LES of Ignition and Transient Combustion in Fuel Vapor Clouds

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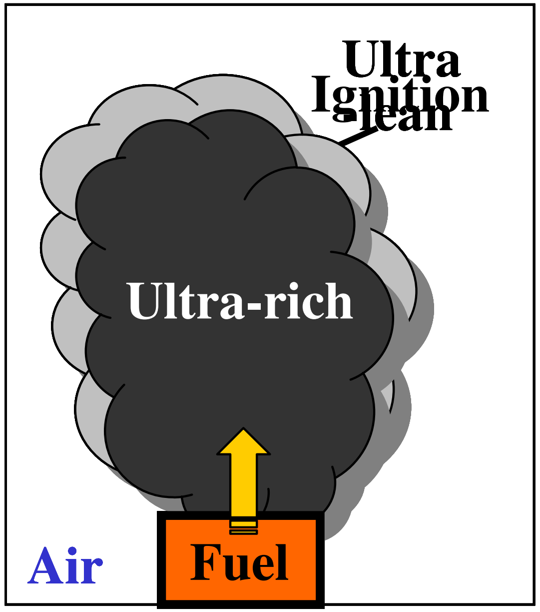
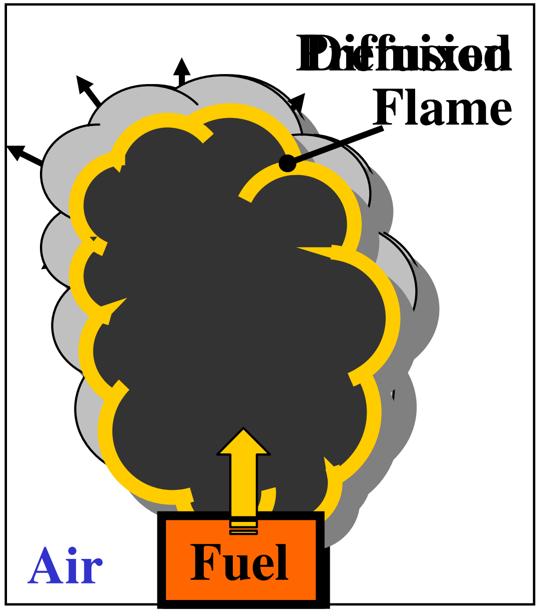
Ignition and Combustion of a Fuel Vapor Cloud

- Basic scenario:
  - Accidental release of gaseous fuel in ambient air
  - Turbulent mixing of fuel and air (delayed ignition)
  - Ignition (in flammable region of vapor cloud)
  - Combustion
    - Explosion: detonation (blast)
    - Flash fire: deflagration (no blast)
    - Fireball: diffusion flame





Fire Dynamics Simulator (FDS)

- Advanced CFD solver oriented towards fire applications; developed by NIST, USA (*http://fire.nist.gov/fds*)
- Main features:
  - Large eddy simulation (LES) approach for turbulence
  - Low Mach number formulation
  - Numerical methods: finite difference scheme (2nd order); predictor-corrector time integrator (2nd order); rectangular Cartesian grid; multi-block grid.
  - Software engineering: public domain; open source (Fortran 90); PC-friendly (Windows/Linux/Unix OS) and parallel (MPI-based).
- Current combustion modeling capability: non-premixed combustion
- Objective: adapt FDS to treat ignition and partially-premixed combustion events (flash fires, fireballs, mixed modes)

Diffusion Flame Modeling

- Model expressions for the LES-filtered HRR [W/m^3]:

$$\boxed{(\overline{\dot{q}'''_d})_{eq} = \underbrace{\frac{\overline{\rho} Y_F^{\infty}}{(1 - Z_{st})} \times (\frac{\nu_t}{Sc_t}) \left|\nabla \tilde{Z}\right|^2 \times \delta(\tilde{Z} - Z_{st})}_{-\overline{\dot{\omega}'''_F}} \times \Delta H_F}$$

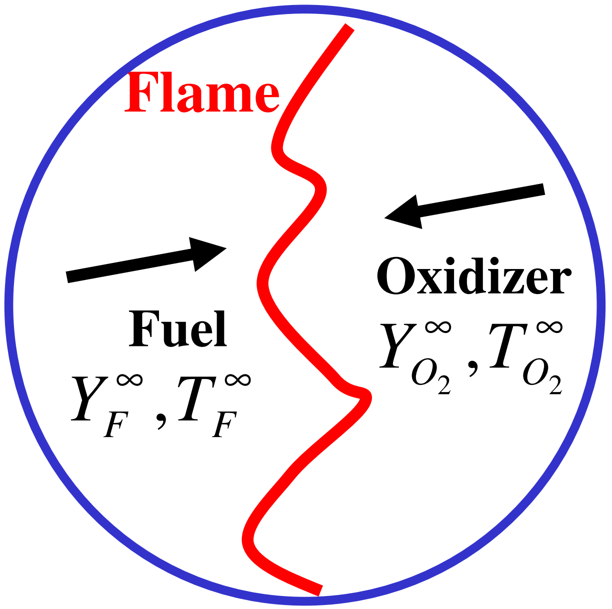
(FDS v4)
(Flame Surface)

$$\boxed{(\overline{\dot{q}'''_d})_{eq} = \underbrace{\overline{\rho} \times \frac{\min(\tilde{Y}_F ; \tilde{Y}_{O_2} / r_s)}{\tau}}_{-\overline{\dot{\omega}'''_F}} \times \Delta H_F}$$

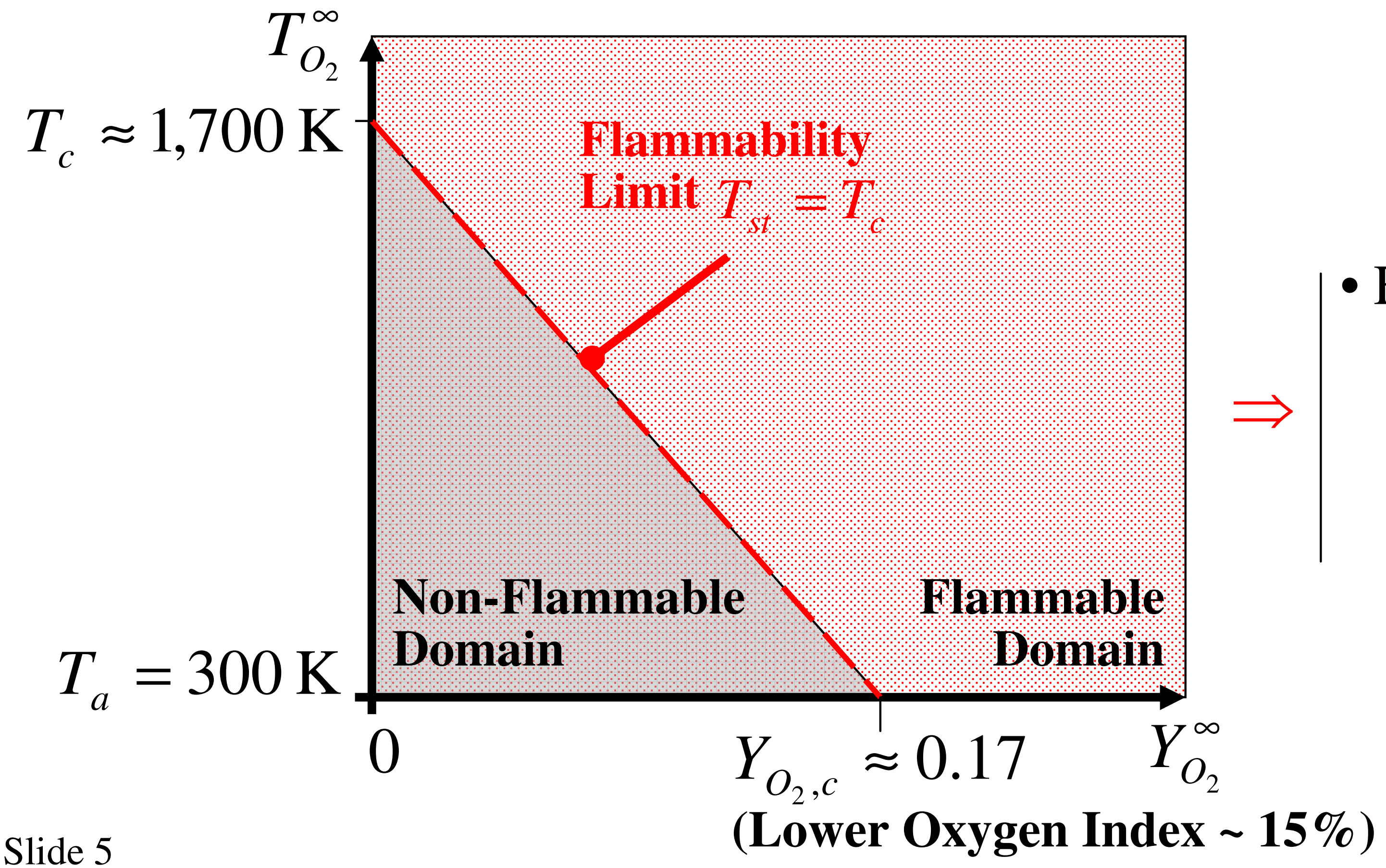
(FDS v5)
(Eddy Break-Up)

- ➢ Flame: chemically-active region located where fuel and air meet in stoichiometric proportions
- ➢ Burning rate limited by fuel-air mixing occurring at the flame surface
- ➢ Flame extinction remains unlikely in (well-ventilated) fire applications

Diffusion Flame Modeling



- Flame extinction due to air vitiation
  - Flammability diagram (for diffusion flames) in terms of the oxidizer stream properties



$\Rightarrow$

- Flammable conditions:

$$\boxed{\frac{Y_{O_2}^\infty}{Y_{O_2,c}} - \left(\frac{T_c - T_{O_2}^\infty}{T_c - T_a}\right) \ge 0}$$

Diffusion Flame Modeling

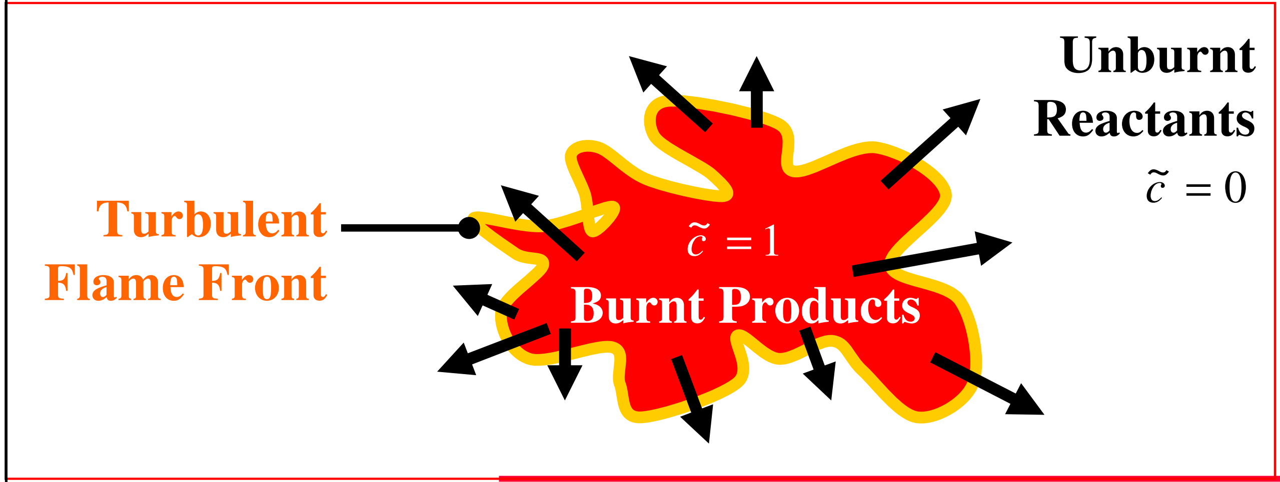
- Modified expression with flame extinction capability:
  - Equilibrium chemistry model expression corrected by a flame extinction factor *FEF*

$$\boxed{\overline{\dot{q}_d'''} = [1 - FEF] \times (\overline{\dot{q}_d'''})_{eq} = [1 - \underbrace{H((\frac{T_c - T_{O_2}^{\infty}}{T_c - T_a}) - \frac{Y_{O_2}^{\infty}}{Y_{O_2,c}})}_{\text{Heaviside function}}] \times (\overline{\dot{q}_d'''})_{eq}}$$

Deflagration Modeling

- Transport equation for the LES-filtered progress variable:
  (Boger *et al.*, *Proc. Combust. Inst.* 1998; Boger & Veynante, 2000)

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{c}) + \frac{\partial}{\partial x_j}(\overline{\rho}\tilde{c}\tilde{u}_j) = \frac{\partial}{\partial x_j}\left(\left(\frac{\rho_u s_L \Delta_c}{16\sqrt{6/\pi}} + \overline{\rho}\frac{\nu_T}{Sc_F}\right)\frac{\partial \tilde{c}}{\partial x_j}\right) + \rho_u s_L \times \Xi \times 4\sqrt{\frac{6}{\pi}}\frac{\tilde{c}(1-\tilde{c})}{\Delta_c} + \overline{\dot{\omega}'''_{ign}}$$



