

A Partially-Stirred Batch Reactor Model for Under-Ventilated Fire Dynamics

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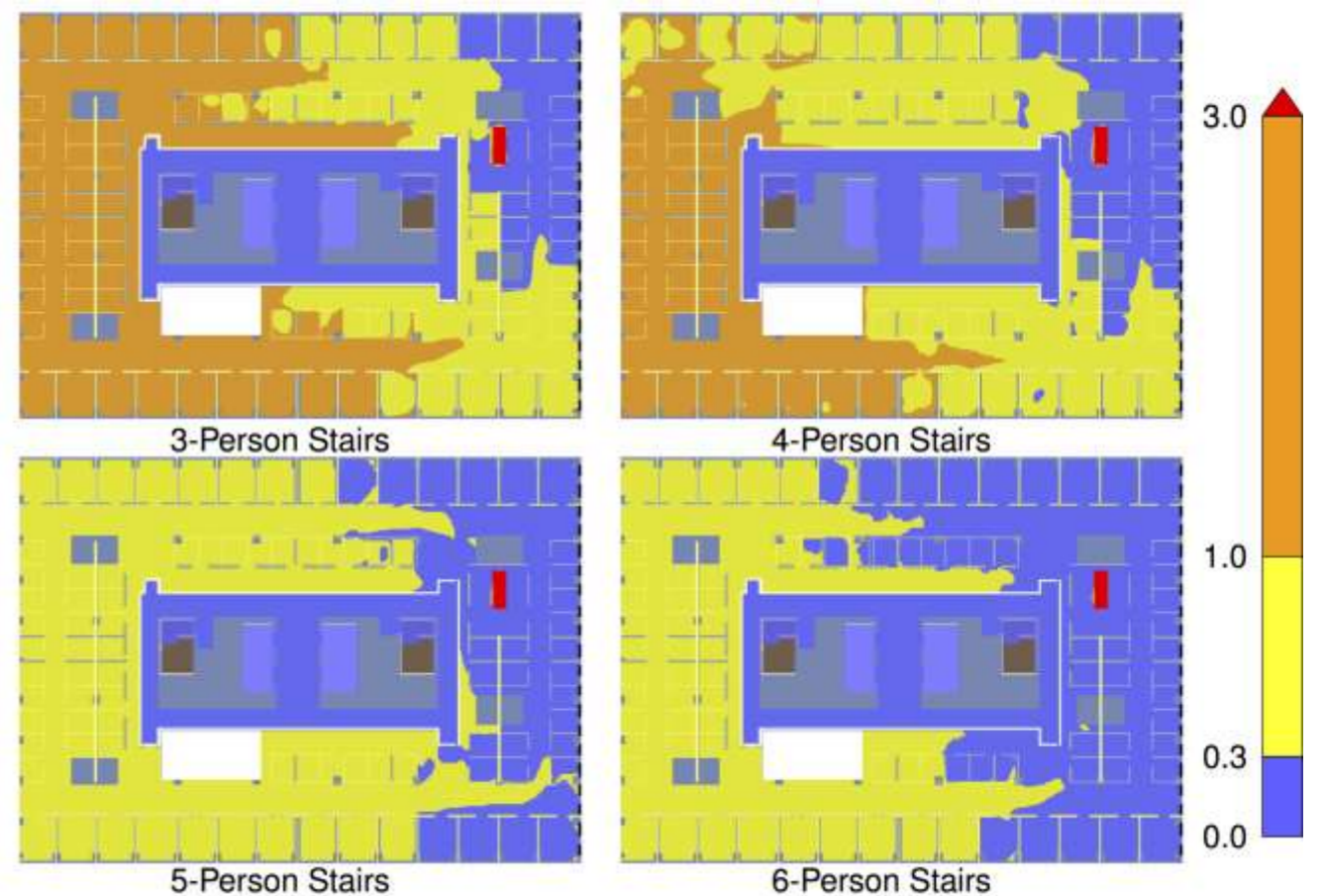
Outline

- **Motivation**
- **Formulation**
 - Lumped species approach
 - Subgrid mixing environment
 - Chemical rate laws
- **Results**

Motivation

The currently accepted IDLH (immediately dangerous to life and health) level for CO exposure is 1,200 ppm at 30 minutes. This ratio is assumed for a healthy, resting nonsmoker who has a resting number of respirations. This equates to a “fractional effective dose,” or FED, of 1.

The CO IDLH of 1,200 ppm should be considerably lower for a firefighter wearing 35 to 40 pounds of gear with elevated respirations (K. Reilly, Fire Engineering, 2006).



Fractional Effective Dose (FED)

FDS 6 Model Formulation

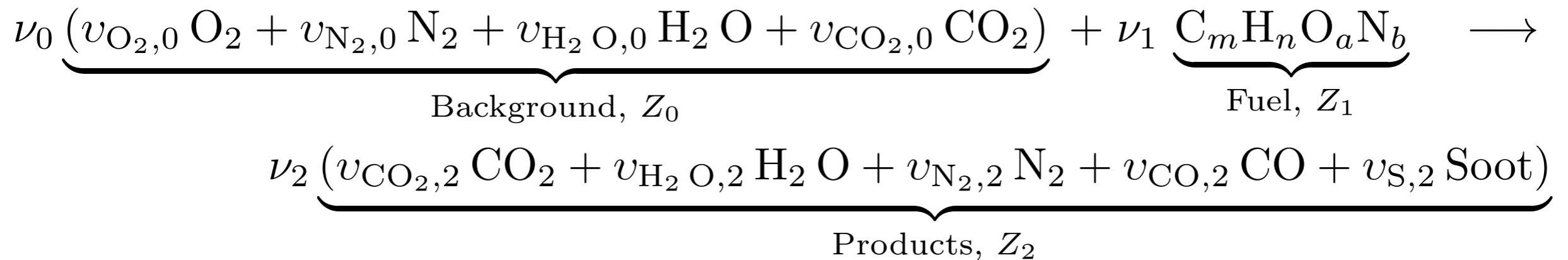
$$\frac{\partial \bar{\rho} \tilde{Y}_\alpha}{\partial t} + \frac{\partial (\bar{\rho} \tilde{Y}_\alpha \tilde{u}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\left[\bar{\rho} D_\alpha + \frac{\mu_t}{Sc_t} \right] \frac{\partial \tilde{Y}_\alpha}{\partial x_i} \right) + \overline{\dot{m}'''_\alpha}$$

- Low-Mach LES, implicit filtering
- **Generalized lumped species**
- Conservative, finite volume, second order
- Explicit time integration
- TVD scalar transport (CHARM, Superbee)
- Deardorff, Vreman, dynamic Smagorinsky
- Constant Sc_t and Pr_t
- **Batch reactor model (turb-chem interaction)**
- **Fast and Arrhenius chemistry (4th order ODE solver with error control)**
- Radiation absorption---diffuse gray gas or RADCAL narrow band model
- Radiation emission---corrected σT^4
- JANAF thermochemical properties
- Formulation to appear in J. Comput. Phys.

Temperature slice, Sandia 1 m CH₄ pool fire

Lumped Species via Simple Chemistry

The default reaction equation in FDS, known as “simple chemistry,” is defined as follows:



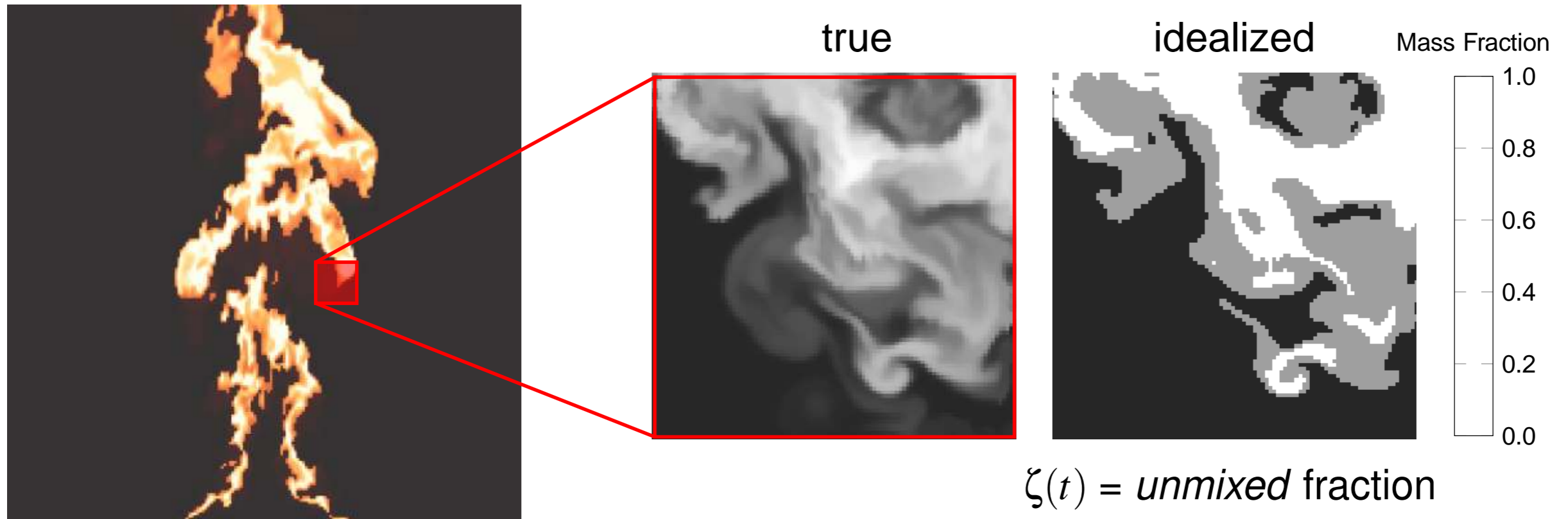
Carbon monoxide and soot yields are zero by default.

The user can specify the CO and soot yields: y_{CO} and y_{S}

$$y_{\text{CO}} = \frac{\text{mass CO in Products}}{\text{mass of Fuel reacted}}$$

$$\nu_2 \nu_{\text{CO},2} = -\nu_1 \frac{W_1}{W_{\text{CO}}} y_{\text{CO}}$$

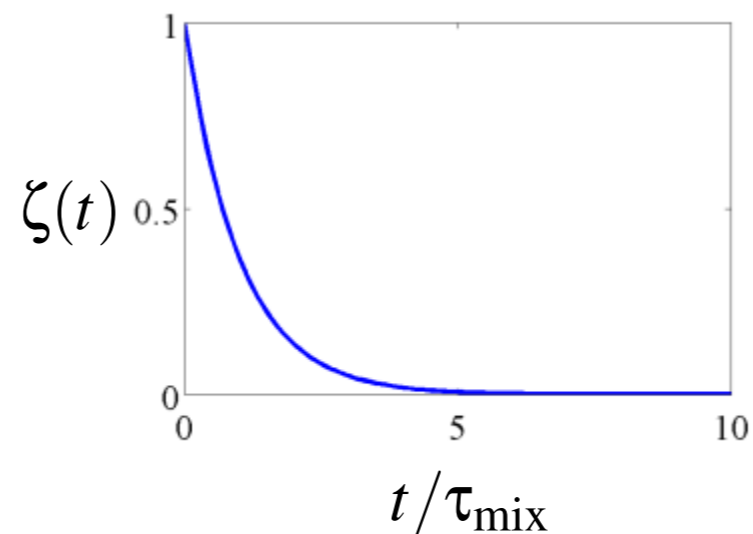
A Simple Subgrid Mixing Environment



$$\tilde{Y}_\alpha(t) = \zeta(t) \tilde{Y}_\alpha^0 + (1 - \zeta(t)) \hat{Y}_\alpha(t)$$

$$\frac{d\zeta}{dt} = -\frac{\zeta}{\tau_{\text{mix}}}$$

$$\zeta(t) = \zeta_0 e^{-t/\tau_{\text{mix}}}$$



The combustion routine:

$$\dot{m}_\alpha''' = \rho \frac{d\tilde{Y}_\alpha}{dt} = \rho \left[\frac{\zeta}{\tau_{\text{mix}}} (\hat{Y}_\alpha - \tilde{Y}_\alpha^0) + (1 - \zeta) \frac{d\hat{Y}_\alpha}{dt} \right]$$

The integration is time split such that mixing is done first, followed by reaction.

