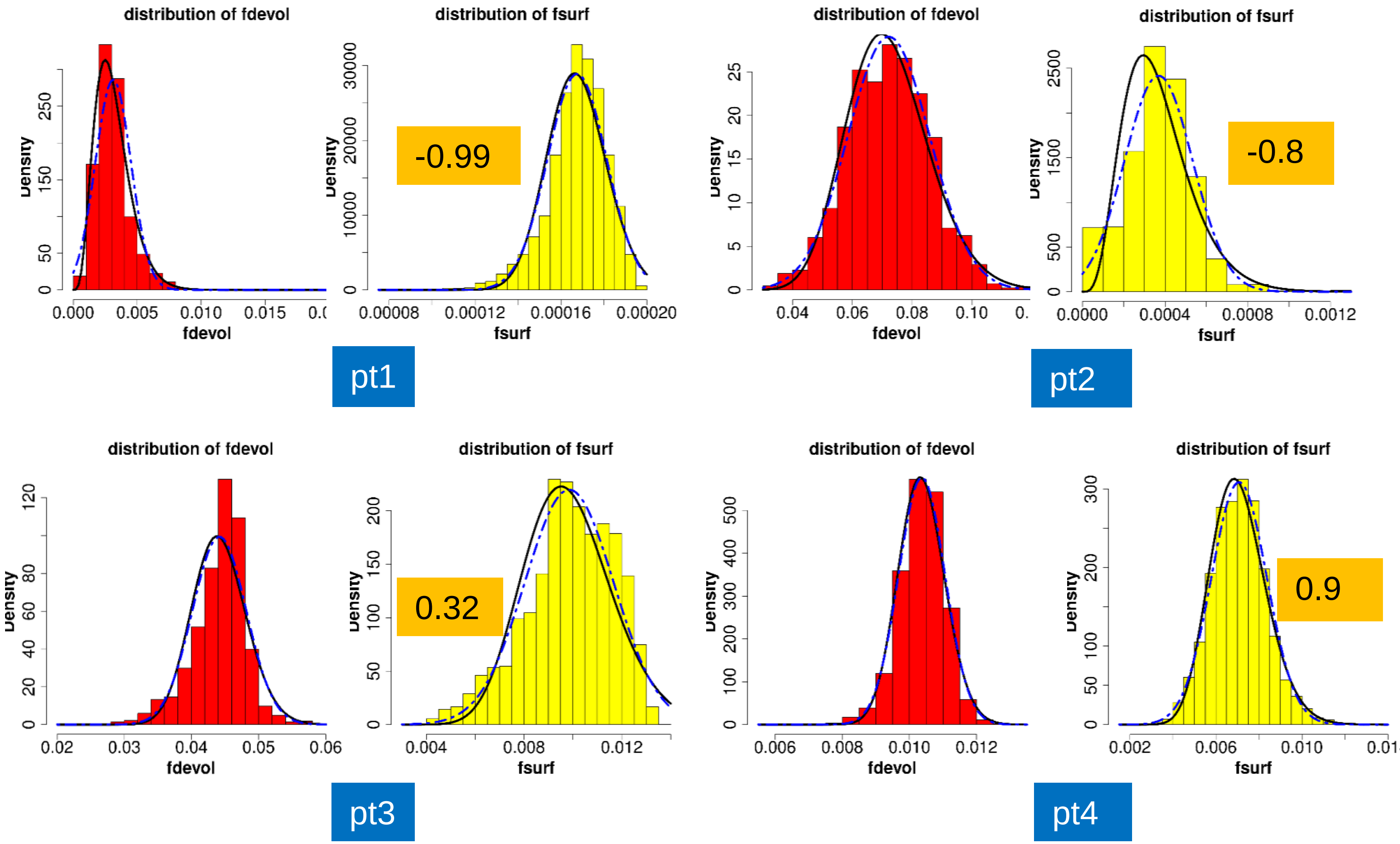
$$f_{devol} = \frac{m_{devol}}{m_{primary} + m_{pilot} + m_{devol}}$$

