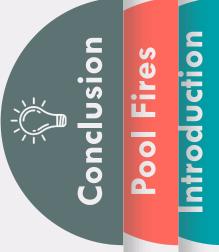
### Transported probability density function modeling of fire extinction

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10/19/2022





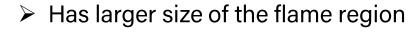
### Introduction

#### Turbulent diffusion combustion



- ➤ Buoyancy controlled
- Low strain
- ➤ Low velocity fuel

#### Objectives of this work



- > Used highly simplified chemical mechanisms
- > Used reduced order turbulence and combustion models





#### Models' accuracy

Highly simplified or reduced-order models cannot capture detailed physics



Use high order model to get accurate prediction of fire extinction limit

# Transported PDF modeling of pool fires

#### Fire Dynamics Simulator (FDS)



FDS (Fire Dynamics Simulator) is a free and open-source software tool provided by the National Institute of Standards and Technology (NIST) of the United States Department of Commerce.

FDS is a large-eddy simulation (LES) code for low-speed flows, emphasizing smoke and heat transport from fires.

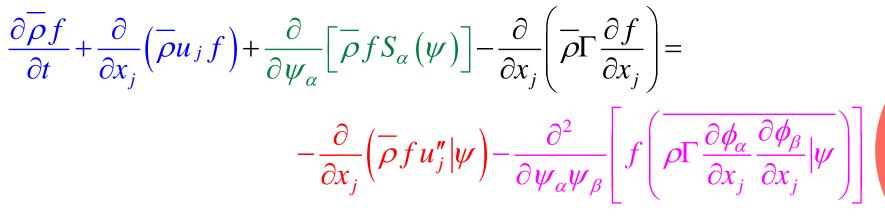
#### Transported PDF model

- PDF represents Probability Density Function
- Transported PDF model represents the turbulent reacting flow by using Joint PDFs of fluid properties
- Advantages:
  - Does not assume a particular mode of combustion
  - Chemical reaction terms are in a closed form
  - Turbulent fluctuations of all species can be represented
  - Applicable to RANS and LES



#### Transported PDF model

A joint pdf transport equation for the velocity and the reactive scalars can be derived \*





local change and convection of the probability density function in physical space source terms due to chemical reaction and it appears in the closed form

spatial flux of the PDF due to residual velocity

molecular mixing in the composition space due to the conditional scalar dissipation

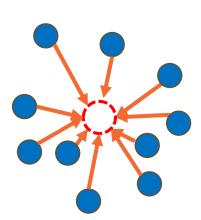
<sup>\*</sup> Pope, S. B. (1985). PDF methods for turbulent reactive flows. Progress in energy and combustion science, 11(2), 119-192.

#### Mixing models implemented in PDF

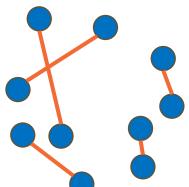
Popular models used in this work

- Interaction by Exchange with the Mean (IEM) model
- Modified Curl (MCurl) model
- Euclidean Minimum Spanning Tree (EMST) model

**IEM** 

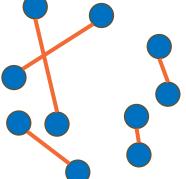


**MCurl** 



Interaction with the mean

$$\frac{d\phi^{(i)}}{dt} = -\frac{1}{2} \frac{C_{\phi}}{\tau} \left( \phi^{(i)} - \tilde{\phi} \right)$$

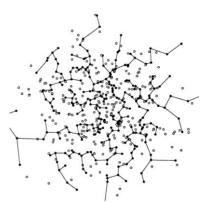


Randomly pairwise mixing

$$\phi^{(i),t+1} = \phi^{(i),t} + h \left( \frac{w^{(i)}\phi^{(i),t} + w^{(j)}\phi^{(j),t}}{w^{(i)} + w^{(j)}} - \phi^{(i),t} \right)$$

$$\phi^{(j),t+1} = \phi^{(j),t} + h \left( \frac{w^{(i)}\phi^{(i),t} + w^{(j)}\phi^{(j),t}}{w^{(i)} + w^{(j)}} - \phi^{(j),t} \right)$$