In FDS we deal with two types of reactions:

- Infinitely fast chemistry
- Finite rate chemistry

The integration is done with a 4th Order Runge-Kutta integrator with error control and variable time-stepping.

For the vast majority of FDS applications the “mixed is burnt” assumption is adequate to model the reaction system.

The mean chemical source term for Fuel is modeled using the Eddy Dissipation Concept (EDC) of Magnussen and Hjertager:

$$\dot{m}_F''' = -\rho \frac{\min(Z_F, Z_A/s)}{\tau_{\text{mix}}}$$

Then the heat release is found by species mass production rates times the respective heats of formation

$$\dot{q}''' \equiv - \sum_{\alpha} \dot{m}_{\alpha}''' \Delta h_{f,\alpha}$$

Chemical Kinetics

$$\frac{d\hat{Y}_F}{dt} = -A T^n \exp(-E_a/(RT)) [\text{Fuel}]^a [\text{Oxidizer}]^b [\text{H}_2\text{O}]^c \quad ; \quad \text{mol}/(\text{cm}^3 \cdot \text{s})$$

ID	Reaction	A	n	E _a [J/mol]	a	b	c
1	CH ₄ + $\frac{3}{2}$ O ₂ → CO + 2 H ₂ O	infinitely fast	0	0	0	0	0
2	CO + $\frac{1}{2}$ O ₂ → CO ₂	1.5 × 10 ⁹	0	4.2 × 10 ⁴	1	0.25	0.5
3	CO ₂ → CO + $\frac{1}{2}$ O ₂	6.2 × 10 ¹³	-0.97	3.3 × 10 ⁵	1	-0.25	0.5

C. K. Westbrook and F. L. Dryer. Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames. *Combustion Science and Technology*, 27:31–43, 1981.

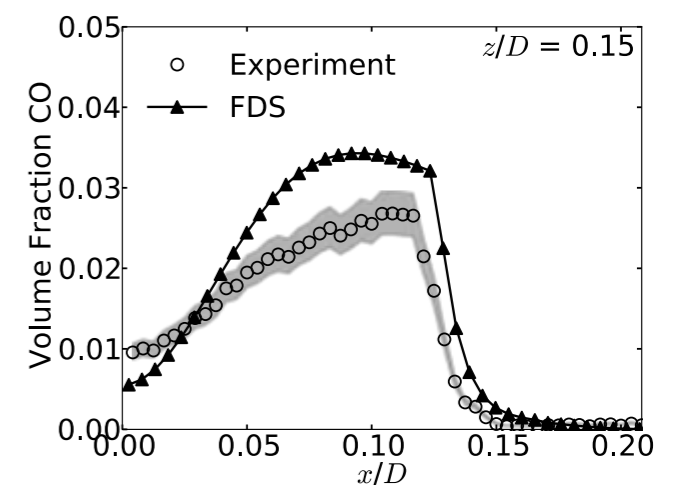
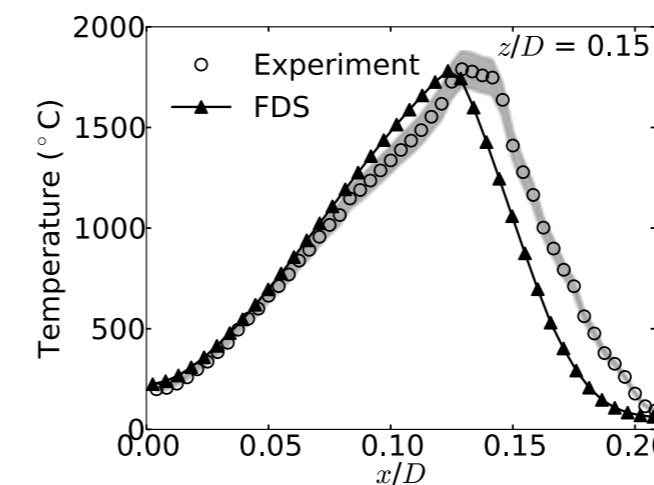
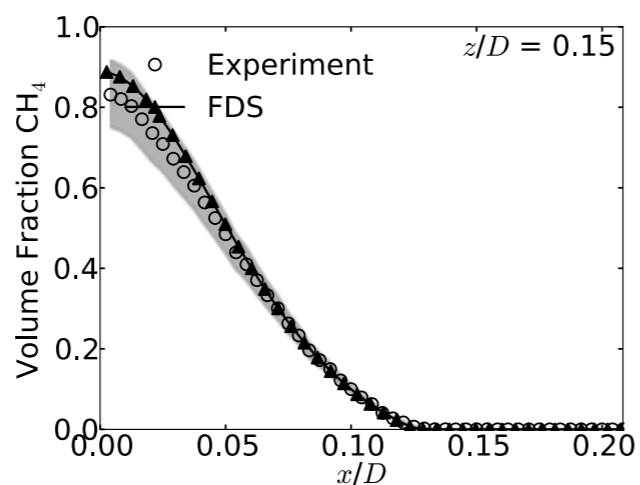
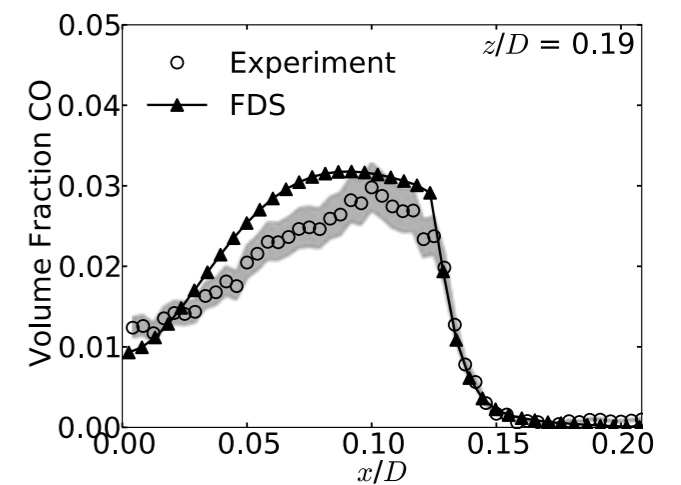
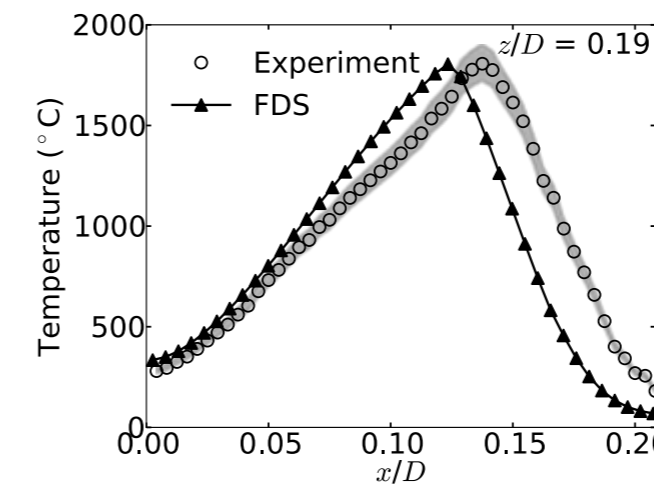
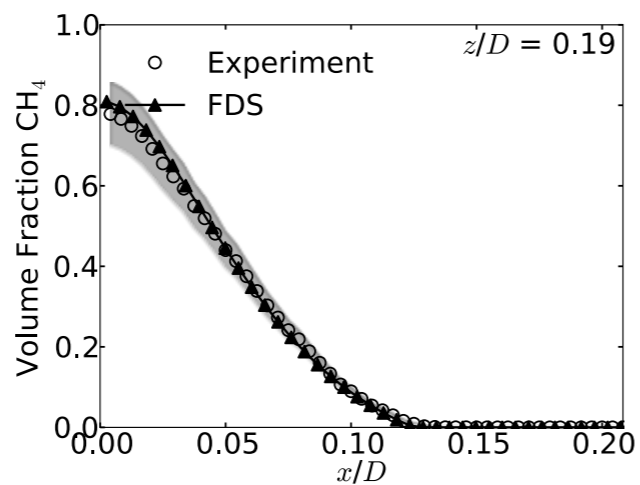
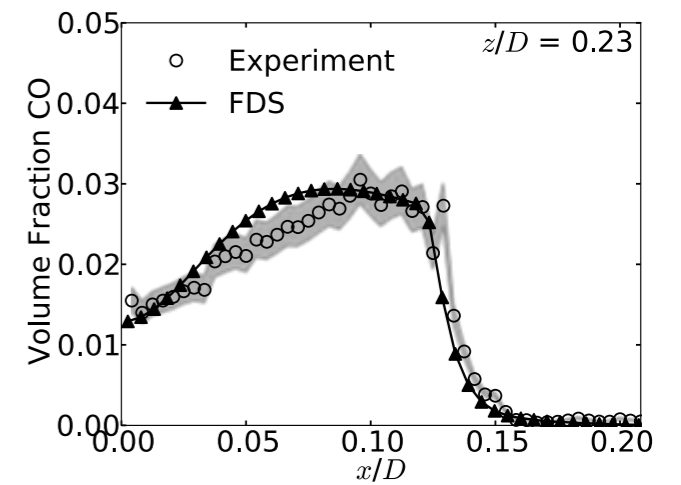
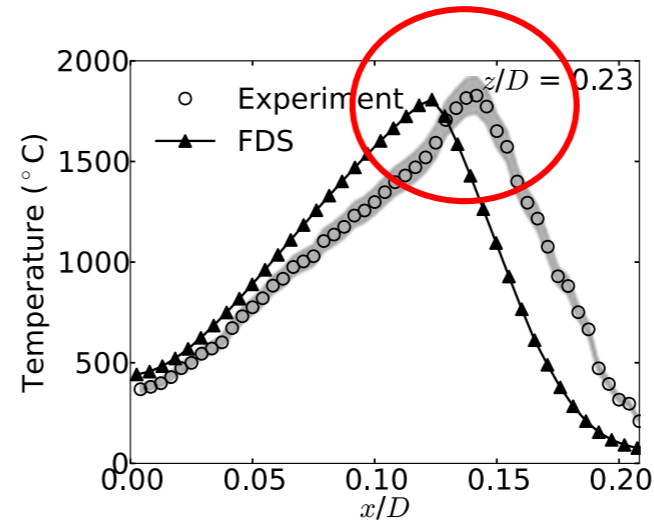
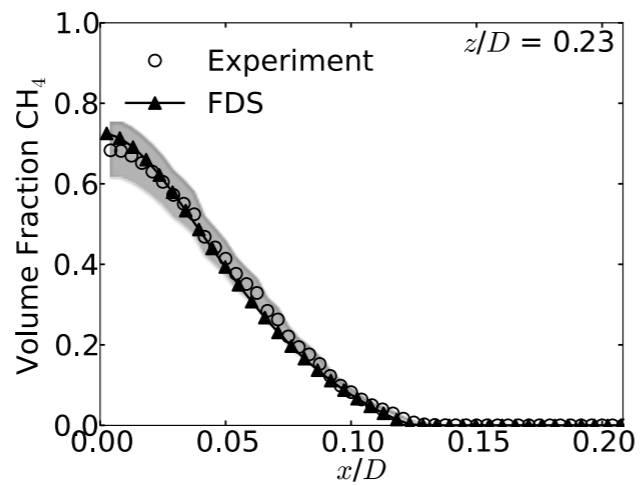
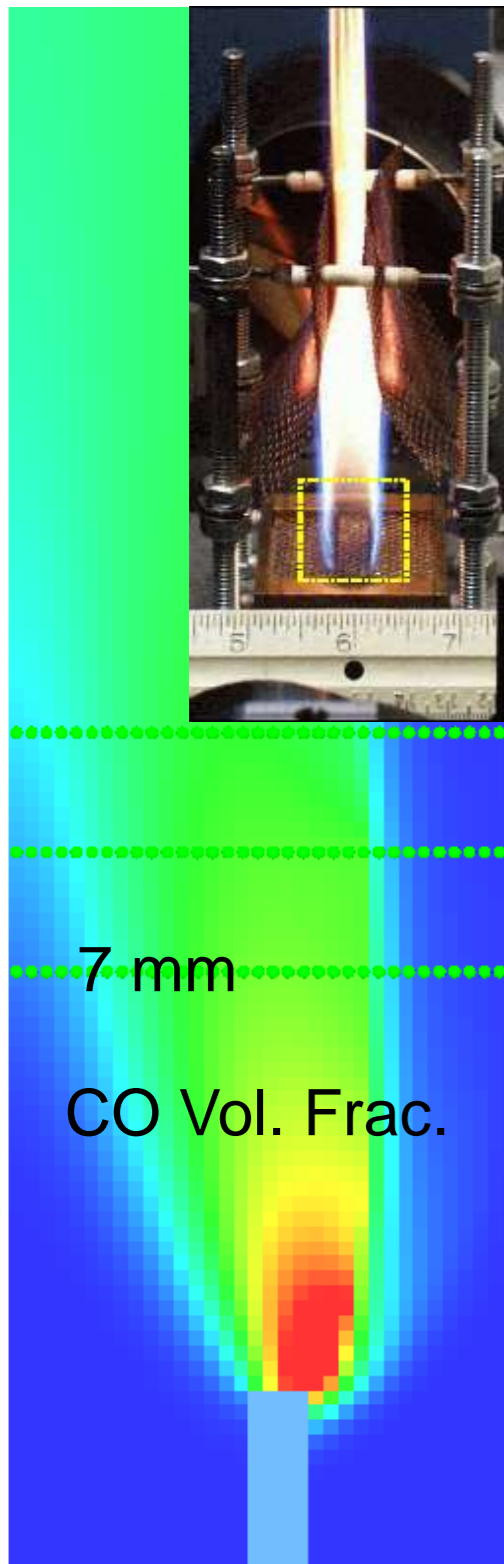
J. Andersen, C. L. Rasmussen, T. Giselsson, and P. Glarborg. Global combustion mechanisms for use in CFD modeling under oxy-fuel conditions. *Energy & Fuels*, 23(3):1379–1389, 2009.