$$f_{surf} = \frac{m_{surf}}{m_{primary} + m_{pilot} + m_{devol} + m_{surf}}$$

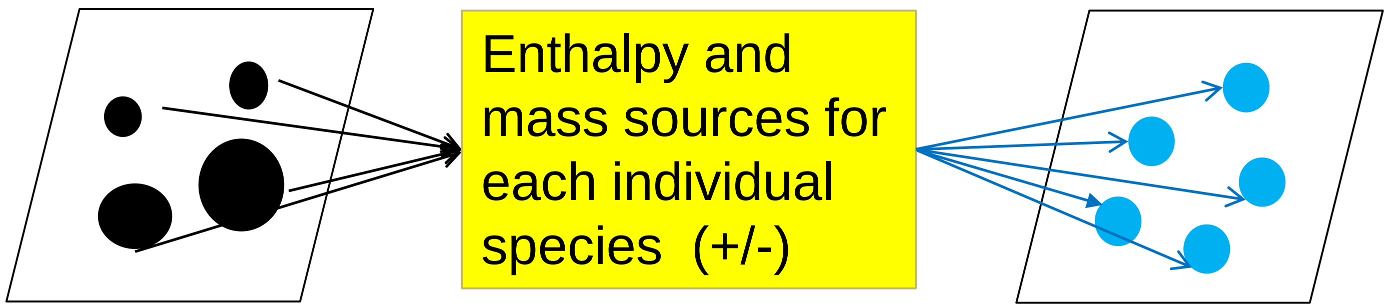




THE ASSUMPTIONS USED IN THE MIXTURE FRACTION BASED METHOD COULD BE TESTED USING HIGH-FIDELITY MODELS.



DIFFICULTIES IN USING HIGH-FIDELITY MODELS



Coal parcels in one cell (solid phase)

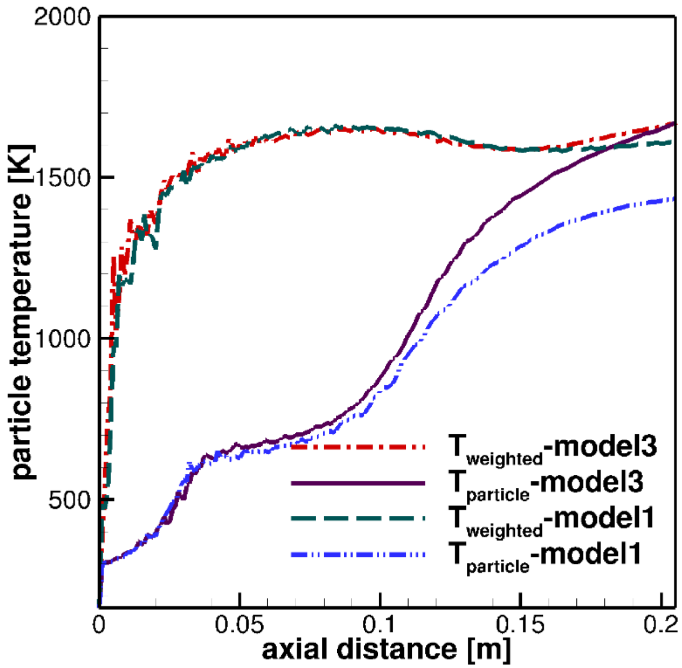
PDF notional particles in one cell (gas phase)