**EMST** 



Interaction with neighboring

particle in composition space

$$\phi^{(j),t+1} = \phi^{(j),t} + h \left( \frac{w^{(i)}\phi^{(i),t} + w^{(j)}\phi^{(j),t}}{w^{(i)} + w^{(j)}} - \phi^{(j),t} \right) \qquad \frac{d\phi_{\alpha}^{(i)}}{dt} = -\frac{1}{w^{(i)}} M_{ij}\phi_{\alpha}^{(j)}, \quad i = 1,...,N_p' \left( N_p' \leq N_p \right),$$

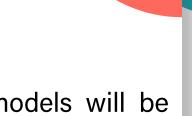
#### Mixing parameters implemented in PDF

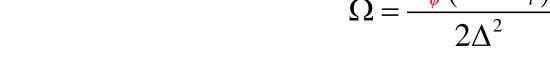
### $\frac{\partial \overline{\rho} f}{\partial t} + \frac{\partial}{\partial x_{i}} \left( \overline{\rho} u_{j} f \right) + \frac{\partial}{\partial \psi_{\alpha}} \left[ \overline{\rho} f S_{\alpha} \left( \psi \right) \right] - \frac{\partial}{\partial x_{i}} \left( \overline{\rho} \Gamma \frac{\partial f}{\partial x_{i}} \right) = 0$

$$-\frac{\partial}{\partial x_{j}} \left( \overline{\rho} f u_{j}'' | \psi \right) - \frac{\partial^{2}}{\partial \psi_{\alpha} \psi_{\beta}} \left[ f \left( \overline{\rho} \Gamma \frac{\partial \phi_{\alpha}}{\partial x_{j}} \frac{\partial \phi_{\beta}}{\partial x_{j}} | \psi \right) \right]$$

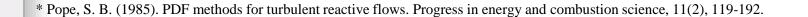
With all the unclosed terms modelled, the transport equation for the PDF is solved numerically by using the Monte Carlo particle method.