“For each set of reaction rate parameters, the pre-exponential terms tabulated here should be regarded as approximate values if they are use in other numerical models... Therefore, for use in other codes, the parameters presented here should be used as initial estimates, with comparisons between computed and experimental data for some reference condition serving to calibrate the pre-exponential factor A.”

- C. K. Westbrook and F. L. Dryer (CST, 1981)

Wolfhard-Parker Burner (2D DNS)

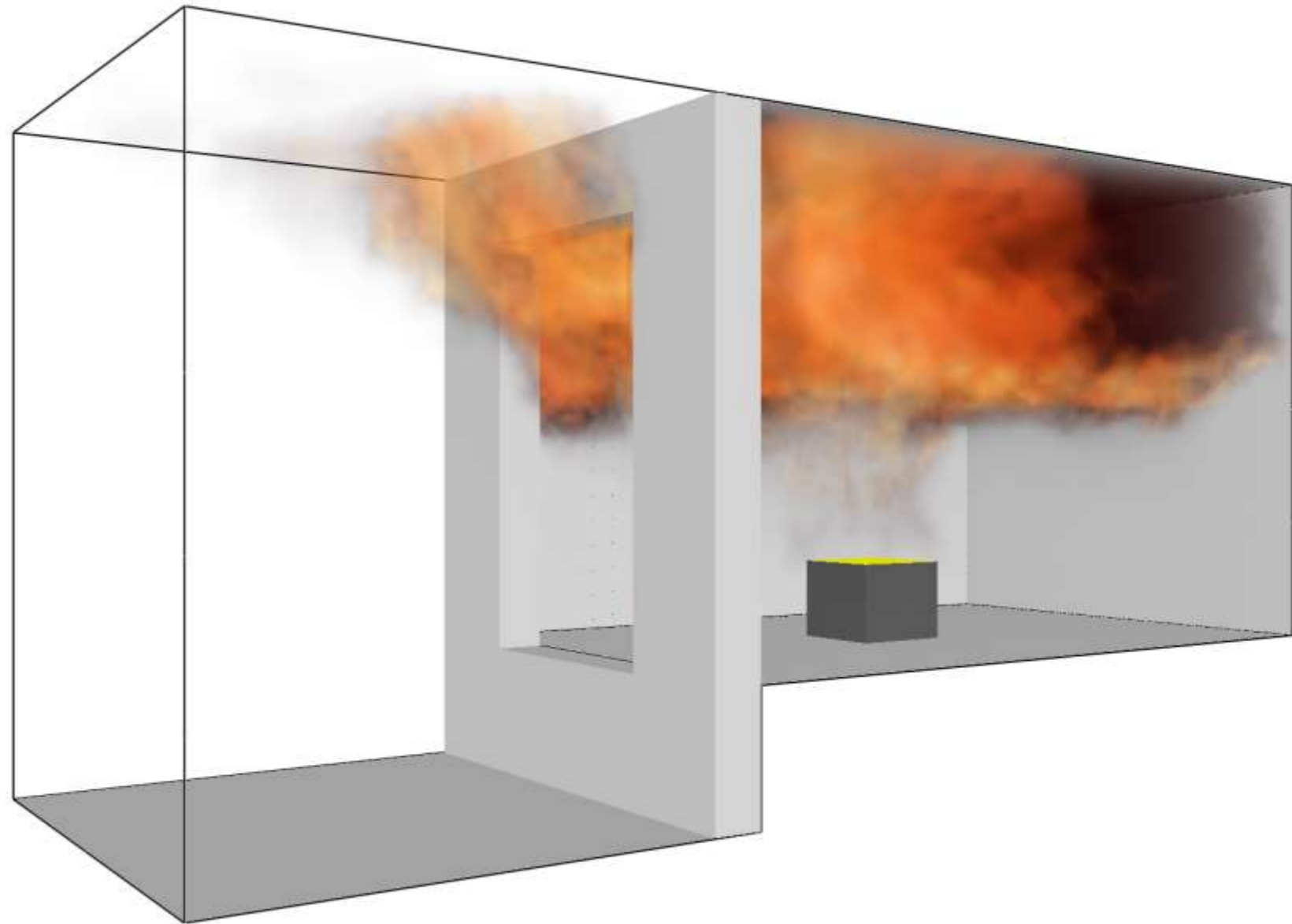
shift due to 3D effects and screen (?)