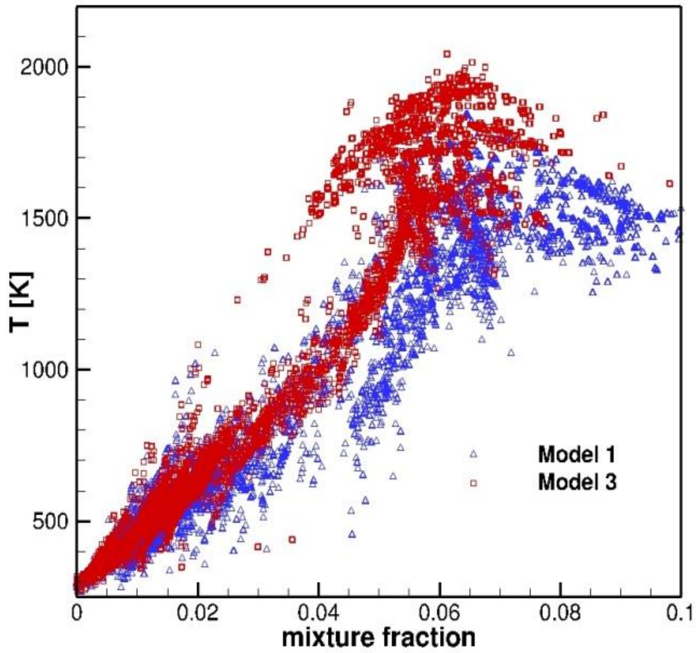
Model 1: distribute cell-level mass and energy source weighted by **notional particle mass (m_p)**

Model 2: distribute cell-level mass and energy source weighted by **notional particle temperature (T_p)**

Model 3: distribute cell-level mass and energy source weighted by **reactivity exp(-C/T_p) (C is a constant)**

MORE VALIDATION WITH EXPERIMENTS OR HIGHER-ORDER MODEL IS NECESSARY.