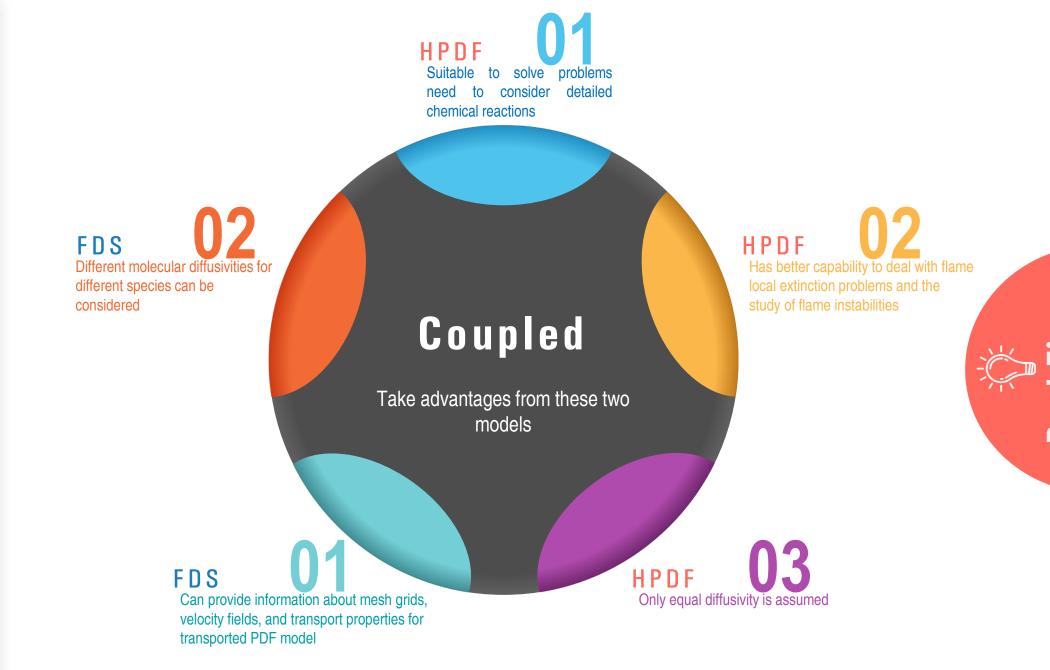




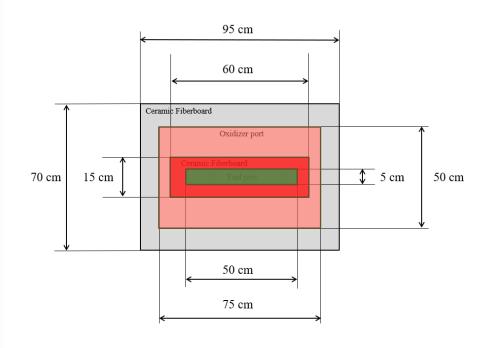
The effects of the mixing parameter  $\,C_{\scriptscriptstyle\phi}\,$  and three different mixing models will be examined.





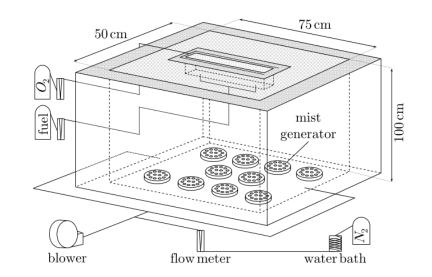


#### UMD line burner



Conclusion

\* J.P. White, Measurement and simulation of suppression effects in a buoyant turbulent line fire, Ph.D. thesis, University of Maryland, College Park, 2016.



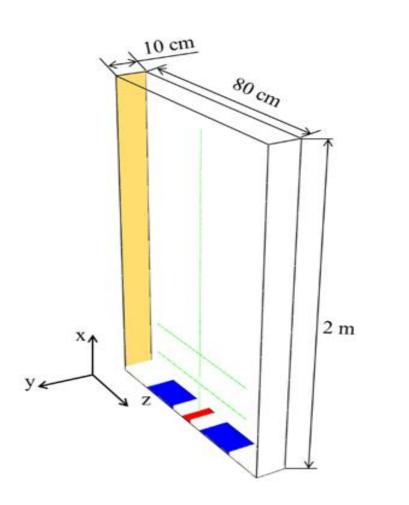


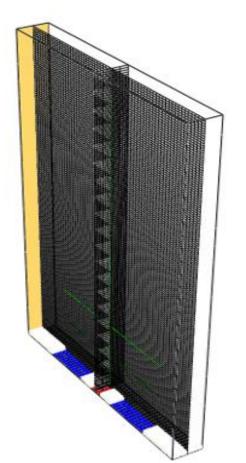
Plane view

**Experimental setup** 

## Conclusion

#### Coupled model simulation setup

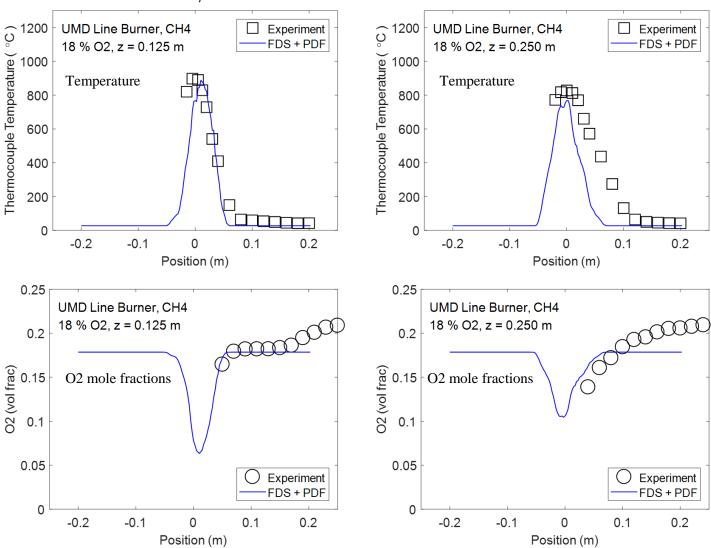






#### Coupled model simulation results

 $C_{\phi} = 3.0$  with EMST model



<sup>\*</sup> Experimental data get from J. P. White, E. D. Link, A. C. Trouve, P. B. Sunderland, A. W. Marshall, J. A. Sheffel, M. L. Corn, M. B. Colket, M. Chaos, H. Z. Yu, Radiative emissions measurements from a buoyant, turbulent line flame under oxidizer-dilution quenching conditions, Fire Safety Journal 76 (2015) pp. 74-84.