NIST Reduced Scale Enclosure (1994) – Natural Gas

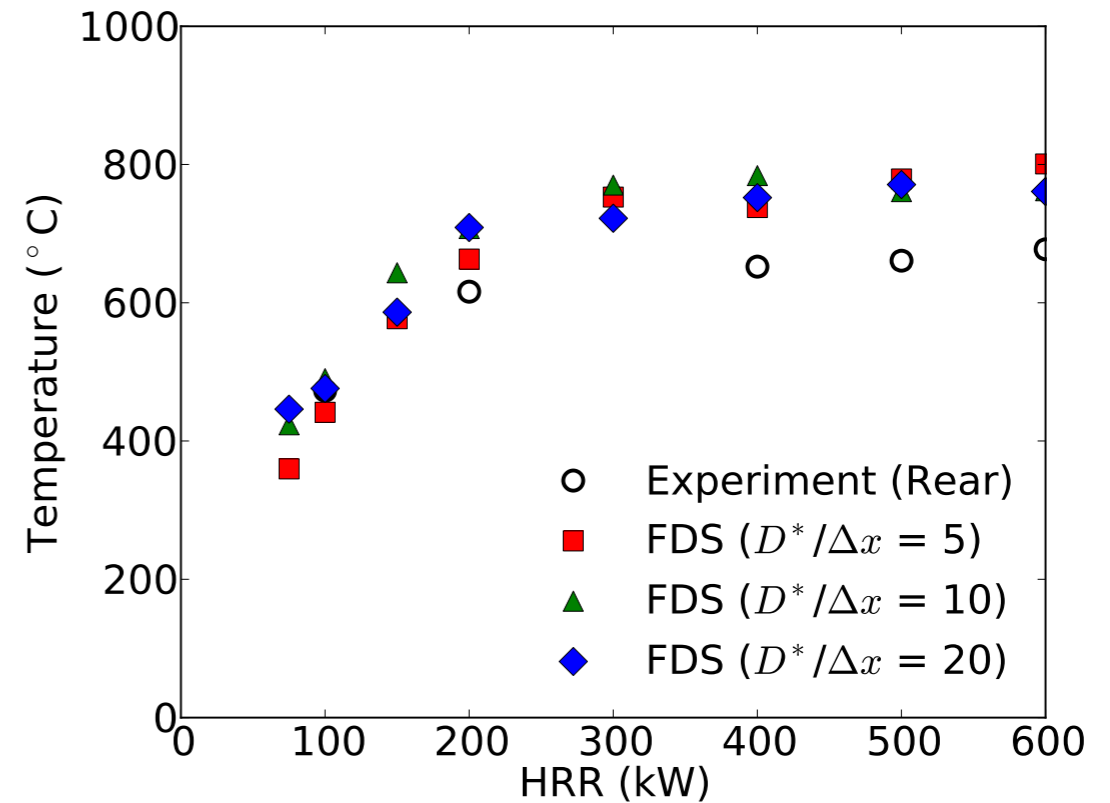
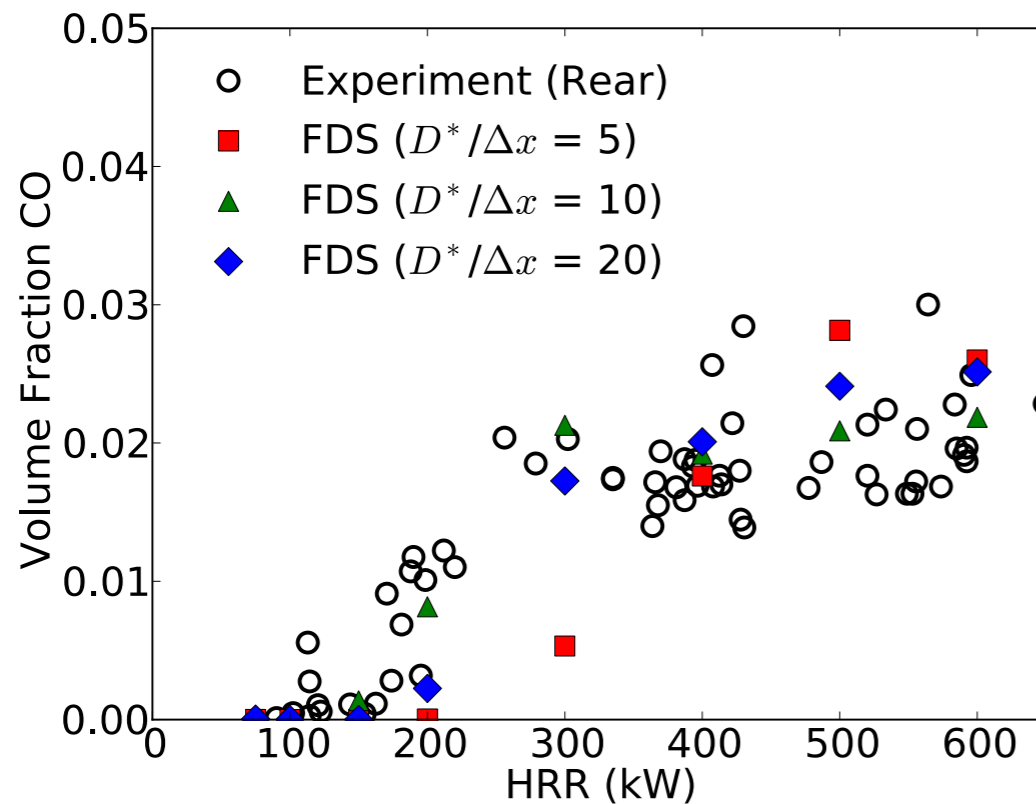
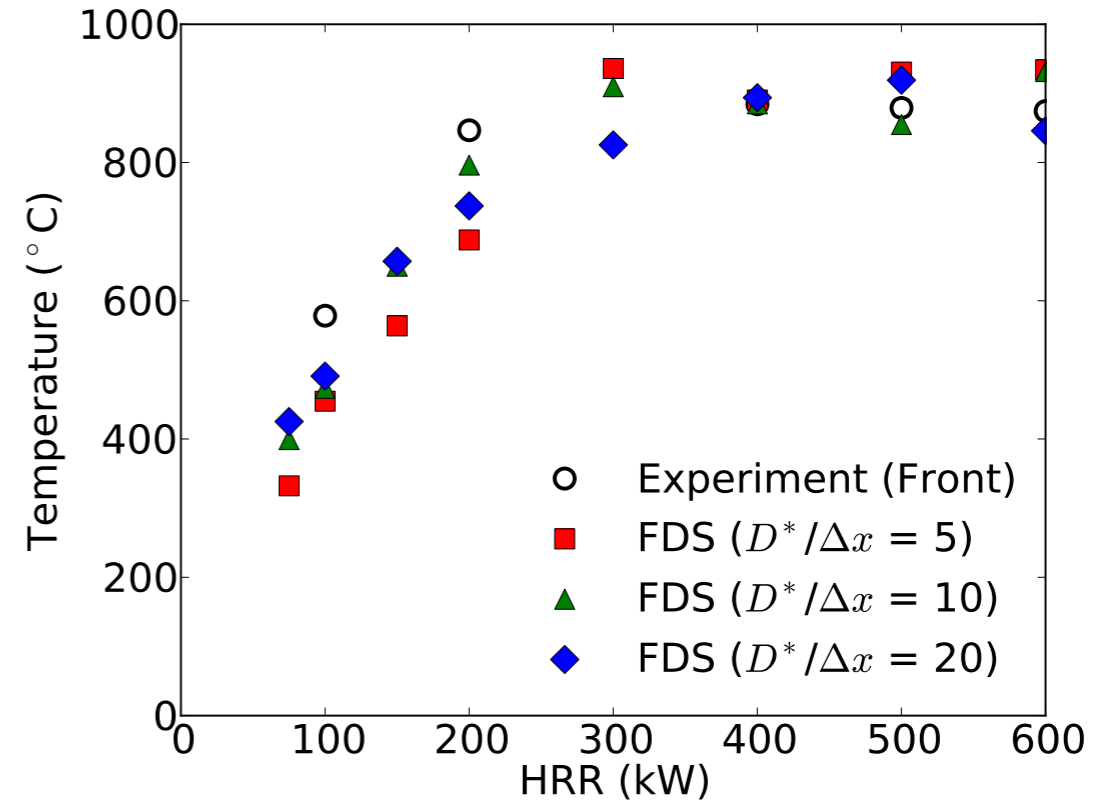
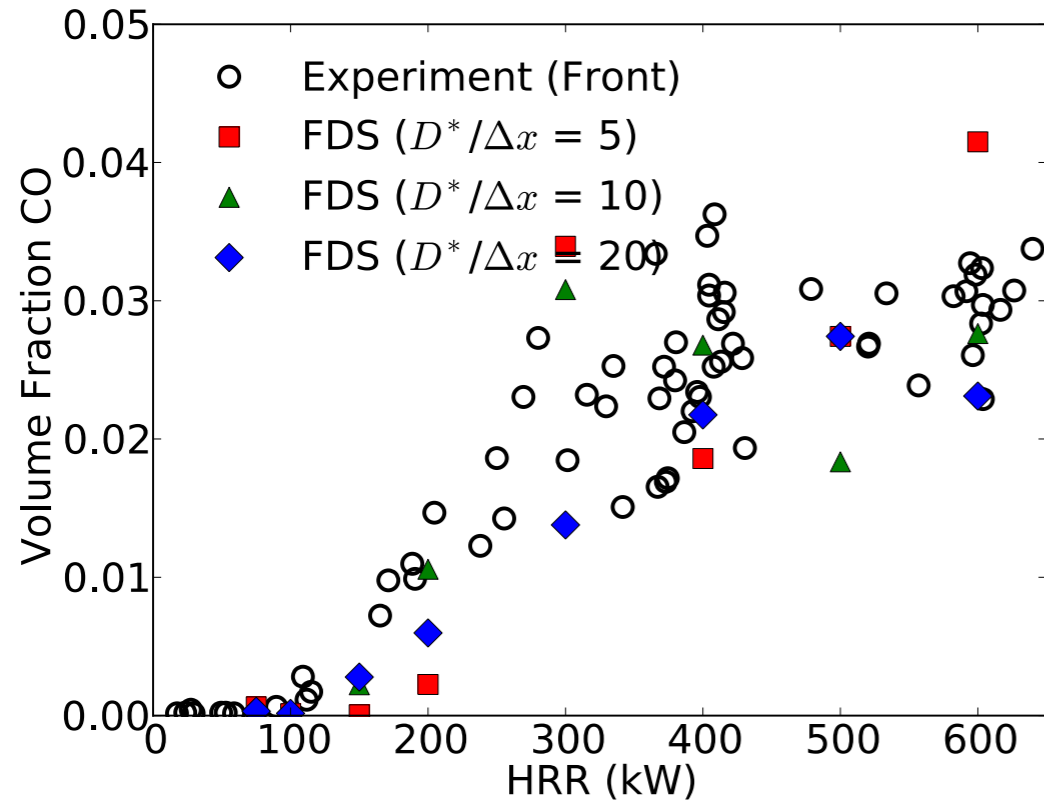


1 m³

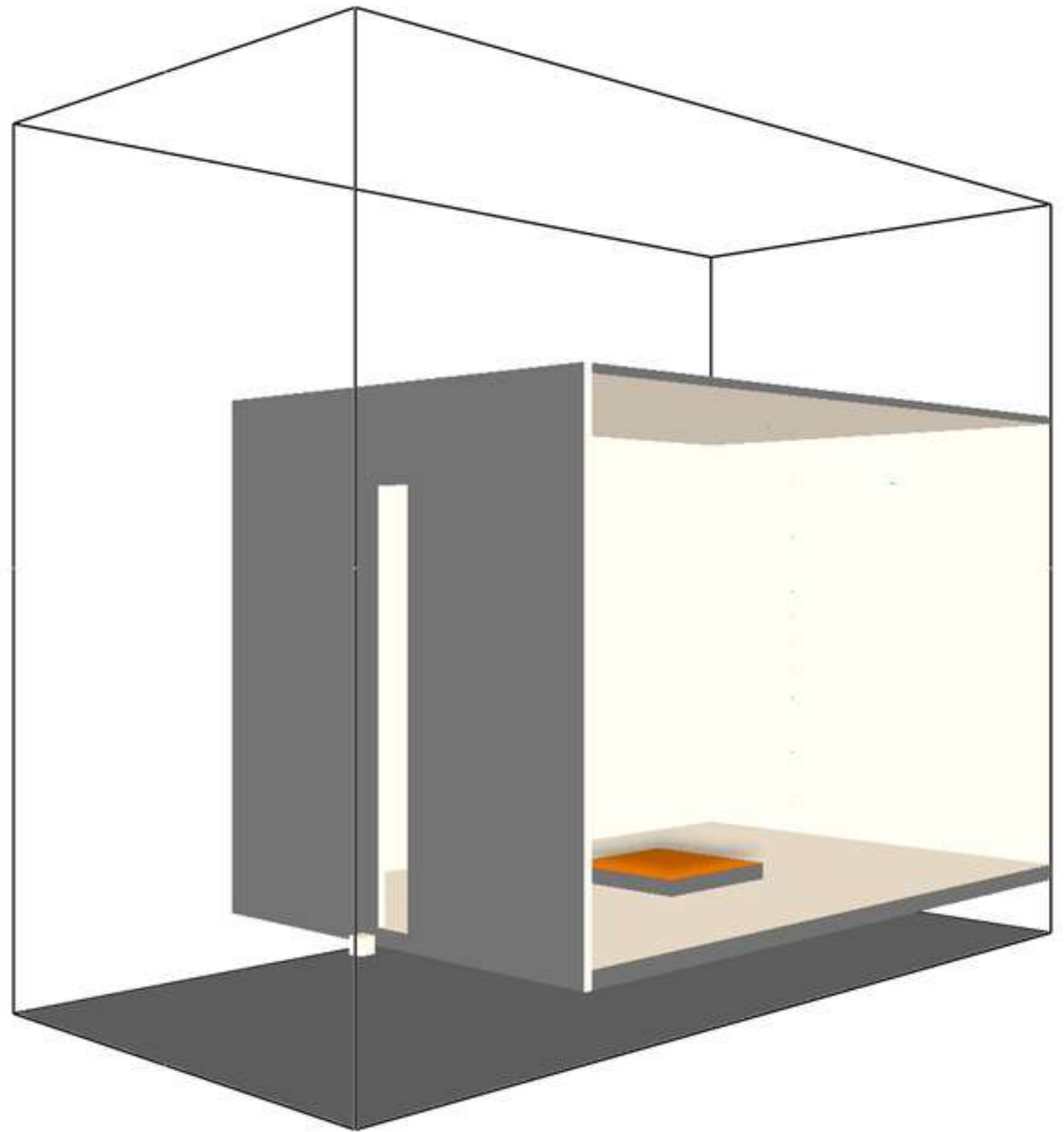


N. Bryner, E. Johnsson, and W. Pitts. Carbon Monoxide Production in Compartment Fires-Reduced-Scale Test Facility. NISTIR 5568, National Institute of Standards and Technology, Gaithersburg, MD, 1994.