Unburnt Reactants

$\tilde{c} = 0$

Turbulent Flame Front

$\tilde{c} = 1$

Burnt Products

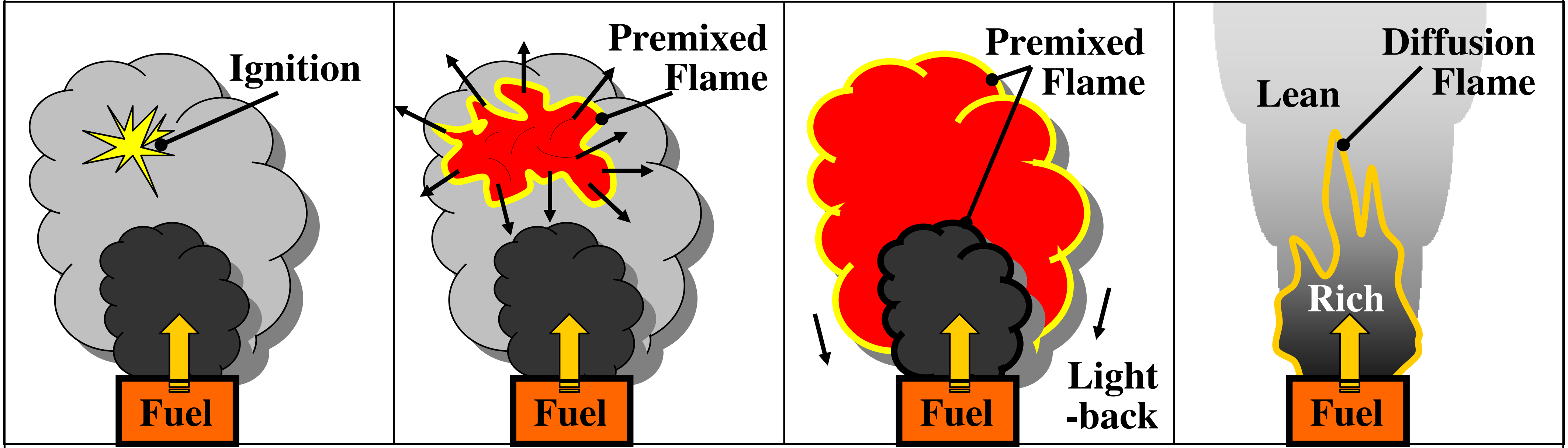
Deflagration Modeling

- Corresponding expression for the HRR [W/m^3]:

$$\boxed{\overline{\dot{q}_p'''} = (\underbrace{\rho_u s_L \times \Xi \times 4\sqrt{\frac{6}{\pi}}\frac{\tilde{c}(1-\tilde{c})}{\Delta_c}}_{\text{propagation}} + \underbrace{\overline{\dot{\omega}_{ign}'''}}_{\text{ignition}}) \times (Y_F^u - Y_F^b)\Delta H_F}$$

Coupling Interface Between Premixed and Non-Premixed Combustion

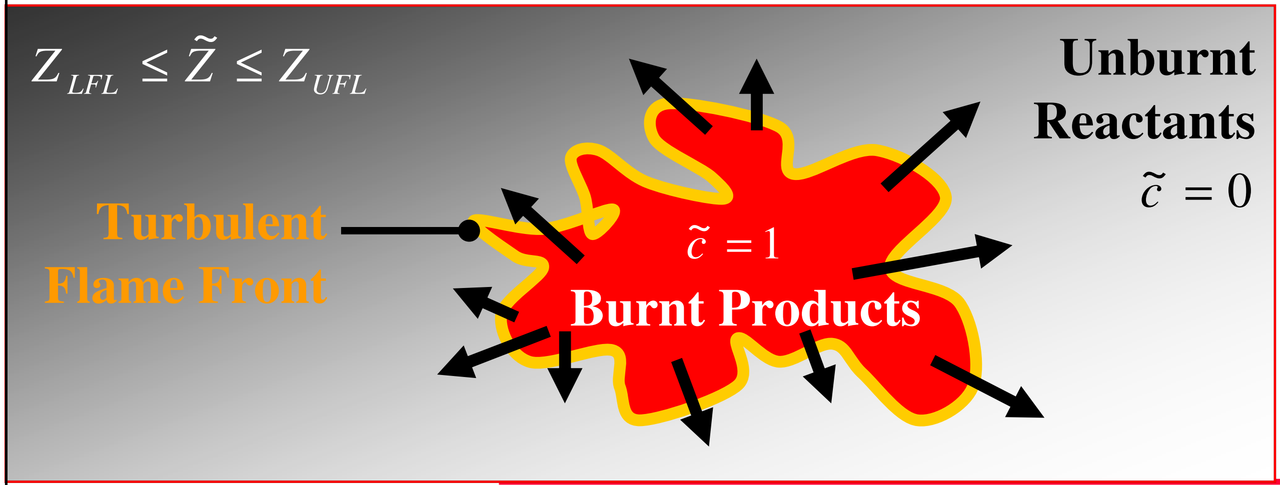
- Adaptation of the filtered reaction progress variable approach to treat deflagrations in non-homogeneous fuel-air mixtures
- Coupling of the deflagration and diffusion burning capabilities to treat partially-premixed combustion events



Coupling Interface Between Premixed and Non-Premixed Combustion

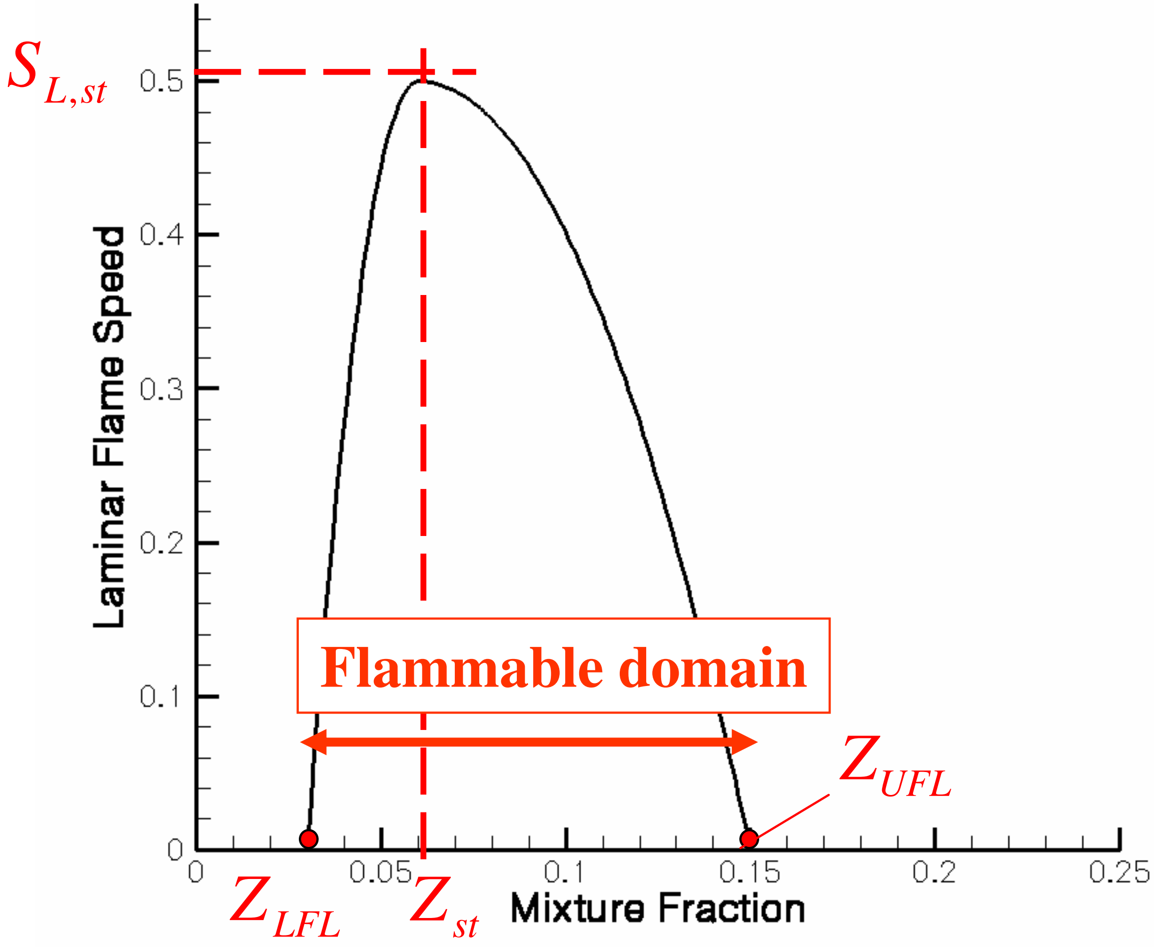
- The variations in fuel-air mixture composition are described using the LES-filtered mixture fraction $\tilde{Z}$:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c})+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{c}\tilde{u}_j)=\frac{\partial}{\partial x_j}\left(\left(\frac{\rho_u \boxed{s_L(\tilde{Z})}\Delta_c}{16\sqrt{6/\pi}}+\bar{\rho}\frac{\nu_T}{Sc_F}\right)\frac{\partial\tilde{c}}{\partial x_j}\right)$$
$$+\rho_u \boxed{s_L(\tilde{Z})}\times\Xi\times 4\sqrt{\frac{6}{\pi}}\frac{\tilde{c}(1-\tilde{c})}{\Delta_c}+\overline{\dot{\omega}_{ign}'''}$$



Coupling Interface Between Premixed and Non-Premixed Combustion

- The variations of laminar flame speed with mixture strength are described using a presumed polynomial function:
  - Input parameters (fuel properties): Z_{LFL}, Z_{UFL}, Z_{st}, $S_{L,st}$



Coupling Interface Between Premixed and Non-Premixed Combustion

- Modified expression for the HRR [W/m^3]:
  - Non-homogeneous premixed combustion:

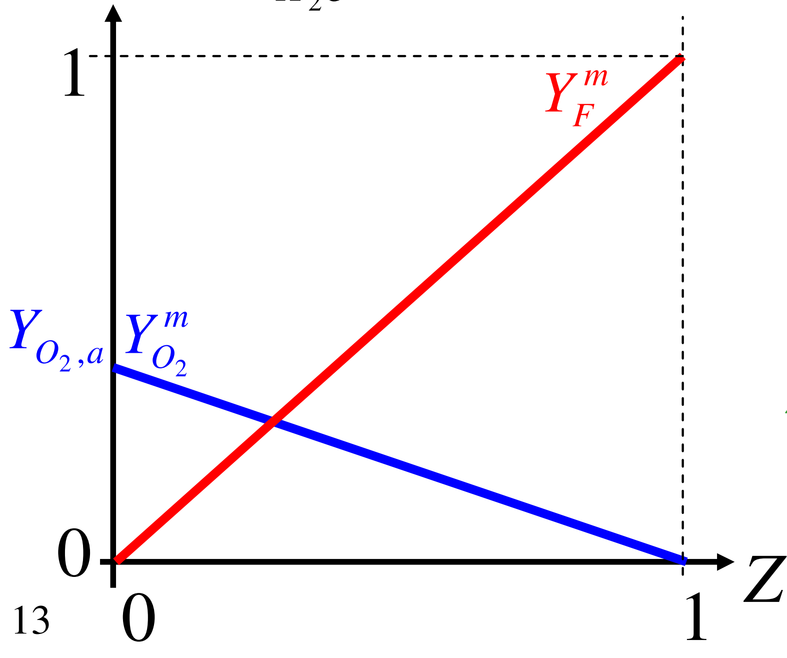
$$\overline{\dot{q}_p'''} = \overbrace{(\underbrace{\rho_u s_L(\tilde{Z}) \times \Xi \times 4\sqrt{\frac{6}{\pi}}\frac{\tilde{c}(1-\tilde{c})}{\Delta_c}}_{\overline{\dot{\omega}_c'''}}) \times (Y_F^m(\tilde{Z}) - Y_F^{eq}(\tilde{Z}))}^{-\overline{\dot{\omega}_F'''}} \times \Delta H_F$$

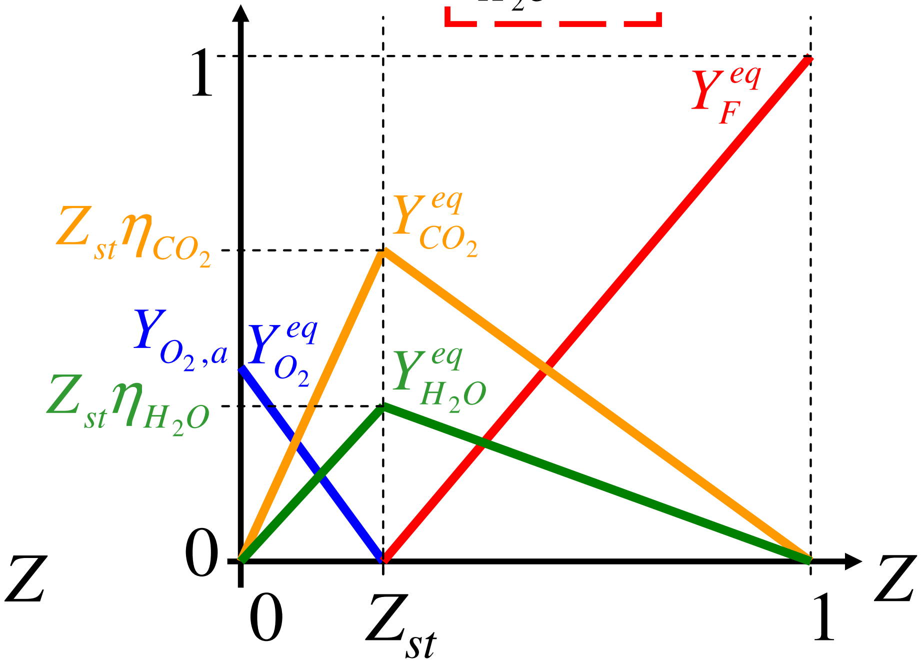
Coupling Interface Between Premixed and Non-Premixed Combustion