#### Coupled model simulation results

• White, J. P. (2016). Measurement and simulation of suppression effects in a buoyant turbulent line fire (Doctoral dissertation).



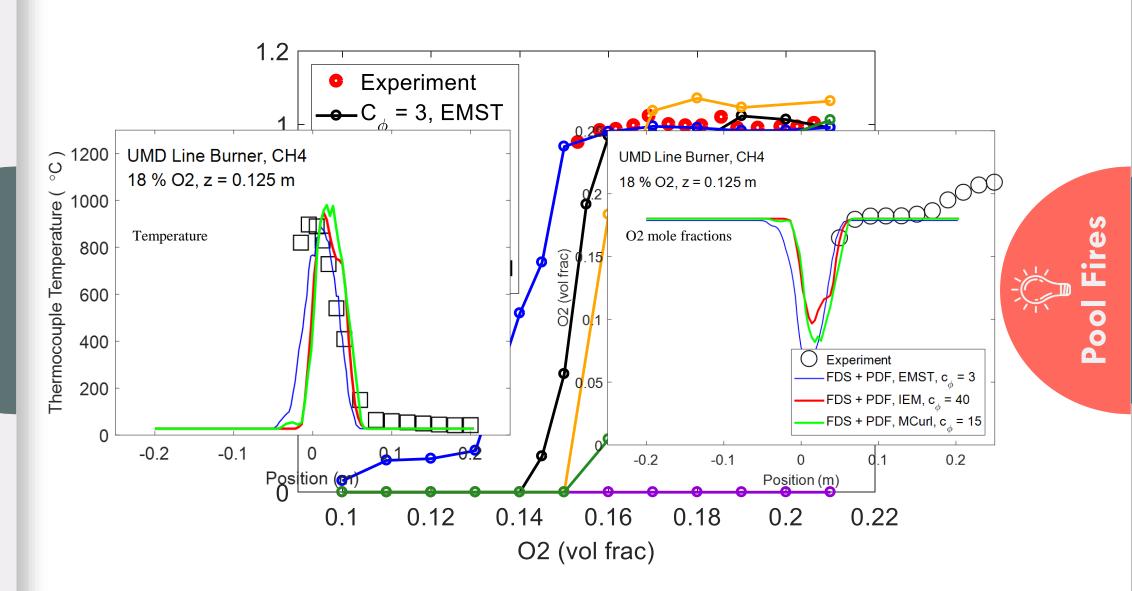


#### Investigation of fire extinction limits prediction



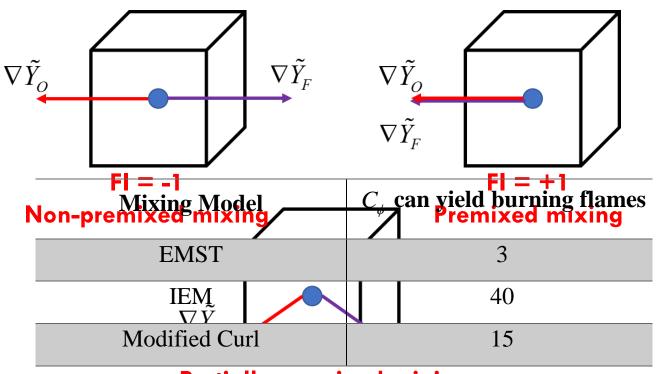


#### Investigation of fire extinction limits prediction





#### Flame regime identification by using flame index



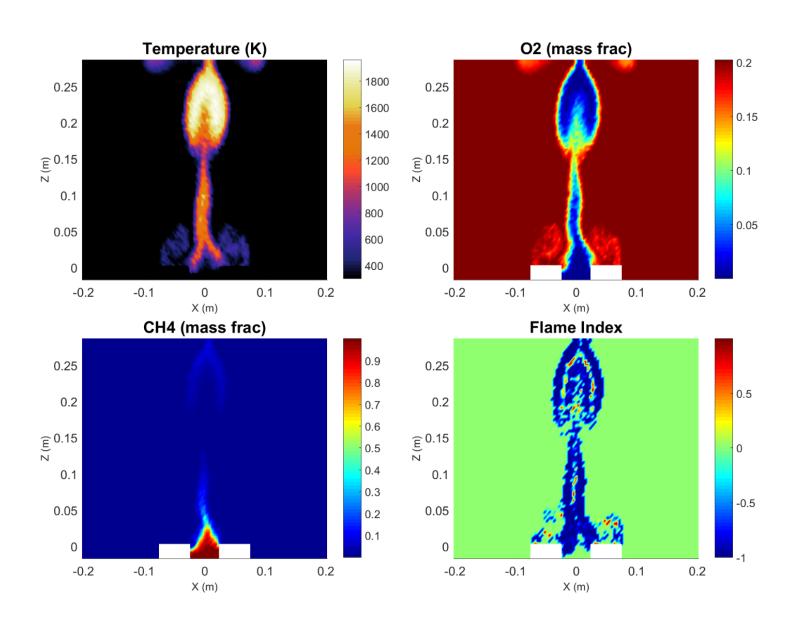


$$FI = \begin{cases} 0 & \left( \left| \tilde{Y}_{O} \right| < \beta\% \left( \max \left| \tilde{Y}_{O} \right| \right), \left| \tilde{Y}_{F} \right| < \beta\% \left( \max \left| \tilde{Y}_{F} \right| \right) \right) \\ & \frac{\nabla \tilde{Y}_{O} \cdot \tilde{Y}_{F}}{\left| \tilde{Y}_{O} \right| \left| \tilde{Y}_{F} \right|} \end{cases}$$



## Conclusion

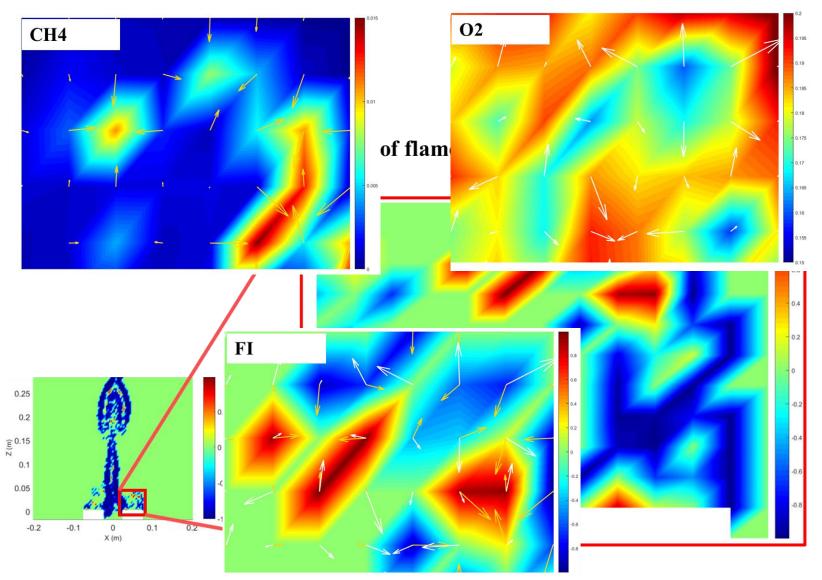
#### Flame regime identification by using flame index





## Conclusion

#### Flame regime identification by using flame index







### Conclusions



#### Conclusions

Buoyancy-controlled pool fires

Discovered the method that combines the NIST Fire Dynamics Simulator (FDS) code of LES and our in-house PDF code, HPDF

The EMST model can yield burning flames without difficulty and perfectly match the measured combustion efficiency

The IEM model and Modified Curl model need a high value of  $C_{\phi}$  to yield burning and constantly underpredict the combustion efficiency

The premixed combustion regimes are enriched in the pool fire's root, which could be the main reason behind the mixing models' performance differences

Fire extinction limit is very sensitive to the different mixing models and mixing parameters. That suggests the importance of mixing modeling in fire simulations.



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