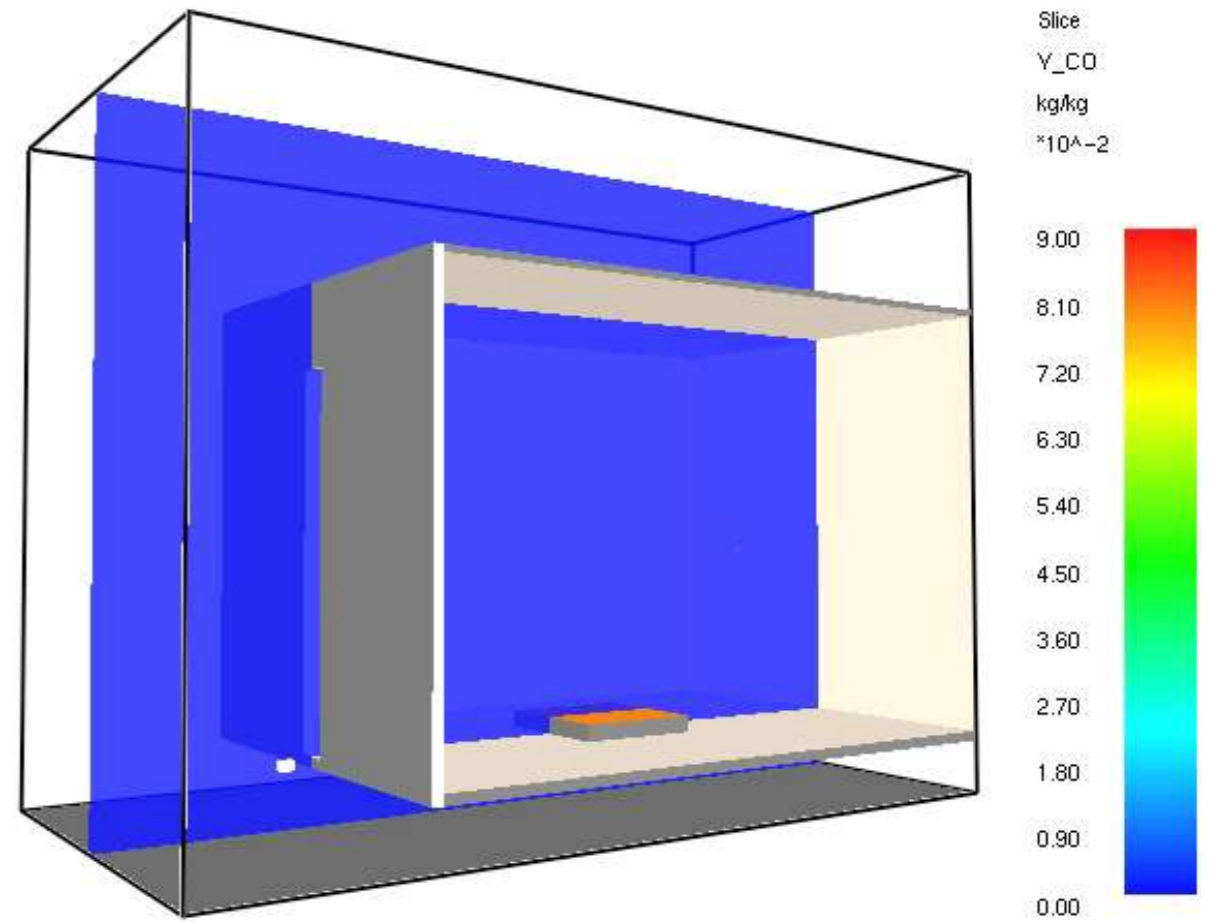
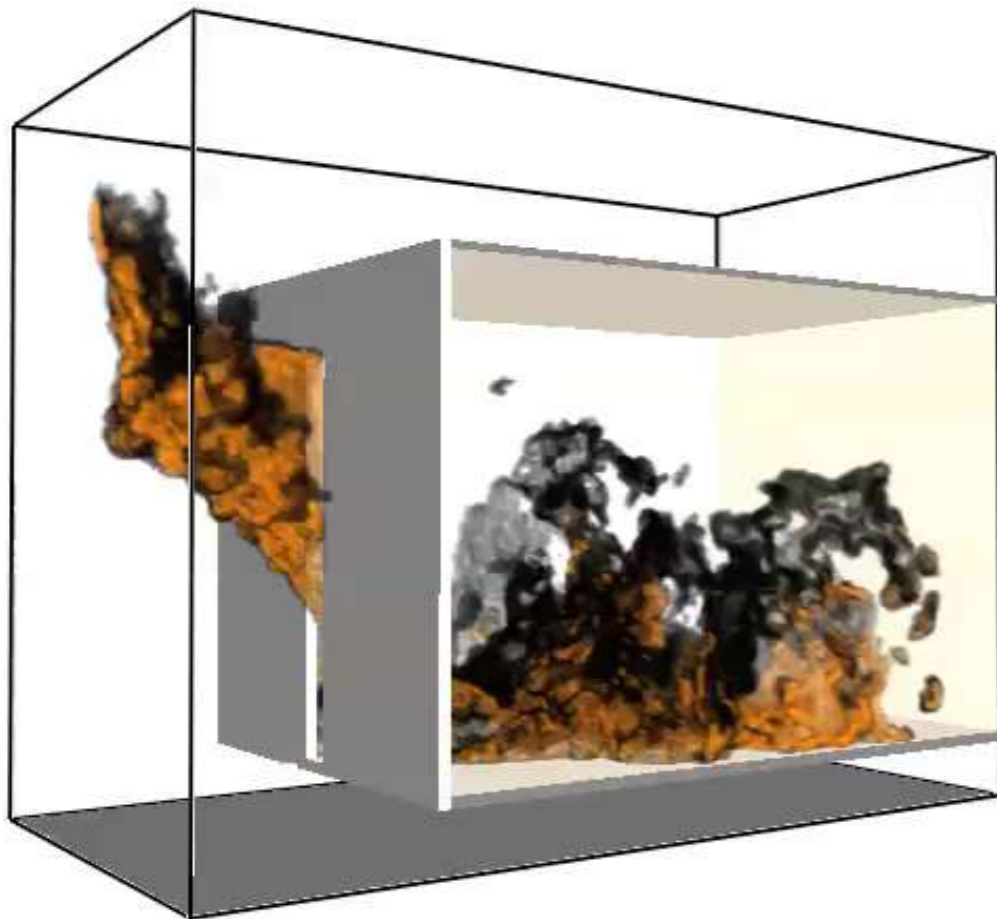
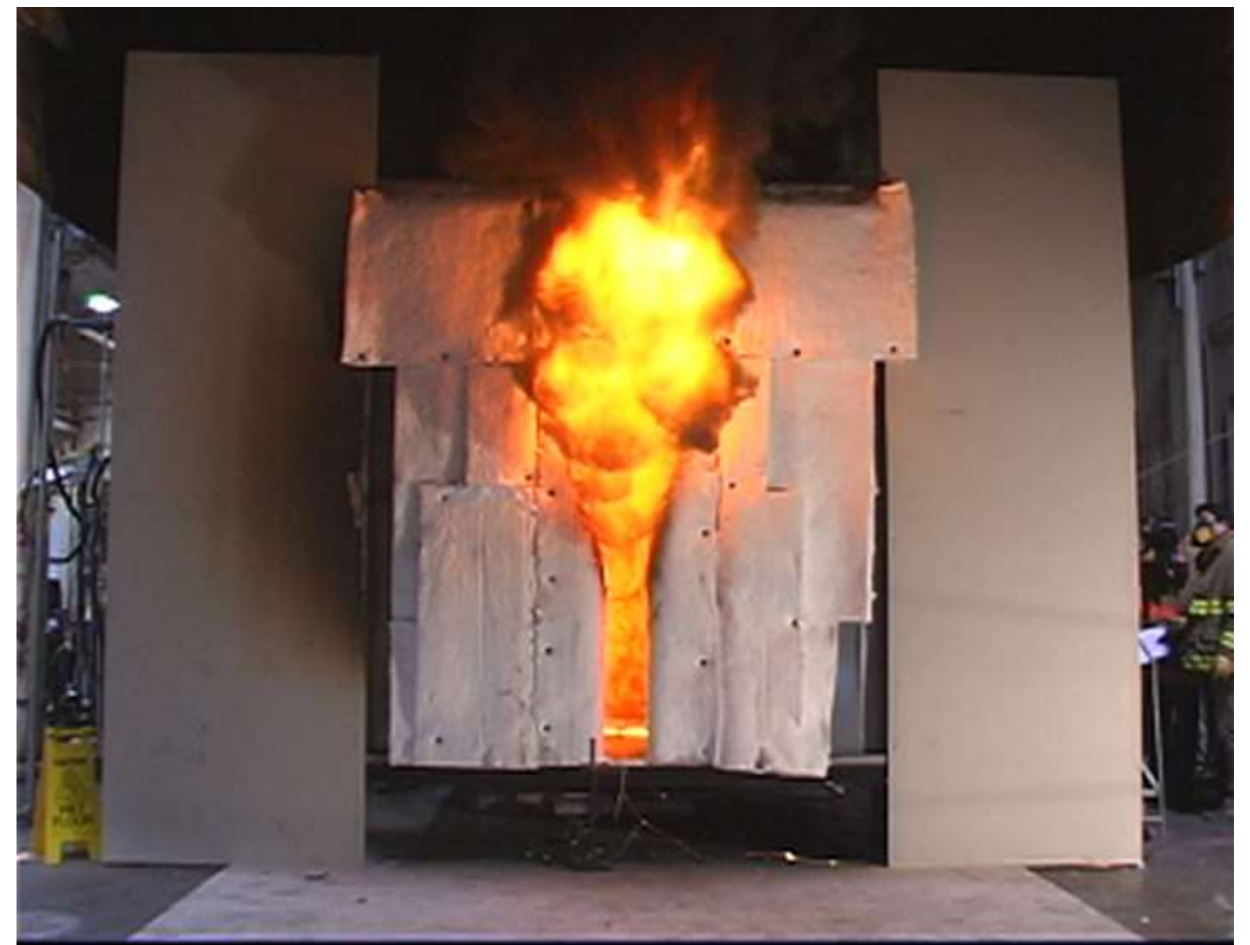
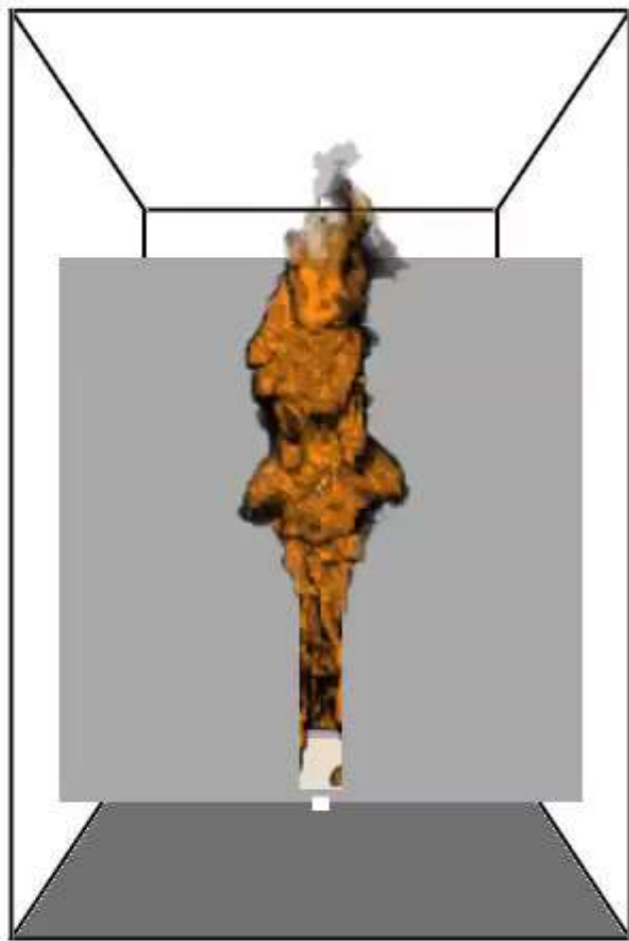
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