- Two-variable description of the reactive mixture composition (state relationships):

$$
\begin{aligned}
\tilde{Y}_F &= (1-\tilde{c})\times \overbrace{Y_F^m(\tilde{Z})}^{\text{Pure mixing solution}} &+& \quad \tilde{c}\times \overbrace{Y_F^{eq}(\tilde{Z})}^{\text{Equilibrium solution}} \\
\tilde{Y}_{O_2} &= (1-\tilde{c})\times Y_{O_2}^m(\tilde{Z}) &+& \quad \tilde{c}\times Y_{O_2}^{eq}(\tilde{Z}) \\
\tilde{Y}_{CO_2} &= (1-\tilde{c})\times 0 &+& \quad \tilde{c}\times Y_{CO_2}^{eq}(\tilde{Z}) \\
\tilde{Y}_{H_2O} &= (1-\tilde{c})\times 0 &+& \quad \tilde{c}\times Y_{H_2O}^{eq}(\tilde{Z})
\end{aligned}
$$

Original FDS model





Coupling Interface Between Premixed and Non-Premixed Combustion

- Basic expressions for the HRR [W/m^3]:
  - Premixed combustion:

$$\boxed{\overline{\dot{q}'''_p} = (\rho_u s_L(\tilde{Z}) \times \Xi \times 4\sqrt{\frac{6}{\pi}}\frac{\tilde{c}(1-\tilde{c})}{\Delta_c}) \times (Y_F^m(\tilde{Z}) - Y_F^{eq}(\tilde{Z})) \times \Delta H_F}$$

  - Non-premixed combustion:

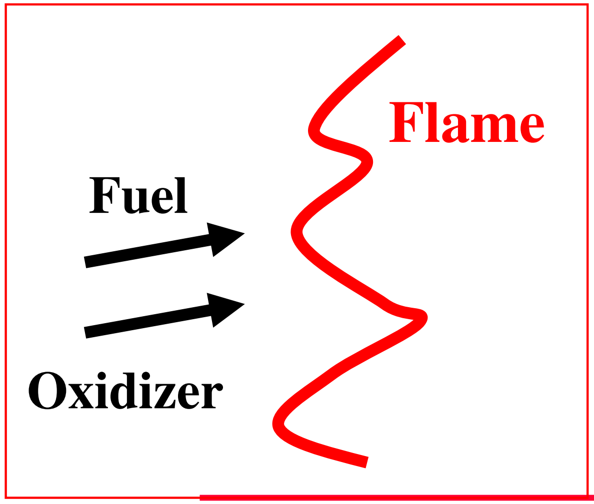
$$\boxed{\overline{\dot{q}'''_d} = [1 - H((\frac{T_c - T_{O_2}^{\infty}}{T_c - T_a}) - \frac{Y_{O_2}^{\infty}}{Y_{O_2,c}})] \times (\overline{\dot{q}'''_d})_{eq}}$$

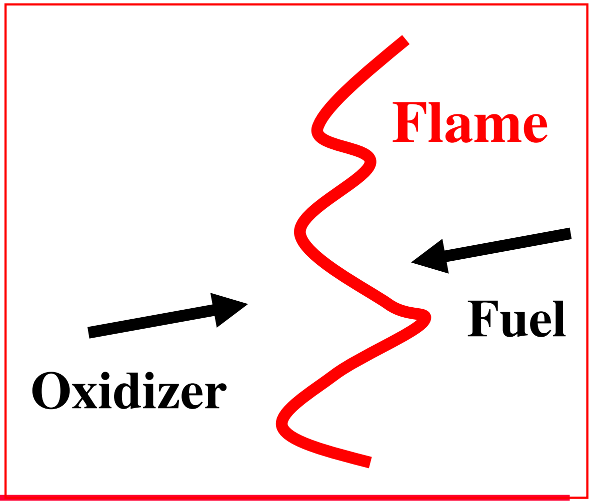
Coupling Interface Between Premixed and Non-Premixed Combustion

- Identification of premixed and non-premixed combustion modes (Domingo, Vervisch & Bray, *Combust. Theory Modelling* 2002)
  - Flame index:

$$FI = \frac{1}{2}\left(\frac{\nabla\tilde{Y}_F . \nabla\tilde{Y}_{O_2}}{\left|\nabla\tilde{Y}_F\right| \times \left|\nabla\tilde{Y}_{O_2}\right|} + 1\right)$$

  - Premixed flamelets: $FI = 1$;   Diffusion flamelets: $FI = 0$





Coupling Interface Between Premixed and Non-Premixed Combustion

- New expression for the HRR (Domingo, Vervisch & Bray, *Combust. Theory Modelling* 2002)
  - Partially-premixed combustion:

$$\boxed{\overline{\dot{q}'''} = FI \times \overline{\dot{q}_p'''} + (1 - FI) \times f_{ign} \times \overline{\dot{q}_d'''}}$$

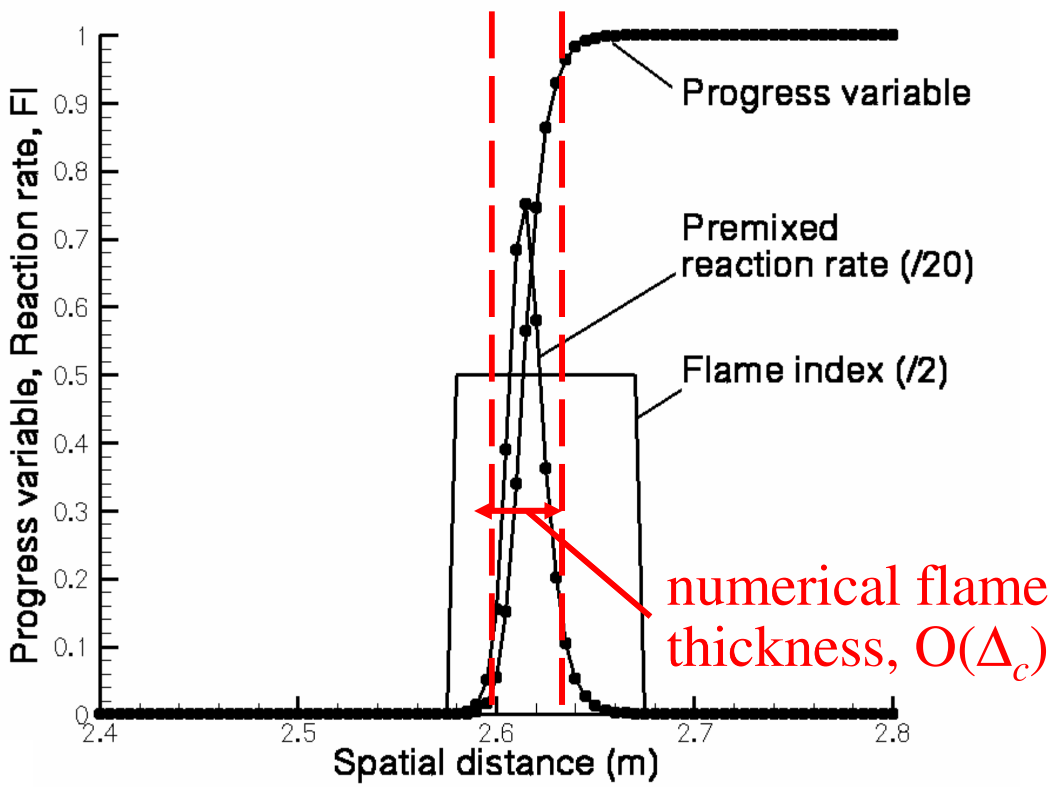
where f_{ign} is an ad hoc ignition factor

$$f_{ign} = (\frac{1}{2} + \frac{1}{2}\tanh(\frac{\tilde{c} - 0.6}{0.05}))$$

Formulated so that the diffusion flame model is initially turned off and is activated as a post-premixed flame event

Numerical Challenges

- Grid resolution requirement of the partially-premixed combustion model formulation
    - Premixed flame must remain <u>smooth on the computational grid</u>

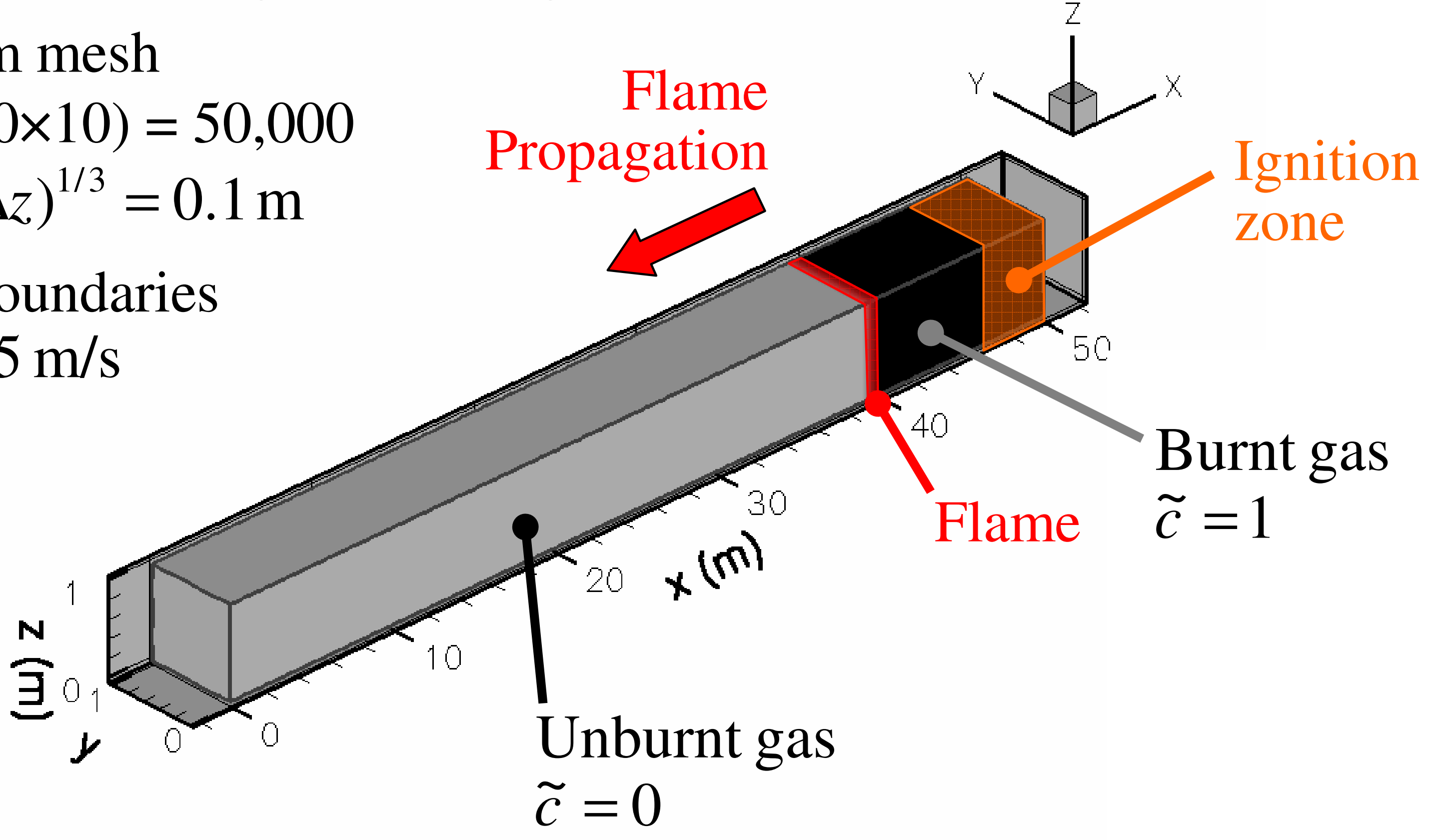


$$\delta_f = \Delta_c \sqrt{\frac{\pi}{6}} \times \sqrt{1 + \frac{16\sqrt{6/\pi}\,\nu_t}{Sc_t s_L \Delta_c}} \approx \Delta_c$$

$$\Rightarrow \boxed{\underbrace{\Delta_c}_{\text{LES } c\text{-filter size}} \geq 4\,\underbrace{(\Delta x \Delta y \Delta z)^{1/3}}_{\text{computational grid cell size}}}$$

Numerical Challenges: Laminar Flame Test

- Simplified conditions: one-dimensional plane configuration, initially quiescent gas, homogeneous fuel-air mixture
  - ➢ Uniform mesh
    $(500\times10\times10) = 50{,}000$
    $(\Delta x\Delta y\Delta z)^{1/3} = 0.1\,\text{m}$
  - ➢ Open boundaries
  - ➢ $s_L = 0.5$ m/s