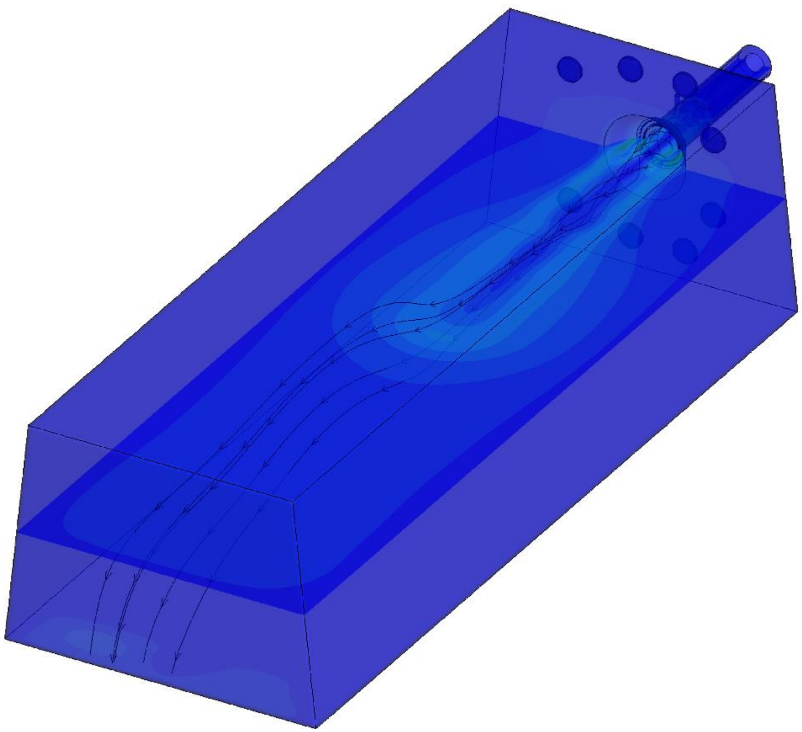


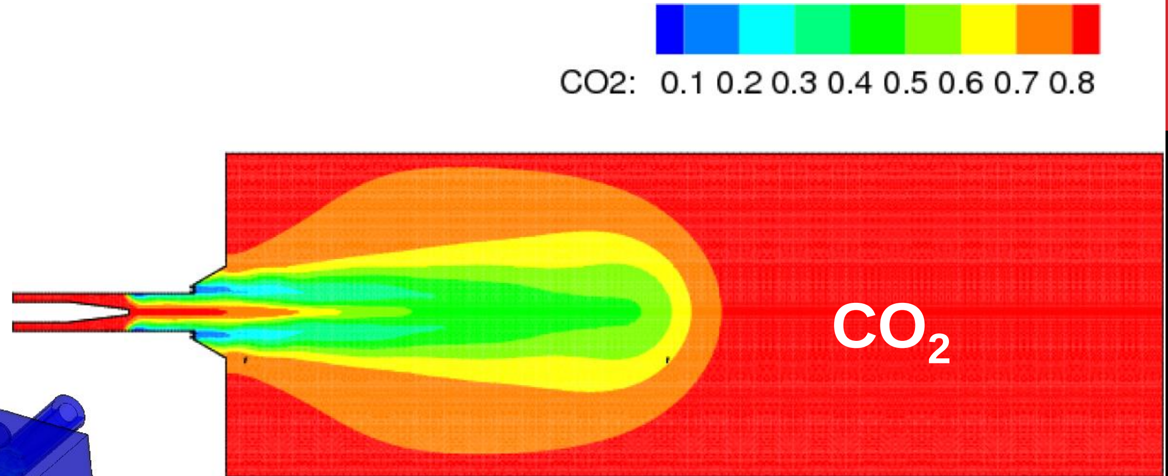


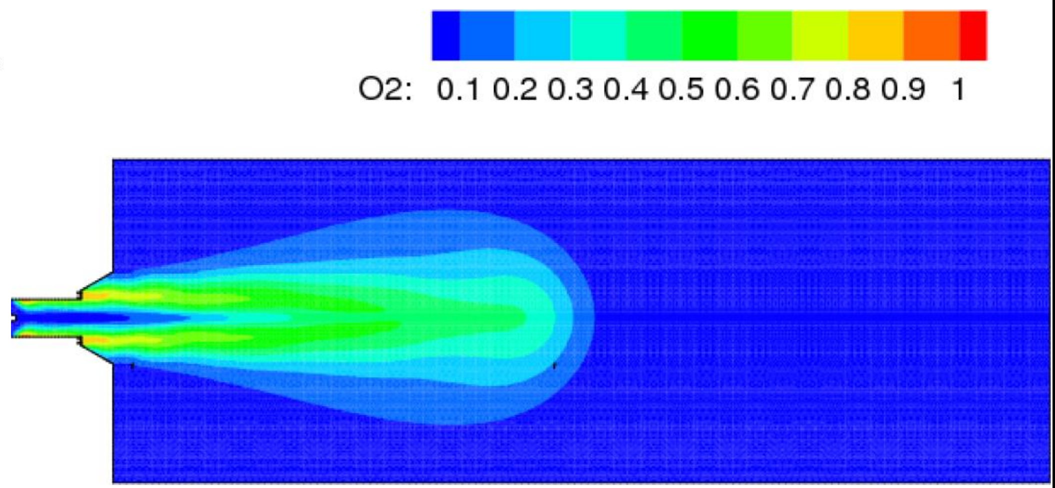
CONCLUSIONS

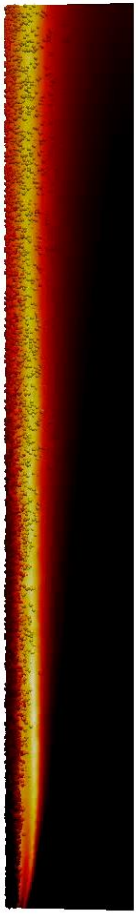
- **A transported PDF model for coal combustion using finite-rate chemistry has been built. Components of the model has be validated through a hierarchy of experimental configurations.**
- **The spectral photon Monte-Carlo method implemented in this work can capture the nongray effect of the high-temperature oxy-combustion environment naturally.**
- **Turbulence-chemistry-radiation interactions can also be captured by the model without additional effort. The interactions are extremely important for pollutants prediction (CO, NO, and soot).**
- **The high-fidelity models developed in this work can be used to guide the development of simpler models.**
- **LES model will be coupled with PDF method to properly predict the particle location.**

POSSIBLE FUTURE WORK









NETL-RUA
Regional University Alliance

PENN STATE
NITTANY LIONS

Thank You !