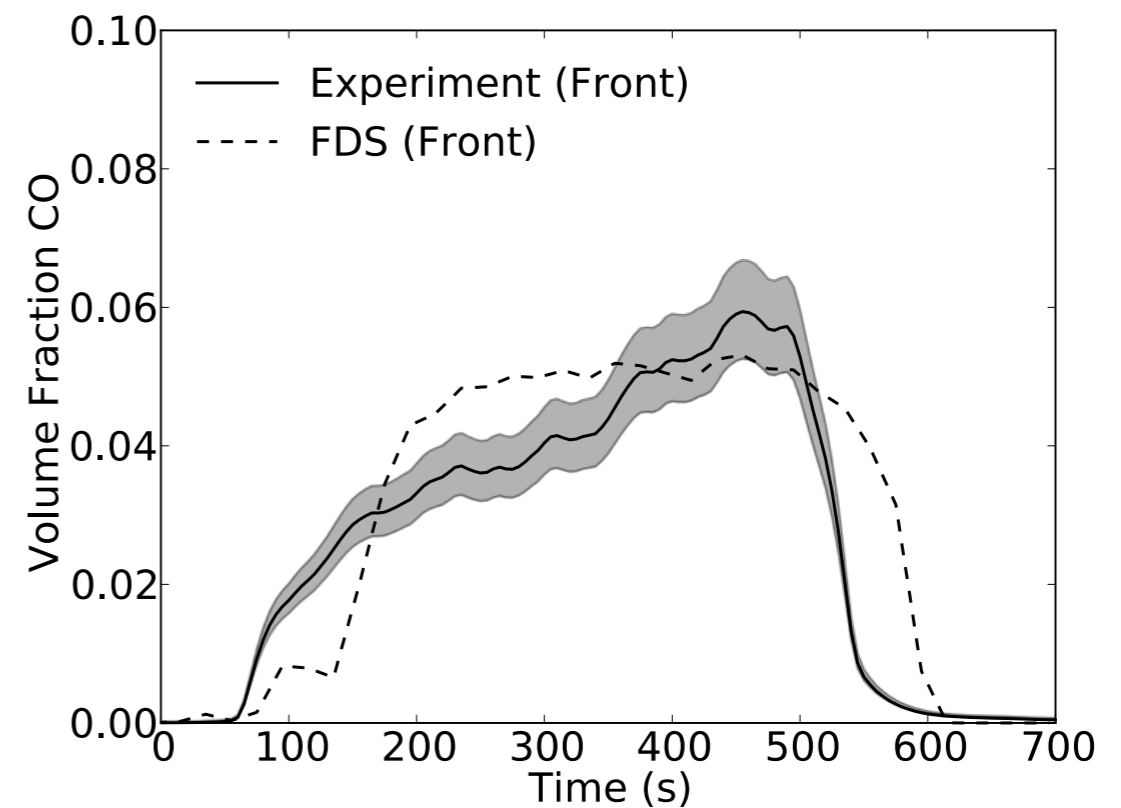
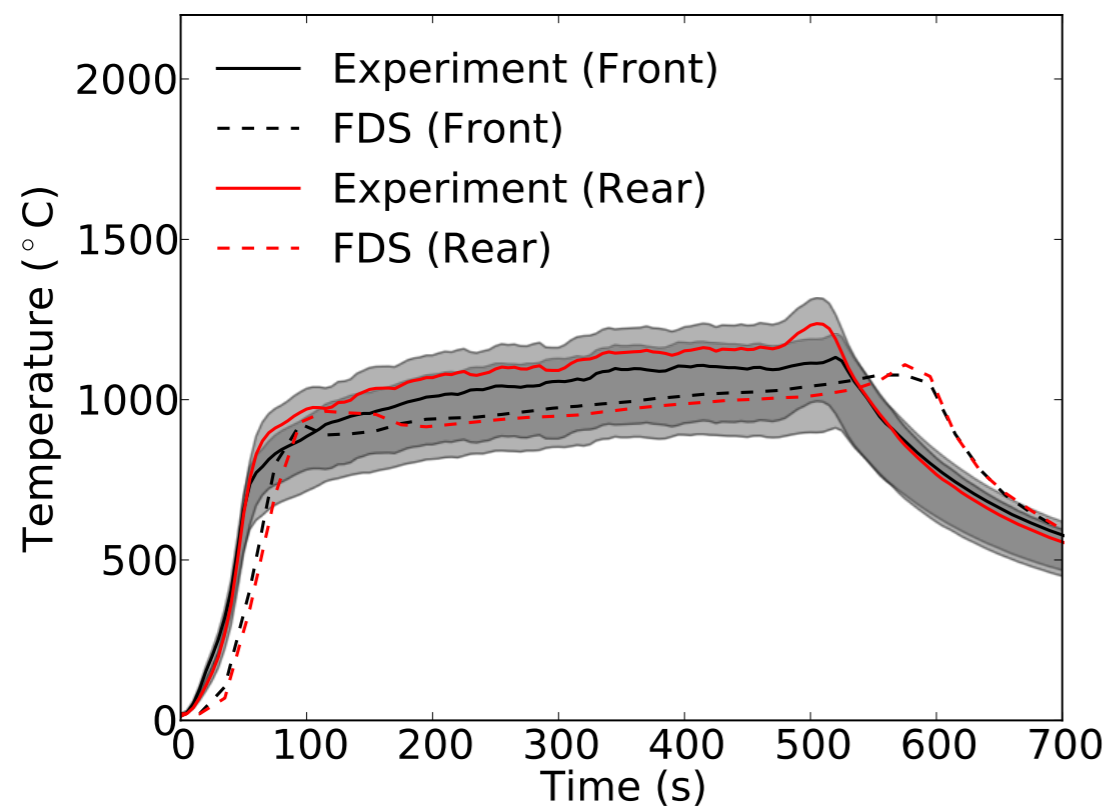
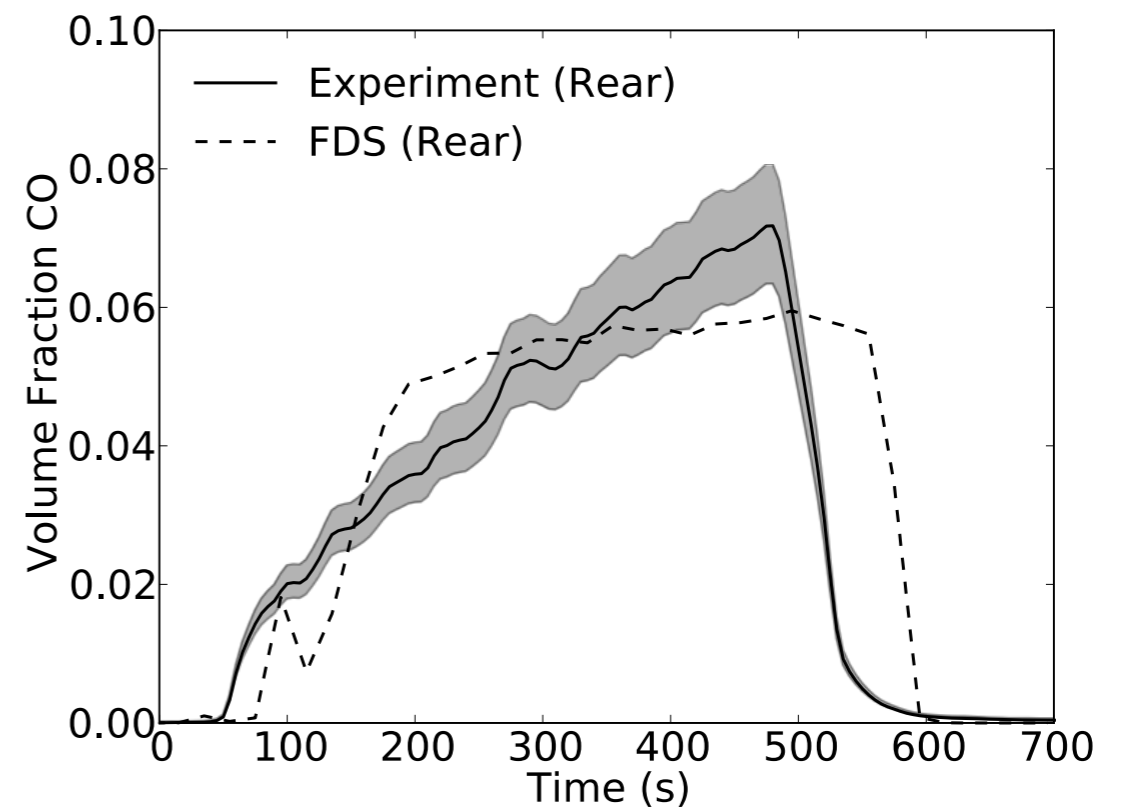
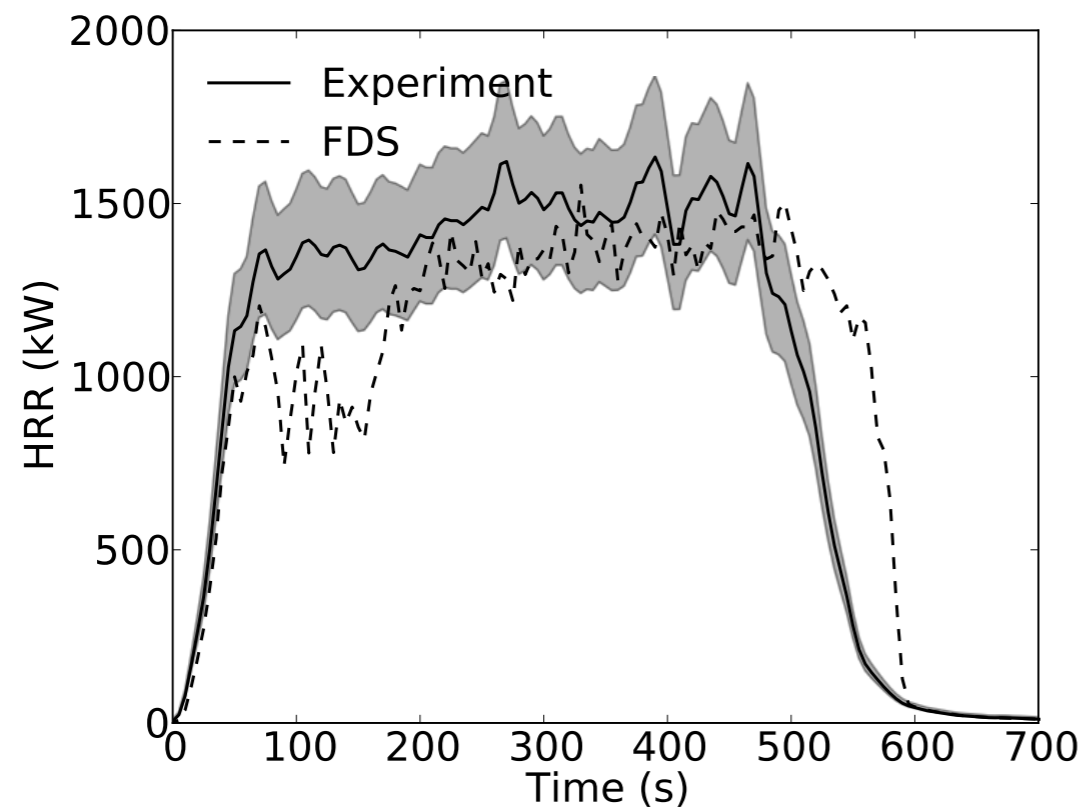
Full-Scale Experiments