Flame Propagation

Ignition zone

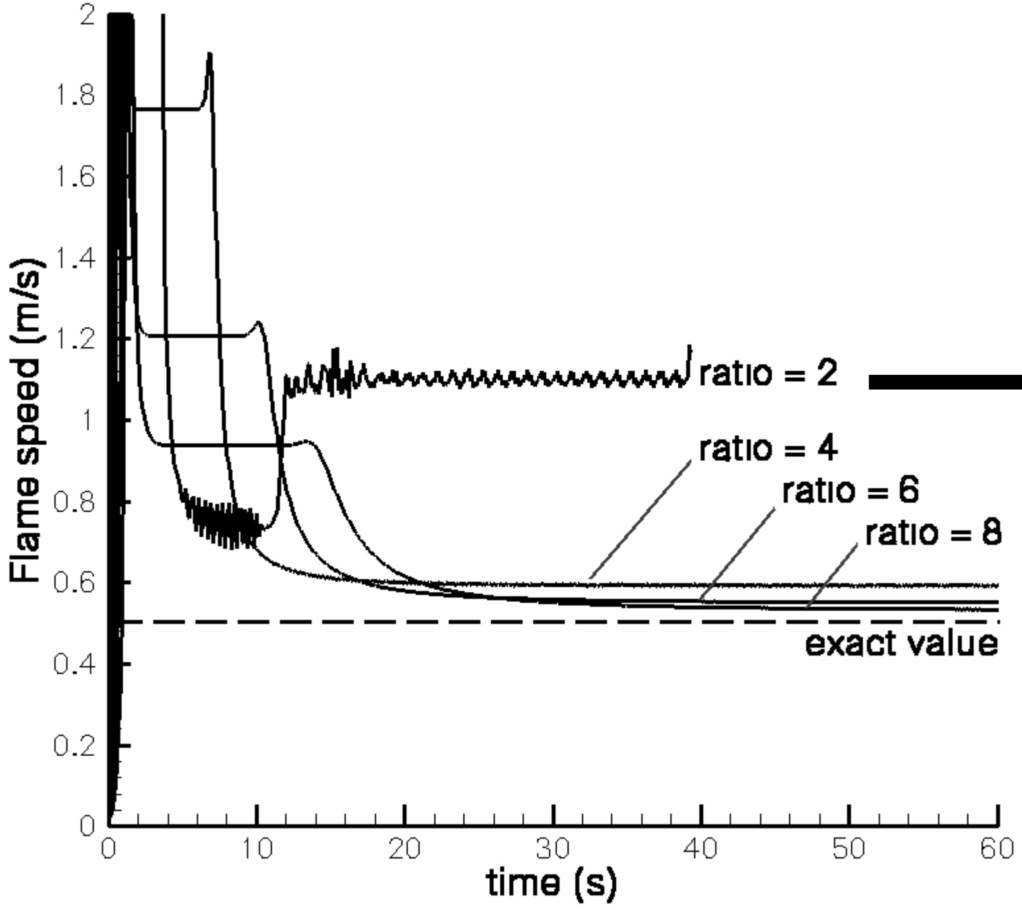
Burnt gas
$\tilde{c} = 1$

Flame

Unburnt gas
$\tilde{c} = 0$

Numerical Challenges: Laminar Flame Test

- Effect of the LES filter-to-grid length scale ratio on the stability and accuracy of the predicted flame speed



$(\Delta_c /(\Delta x \Delta y \Delta z)^{1/3}) = 2$

Unstable and inaccurate

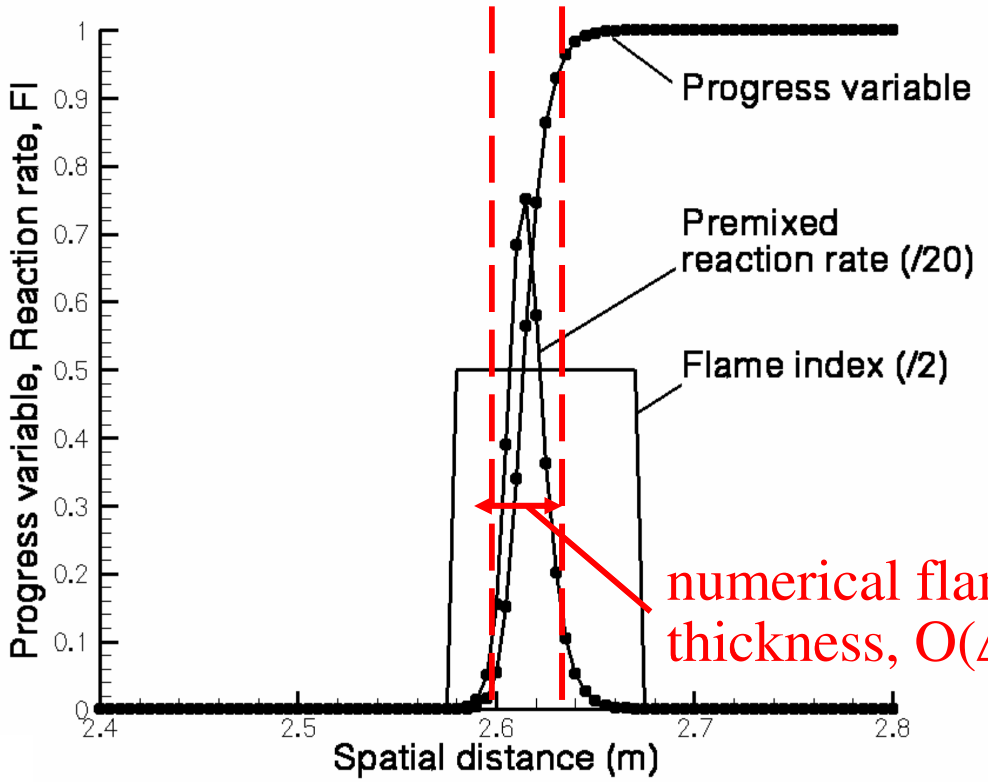
$(\Delta_c /(\Delta x \Delta y \Delta z)^{1/3}) \geq 4$

Stable and accurate

(error less than 20 %)

Numerical Challenges

- Grid resolution requirement of the partially-premixed combustion model formulation
  - Premixed flame must remain <u>thin in mixture fraction space</u>



numerical flame thickness, O(Δ_c)

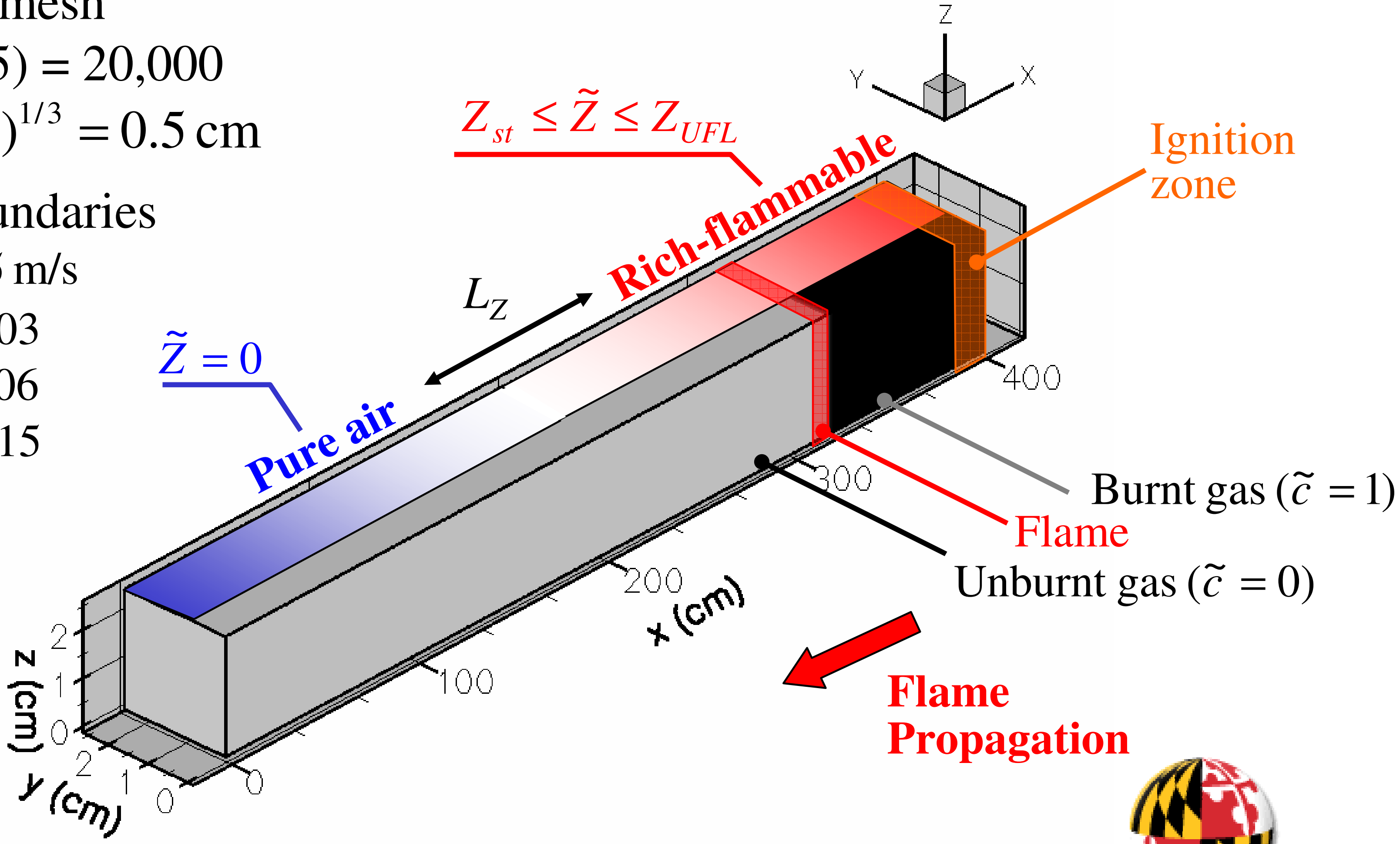
$$\delta_f = \Delta_c \sqrt{\frac{\pi}{6}} \times \sqrt{1 + \frac{16\sqrt{6/\pi}\,\nu_t}{Sc_t s_L \Delta_c}} \approx \Delta_c$$

$$\Rightarrow \boxed{\underbrace{\Delta_c}_{\text{LES } c\text{-filter size}} \le l_Z \approx \frac{Z_{st}}{|(\nabla \tilde{Z})_{\max}|}}$$

characteristic length scale for Z-variations

Numerical Challenges: Laminar Flame Test

- Simplified conditions: one-dimensional plane configuration, initially quiescent gas, non-homogeneous fuel-air mixture
  - Uniform mesh
    $(800 \times 5 \times 5) = 20{,}000$
    $(\Delta x \Delta y \Delta z)^{1/3} = 0.5\ \text{cm}$
  - Open boundaries
  - $s_{L,st} = 0.5\ \text{m/s}$
    $Z_{LFL} = 0.03$
    $Z_{st} = 0.06$
    $Z_{UFL} = 0.15$

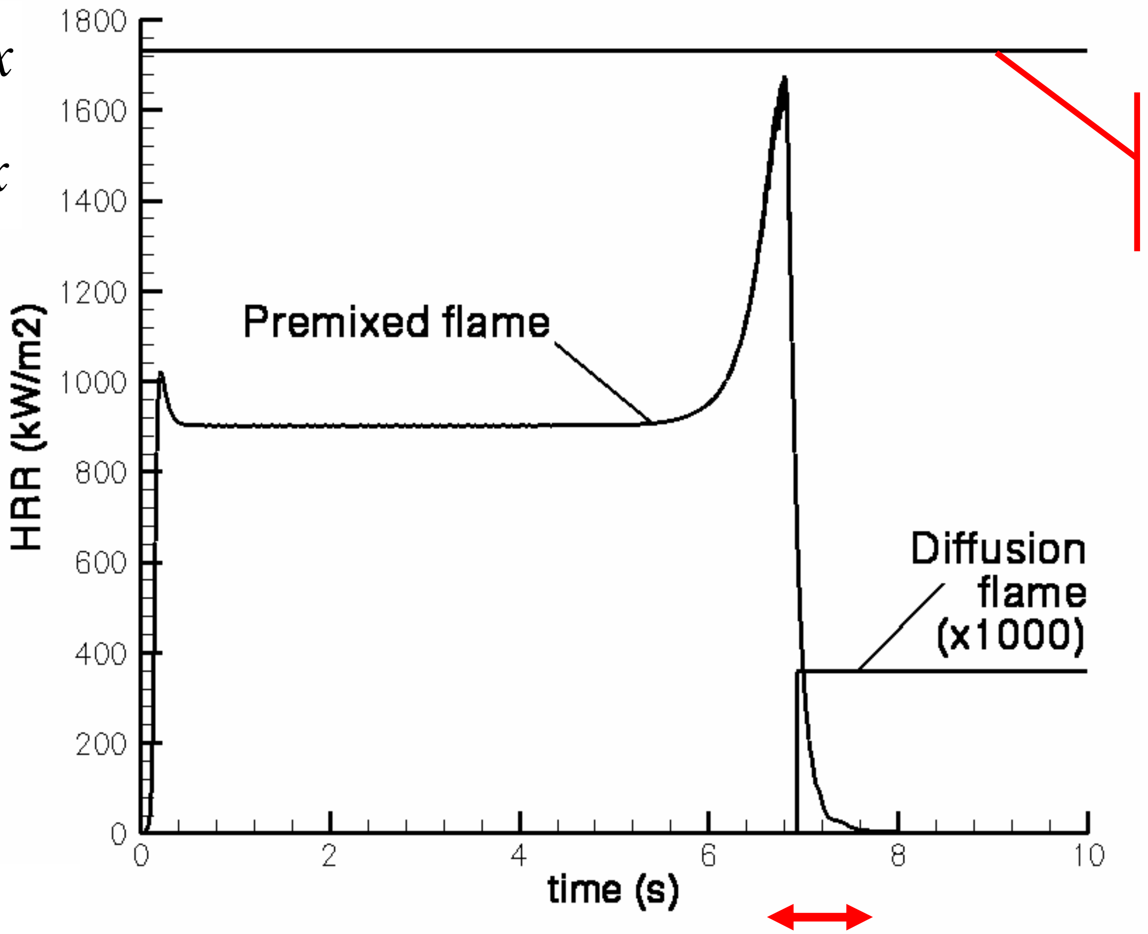


Numerical Challenges: Laminar Flame Test

- Time variations of global HRR (premixed/diffusion components) $(L_Z / \Delta_c) = 10$