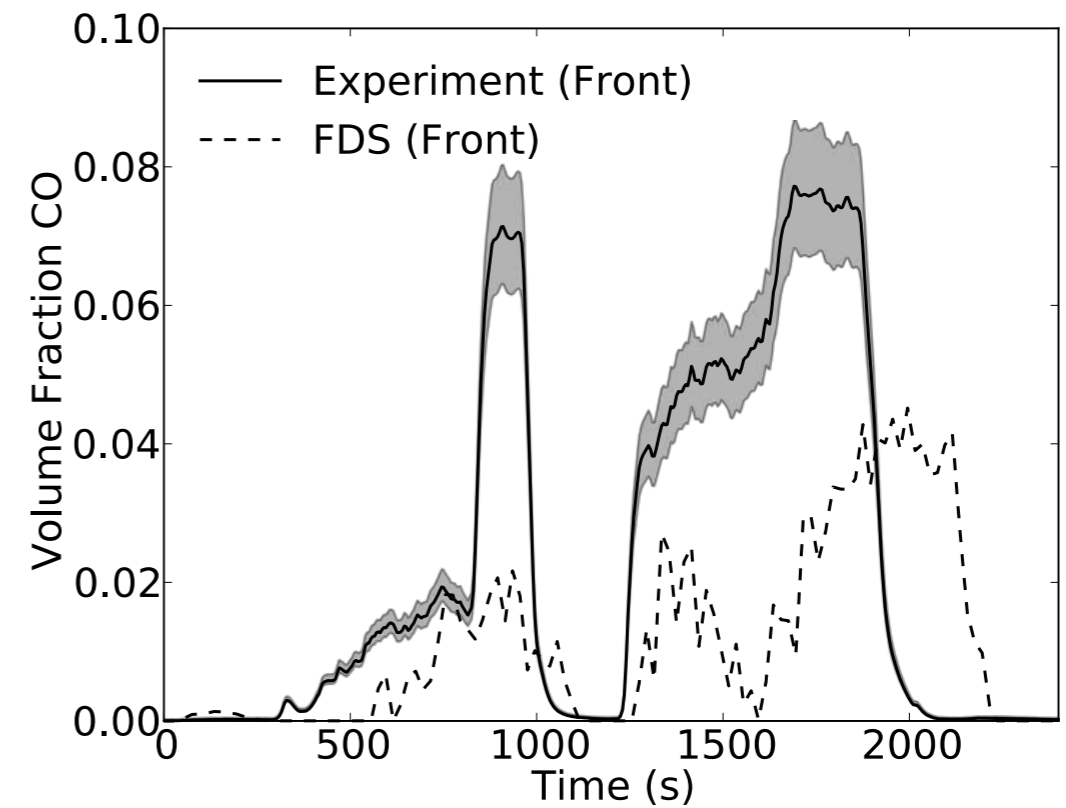
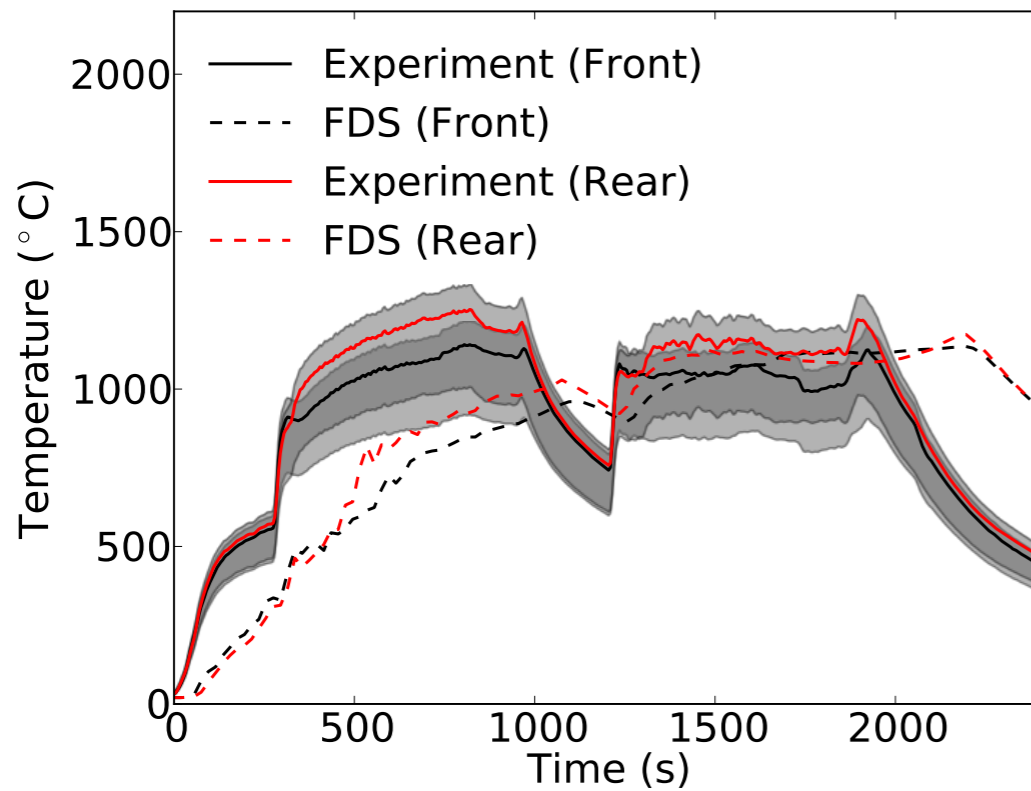
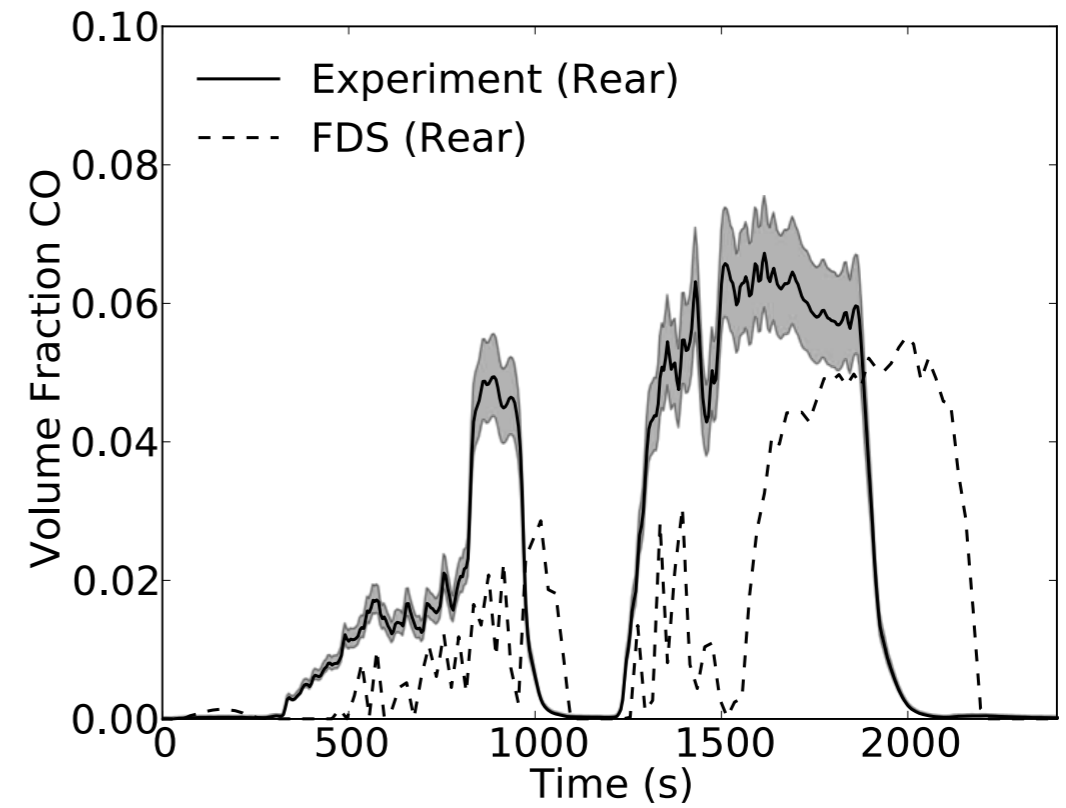
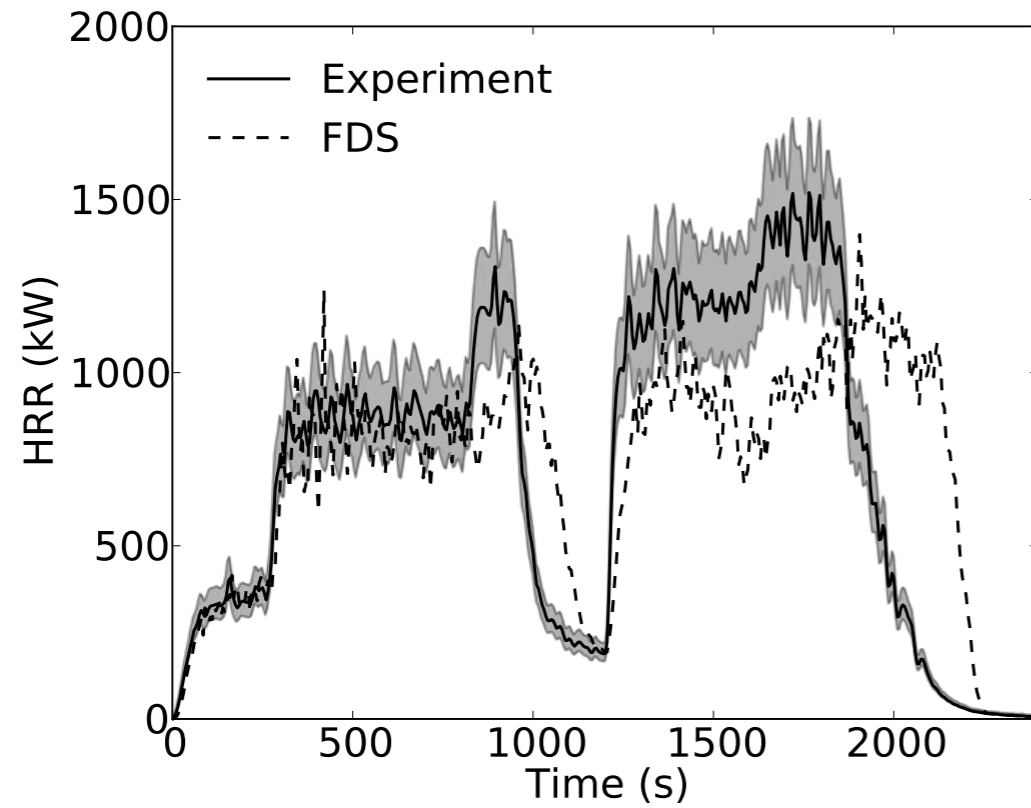
A. Lock, M. Bundy, E.L. Johnsson, A. Hamins, G.H. Ko, C. Hwang, P. Fuss, and R. Harris. Experimental study of the effects of fuel type, fuel distribution, and vent size on full-scale under-ventilated compartment fires in an ISO 9705 room. NISTTN 1603, National Institute of Standards and Technology, Gaithersburg, MD, 2008.