$$\overline{\dot{q}''_p} = \int \overline{\dot{q}'''_p} dx$$

$$\overline{\dot{q}''_d} = \int \overline{\dot{q}'''_d} dx$$



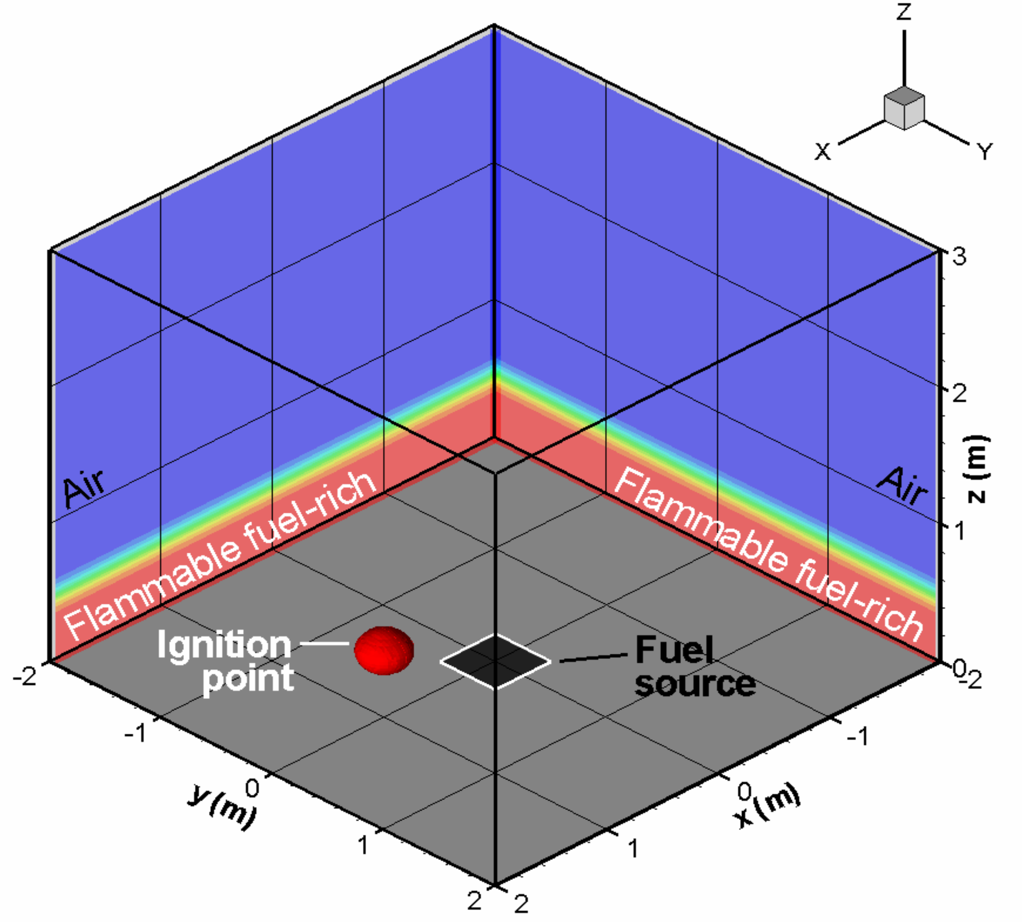
Homogeneous stoichiometric premixed flame

Transition from premixed to non-premixed combustion

Coupling Interface: Turbulent Flame Test

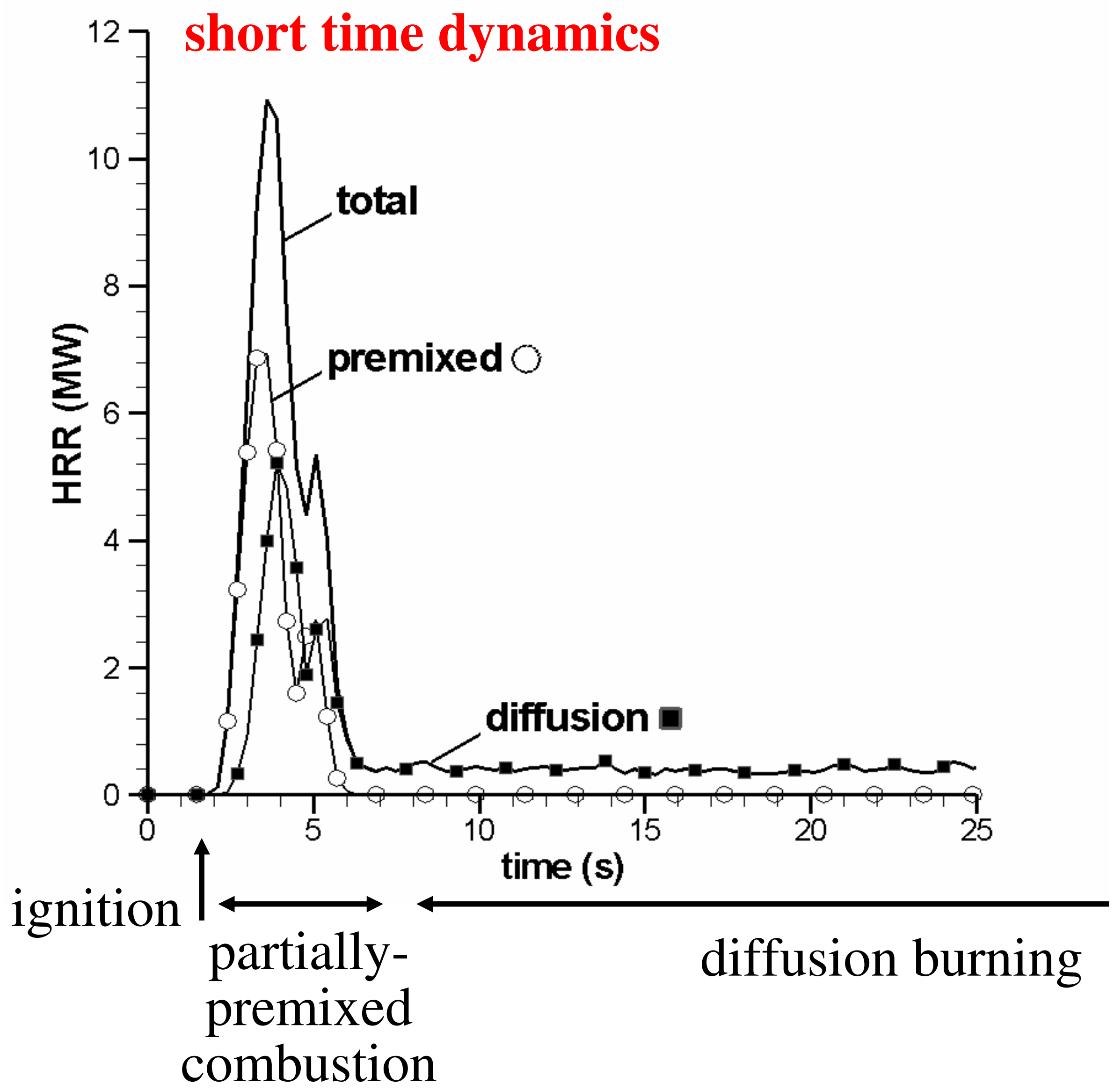
- Model problem: ignition of a fuel vapor cloud in a sealed compartment (FDS v4)
  - Uniform mesh
    $(160\times160\times120) = 3{,}072{,}000$
    $(\Delta x\Delta y\Delta z)^{1/3} = 2.5\,\text{cm}$

$$\left|\begin{array}{l}\text{Fuel: heptane}\\ m_F \approx 1.2\,\text{kg}\\ E_F \approx 55\,\text{MJ}\end{array}\right.$$



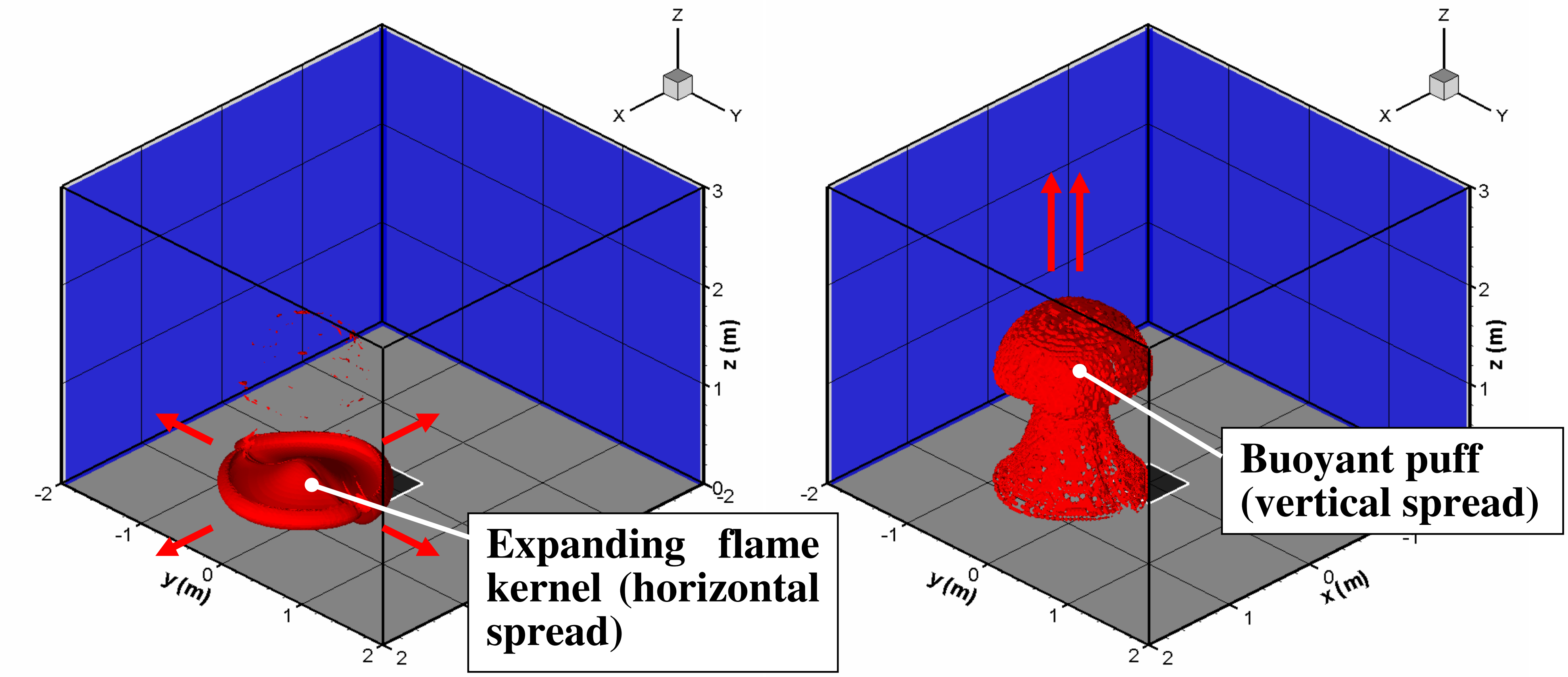
Coupling Interface: Turbulent Flame Test

- Time variations of global HRR (premixed/diffusion flames)



Coupling Interface: Turbulent Flame Test

- Location and structure of premixed and non-premixed flames at $t = 2.5$ s
  - Initiation of partially-premixed combustion



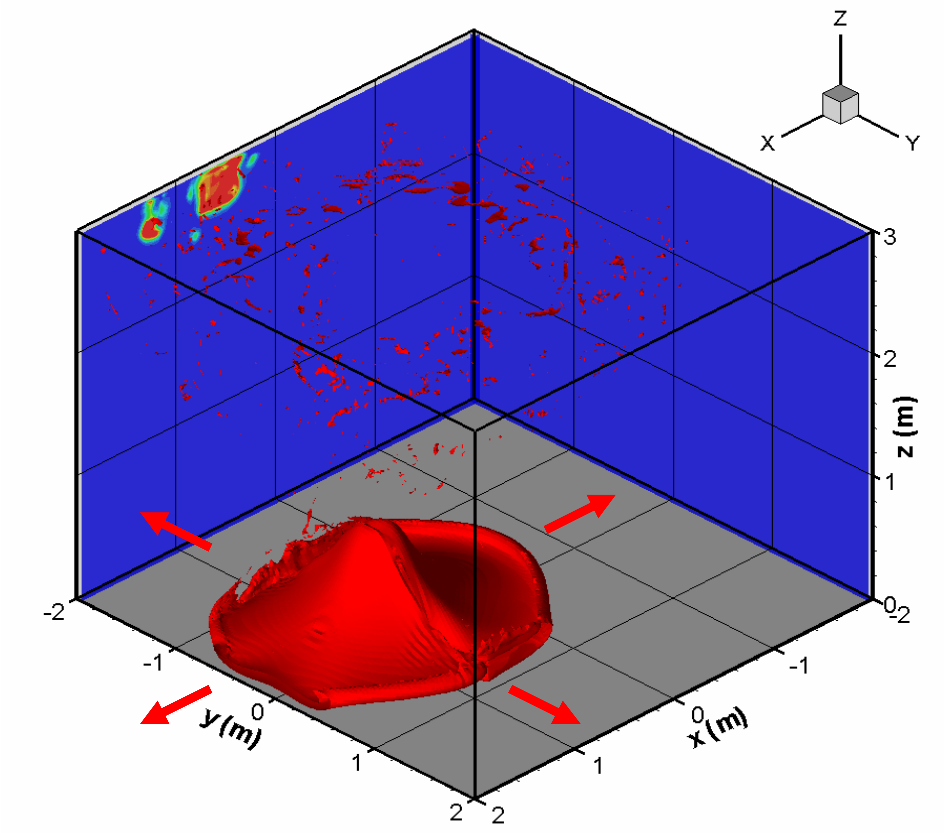
Premixed

Non-premixed

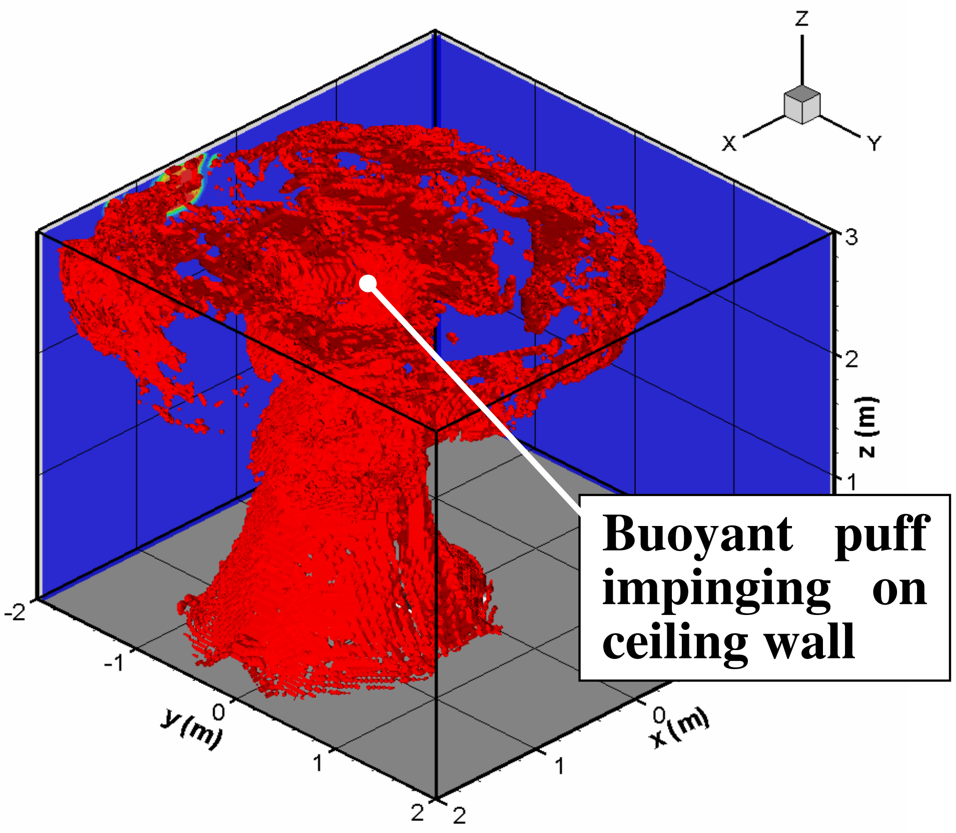
Coupling Interface: Turbulent Flame Test

- Location and structure of premixed and non-premixed flames at $t = 3$ s
  - Partially-premixed combustion

Premixed



Non-premixed

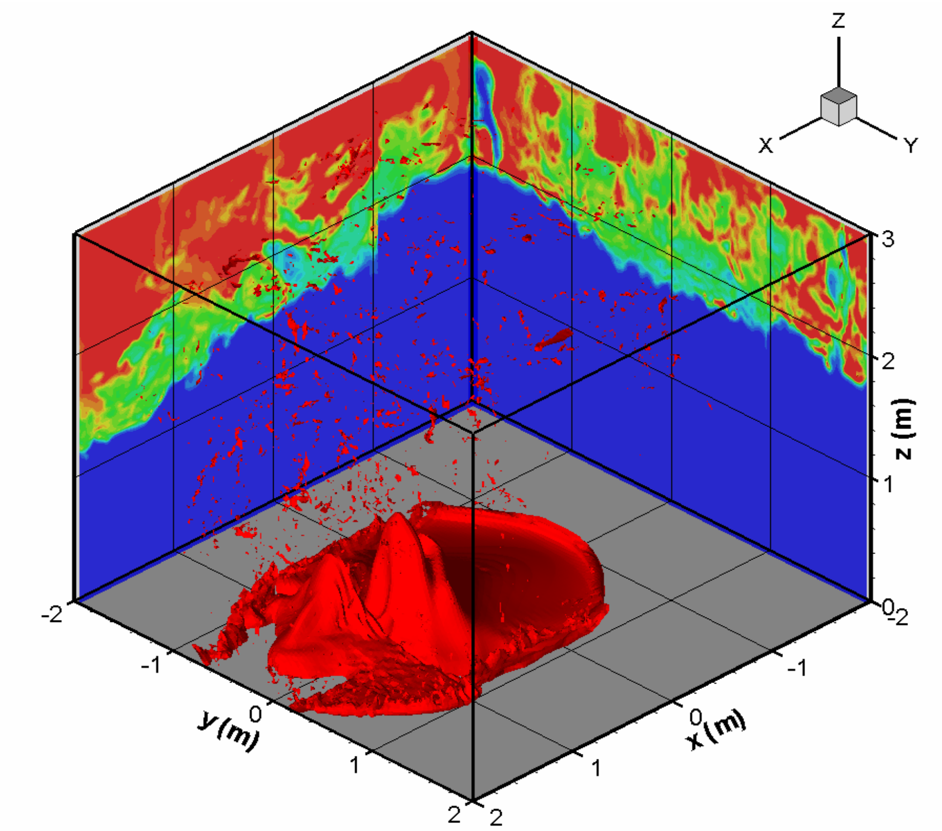


Buoyant puff impinging on ceiling wall

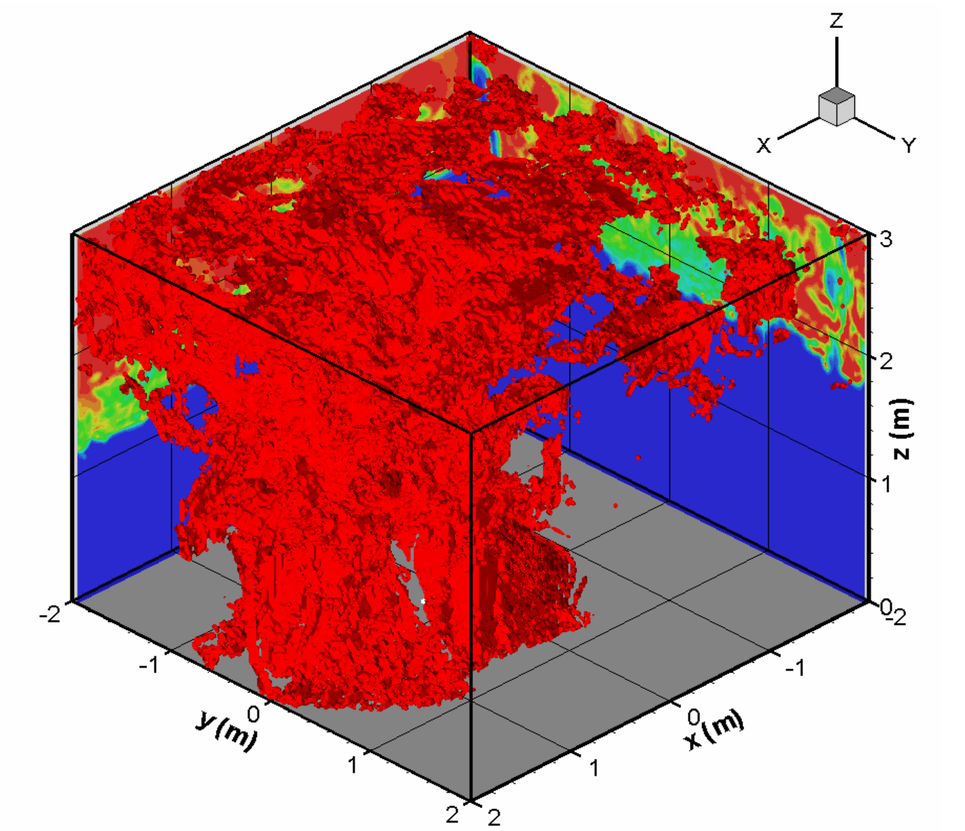
Coupling Interface: Turbulent Flame Test

- Location and structure of premixed and non-premixed flames at $t = 3.5$ s
  - Partially-premixed combustion

Premixed



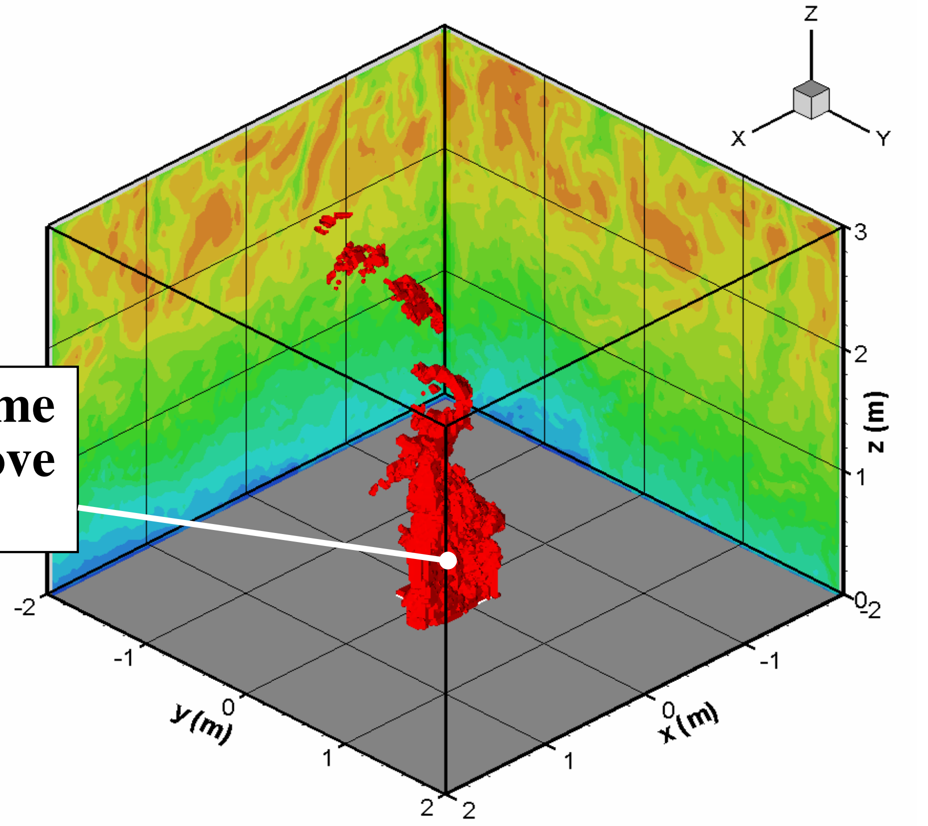
Non-premixed



Coupling Interface: Turbulent Flame Test

- Location and structure of premixed and non-premixed flames at $t = 8$ s
  - Depletion of flammable fuel (due to combustion and pre-mixing) and transition to diffusion burning (attached to the fuel source)