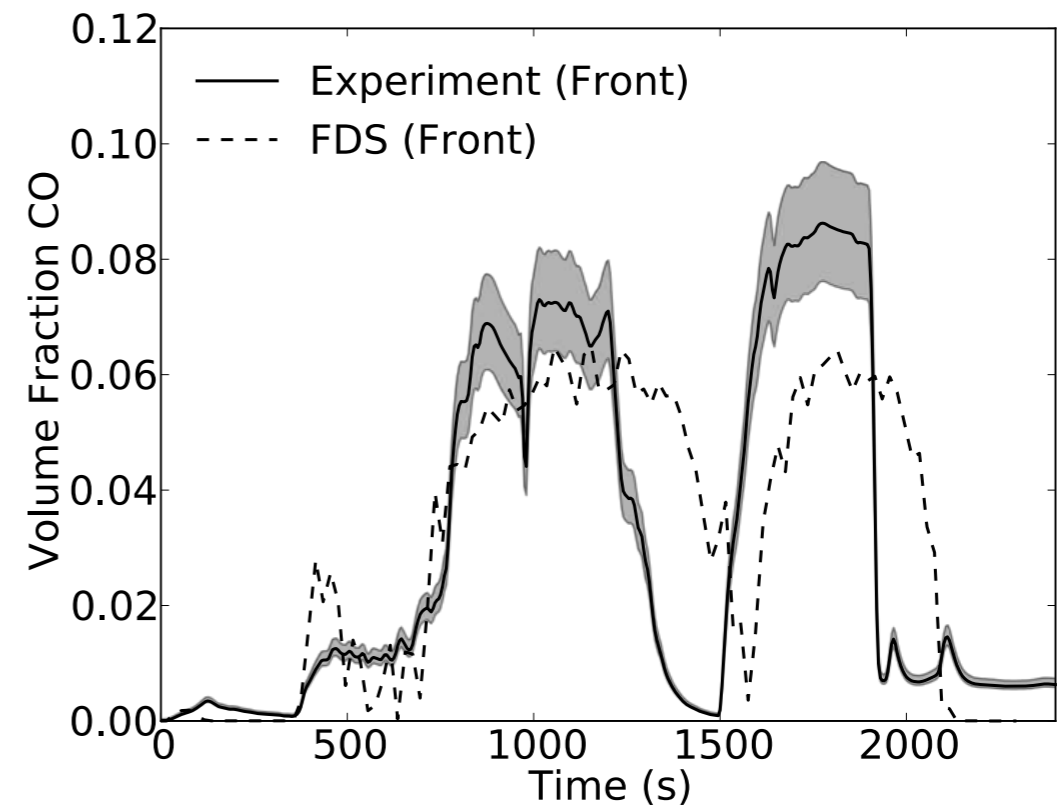
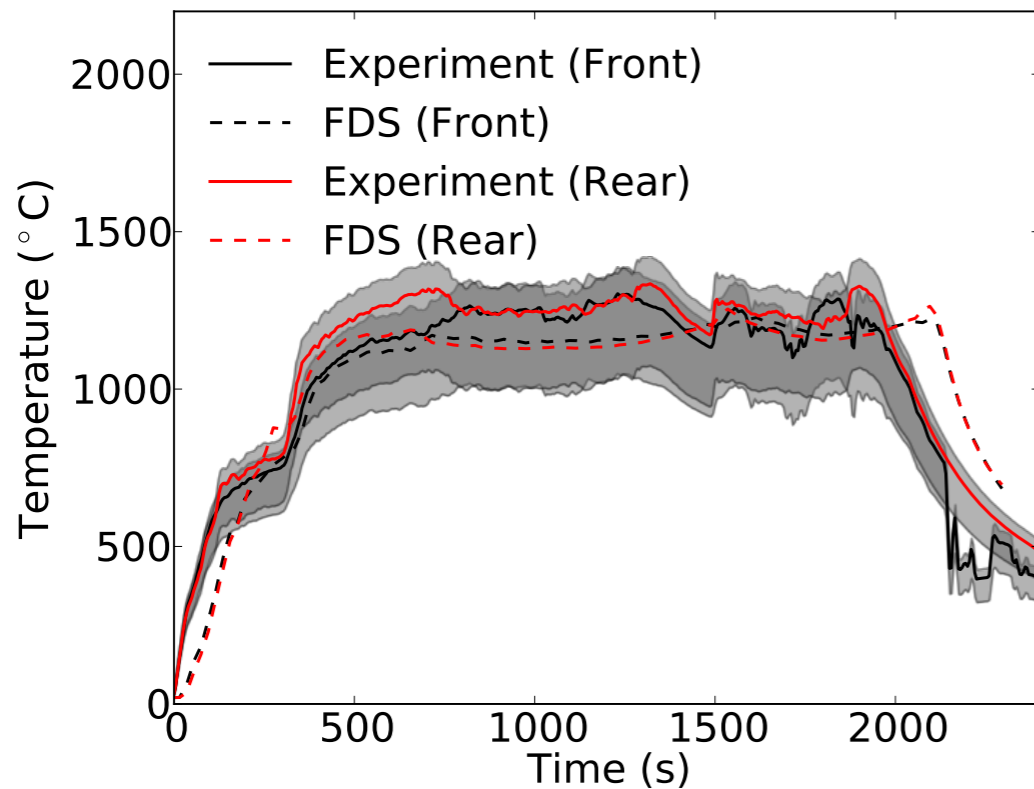
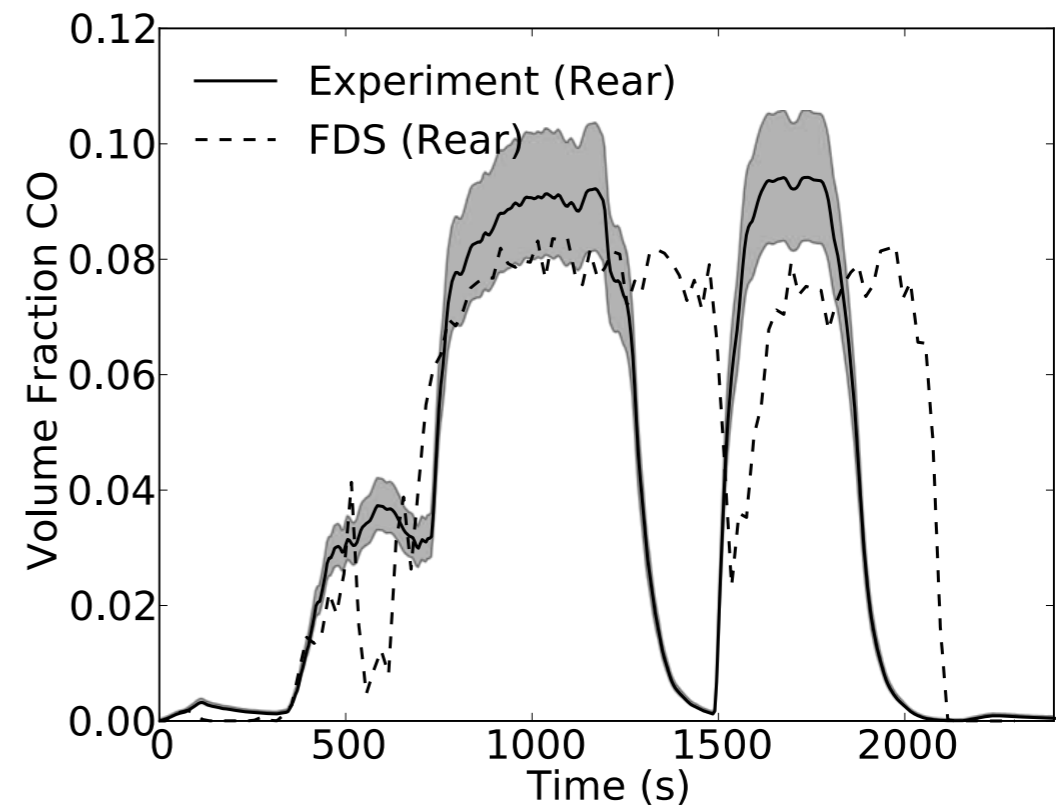
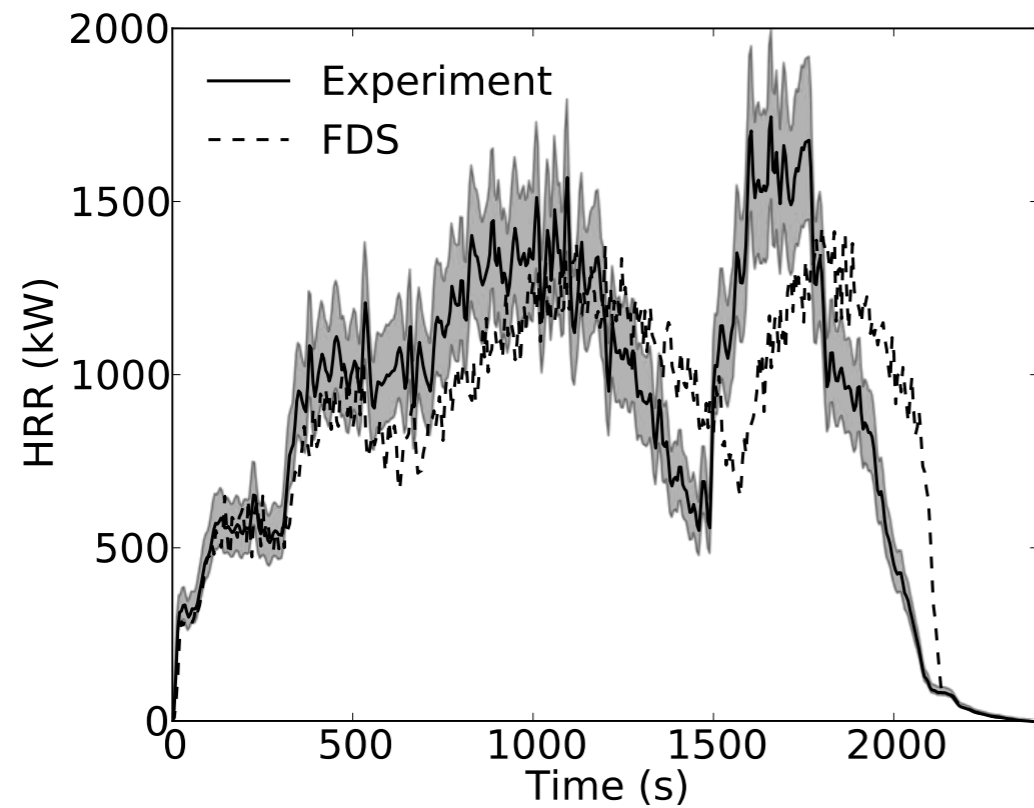
NIST Large Scale Enclosure (2008) – N-Heptane



NIST Large Scale Enclosure (2008) – Isopropanol



NIST Large Scale Enclosure (2008) – Toluene



Conclusions and Future Work

1. The model has three basic components: a subgrid mixing environment, a mixing model, and a set of chemical rate laws, all of which are amenable to improvement.
2. Reasonable results for CO concentrations are obtained using a modified Westbrook-Dryer (1981) mechanism from Andersen et al. (2009). The test cases span two orders of magnitude in length and time scales.
3. Future work will focus on improved modeling of the unmixed fraction and evolution of the subgrid temperature distribution, as well as increasing the complexity of the reaction mechanisms we can handle.
4. Add support for extinction with multiple fast-chemistry reactions.
5. Continue to explore options for mechanisms to predict CO with shortest computation time.

Acknowledgements

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