Non-premixed

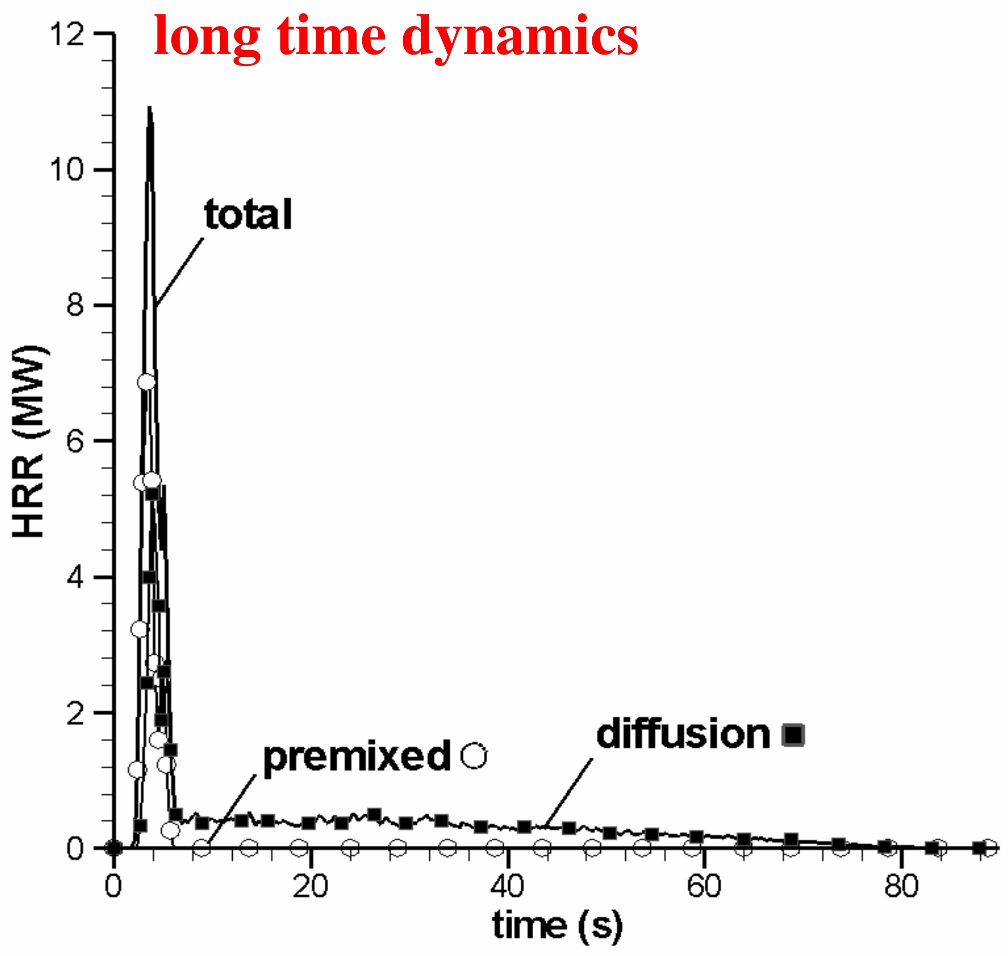


Diffusion flame located above fuel source

(light-back)

Coupling Interface: Turbulent Flame Test

- Time variations of global HRR (premixed/diffusion flames)



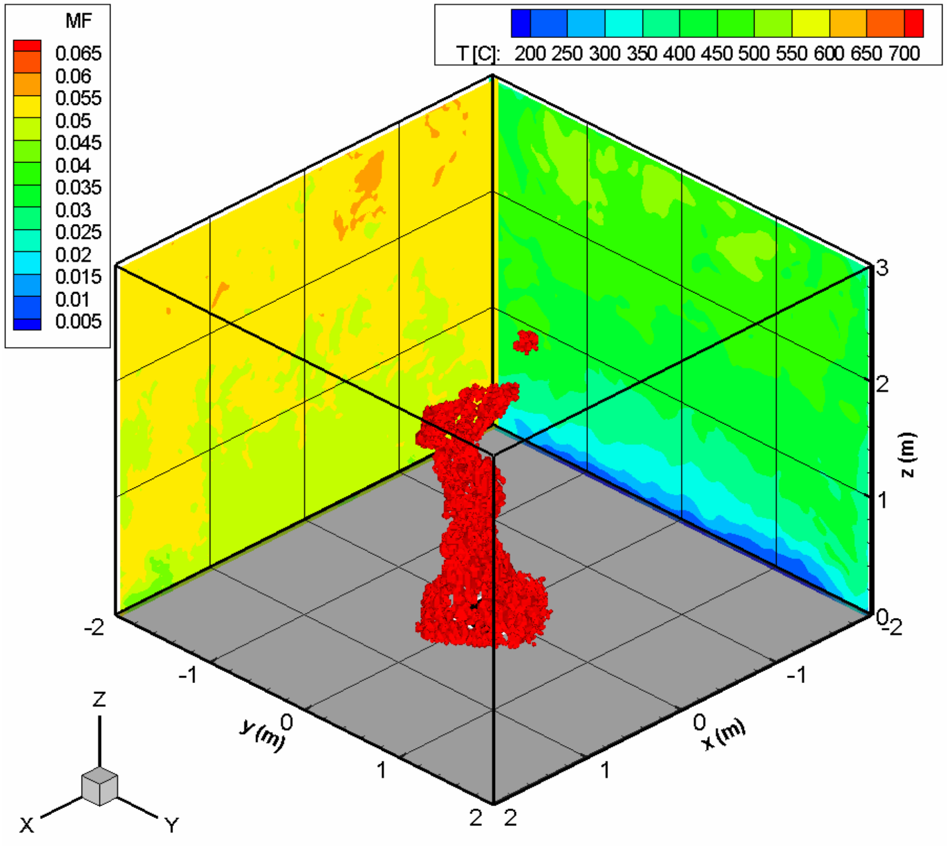
local flame extinctions

global flame extinction

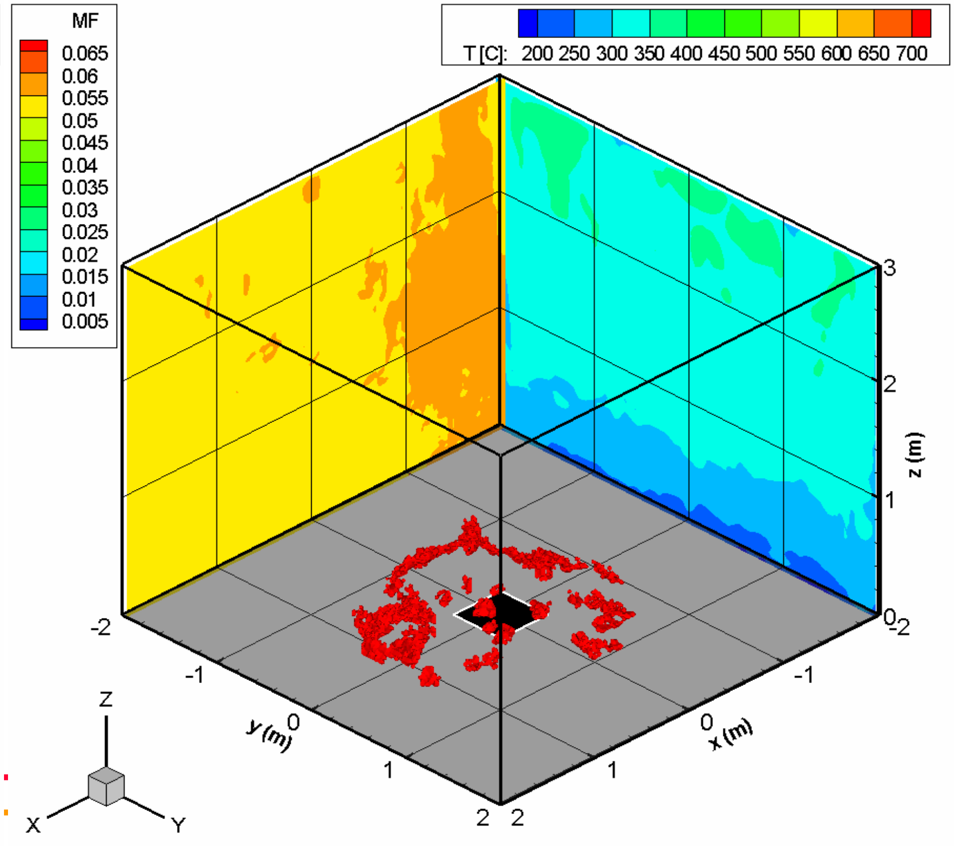
Coupling Interface: Turbulent Flame Test

- Location and structure of non-premixed flame at *t* = 60 and 80 s
  - Flame extinction due to oxygen starvation

t = 60 s

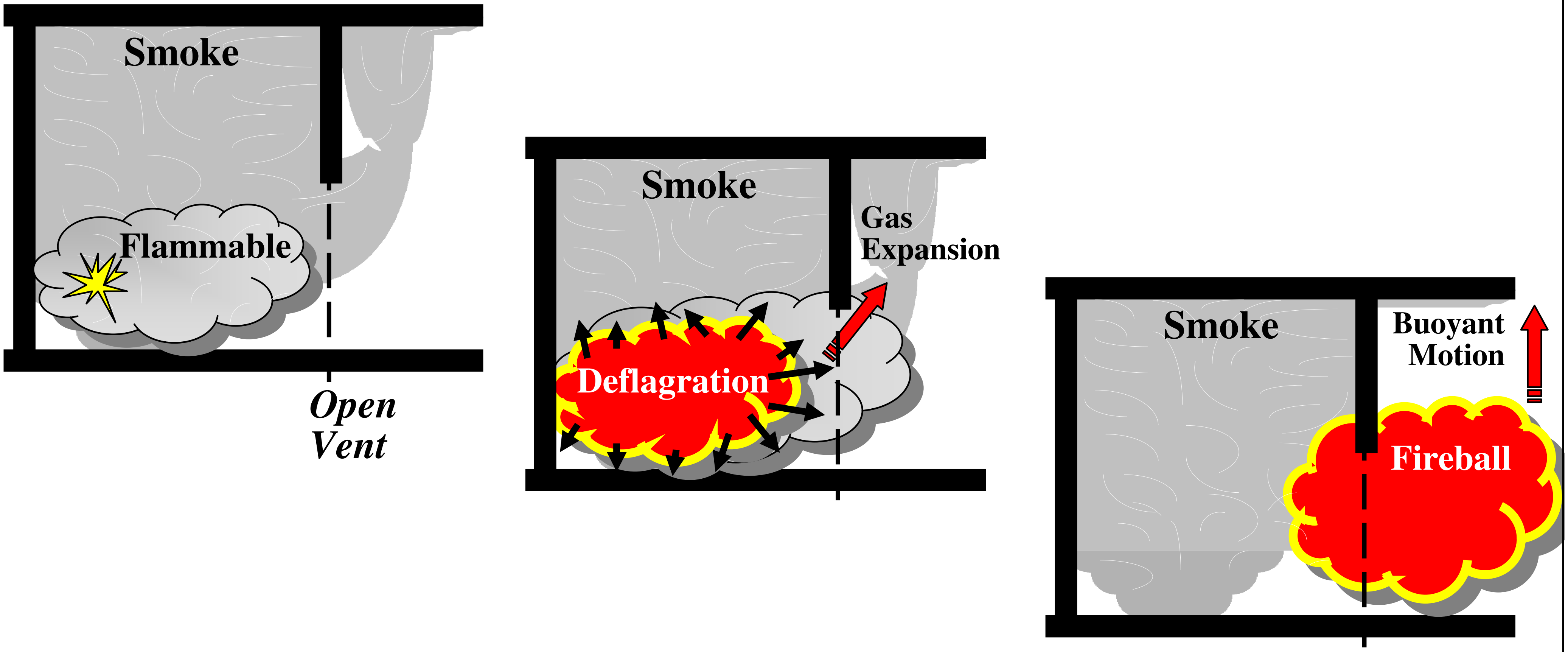


t = 80 s



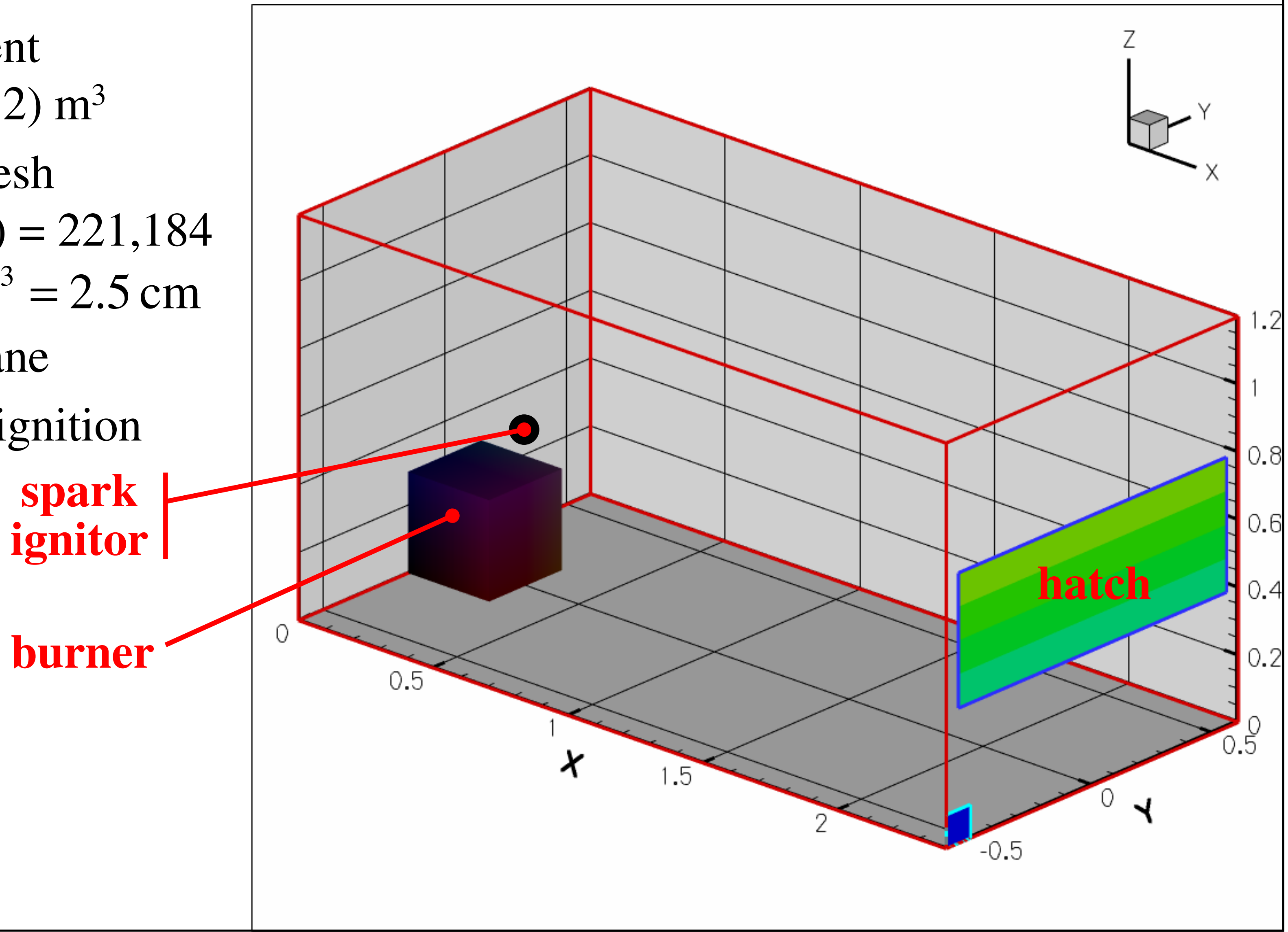
Backdraft

- Basic scenario:
  - Phase II: Ignition followed by a deflagration and fireball event



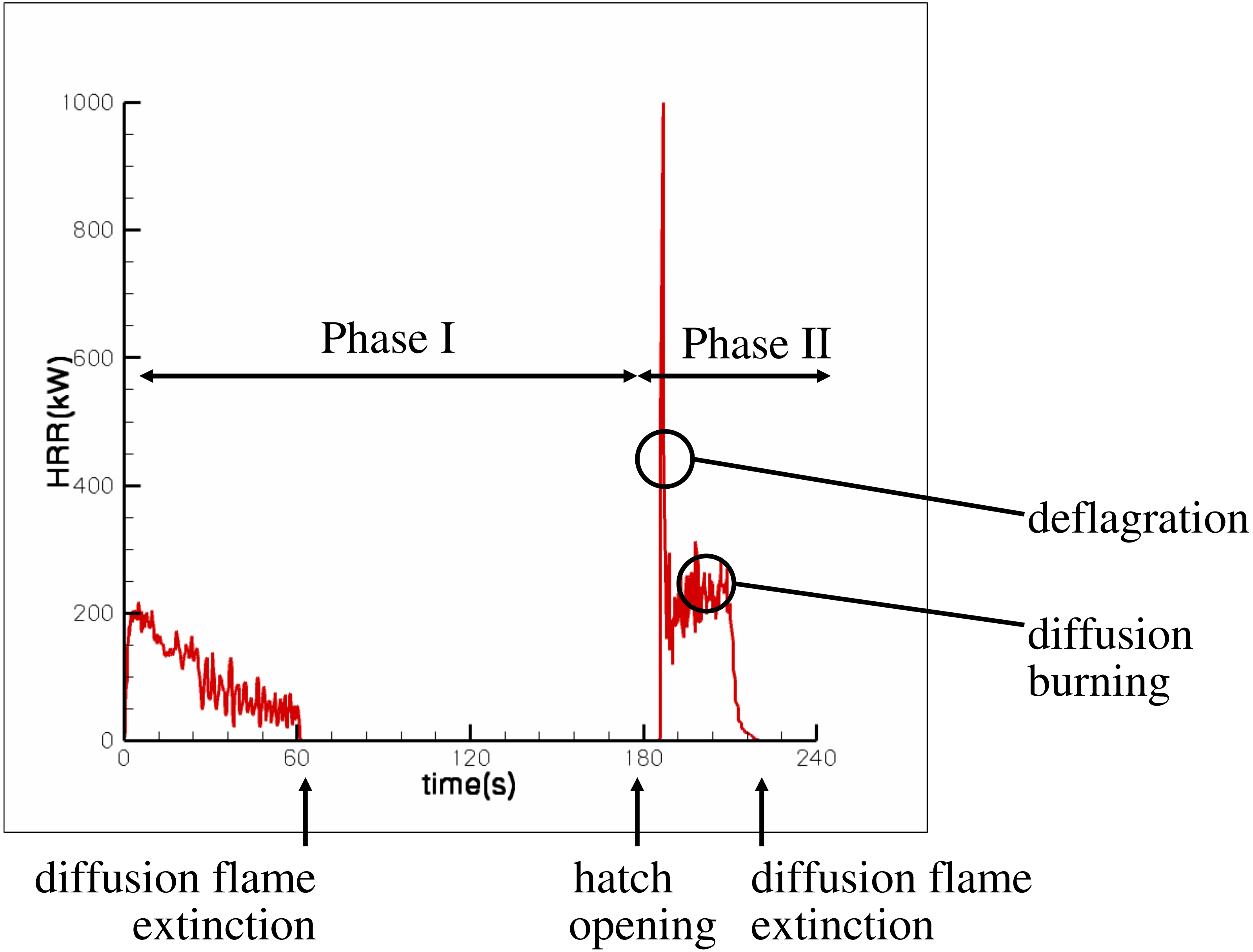
Validation Tests: Simulation of Backdraft

- Reduced-scale backdraft experiment (C. M. Fleischmann, 1994) (FDS v5)
  - Compartment $(2.4\times1.2\times1.2)\ \mathrm{m}^3$
  - Uniform mesh $(96\times48\times48) = 221{,}184$ $(\Delta x\Delta y\Delta z)^{1/3} = 2.5\ \mathrm{cm}$
  - Fuel: methane
  - Controlled ignition location



Validation Tests: Simulation of Backdraft

- Time variations of global HRR (premixed/diffusion flames)



Phase I

Phase II

deflagration

diffusion
burning

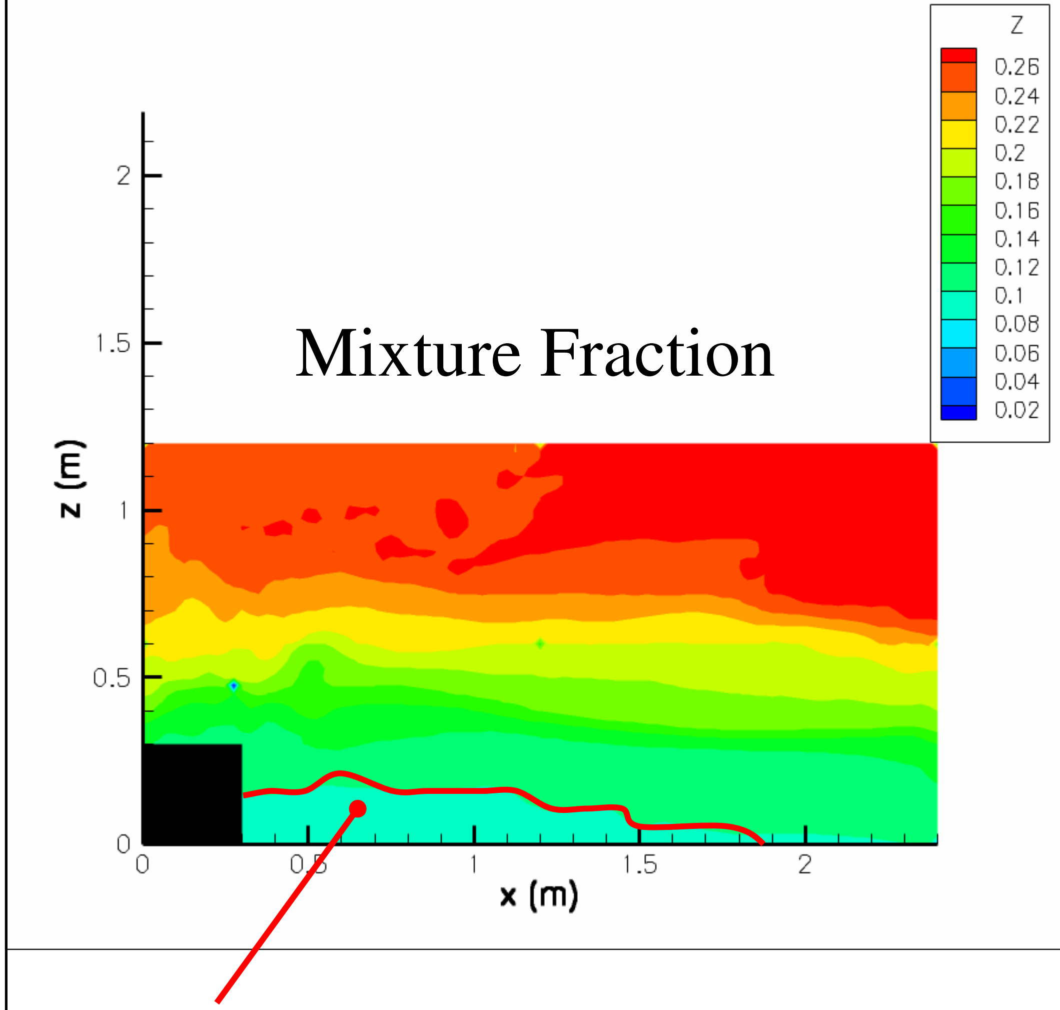
diffusion flame
extinction

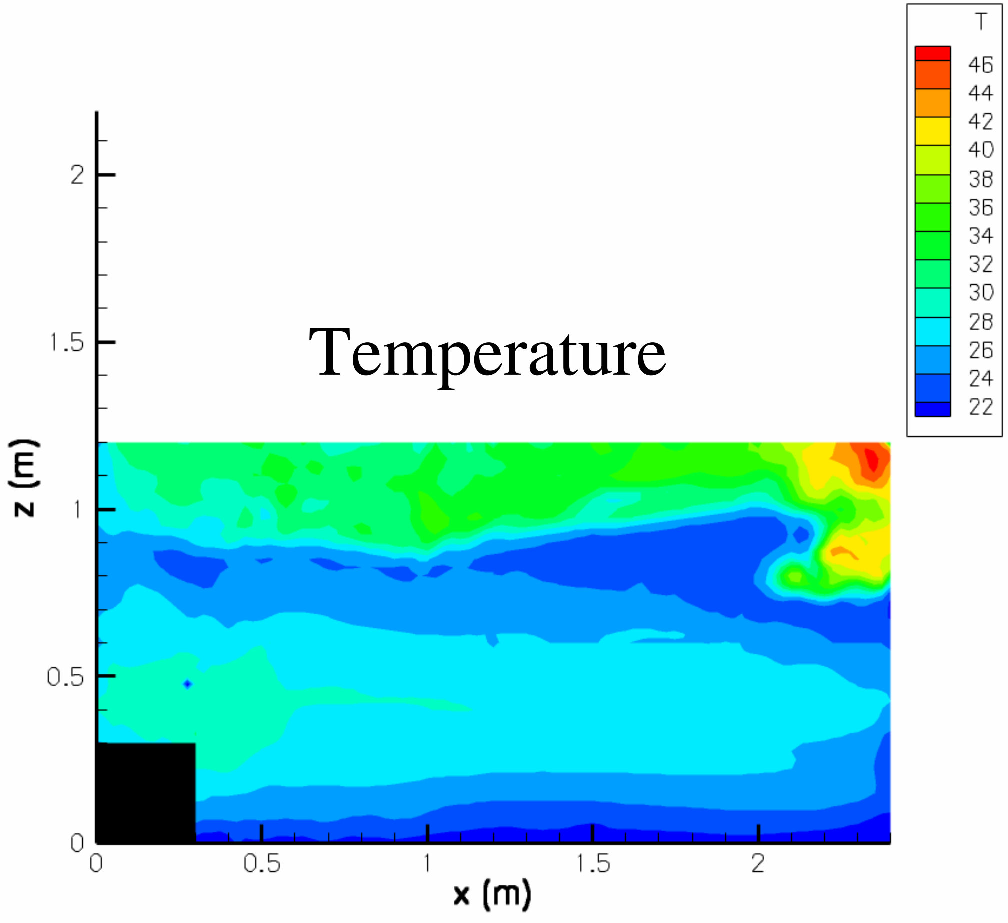
hatch
opening

diffusion flame
extinction

Validation Tests: Simulation of Backdraft

- Phase 2: conditions at time of hatch opening

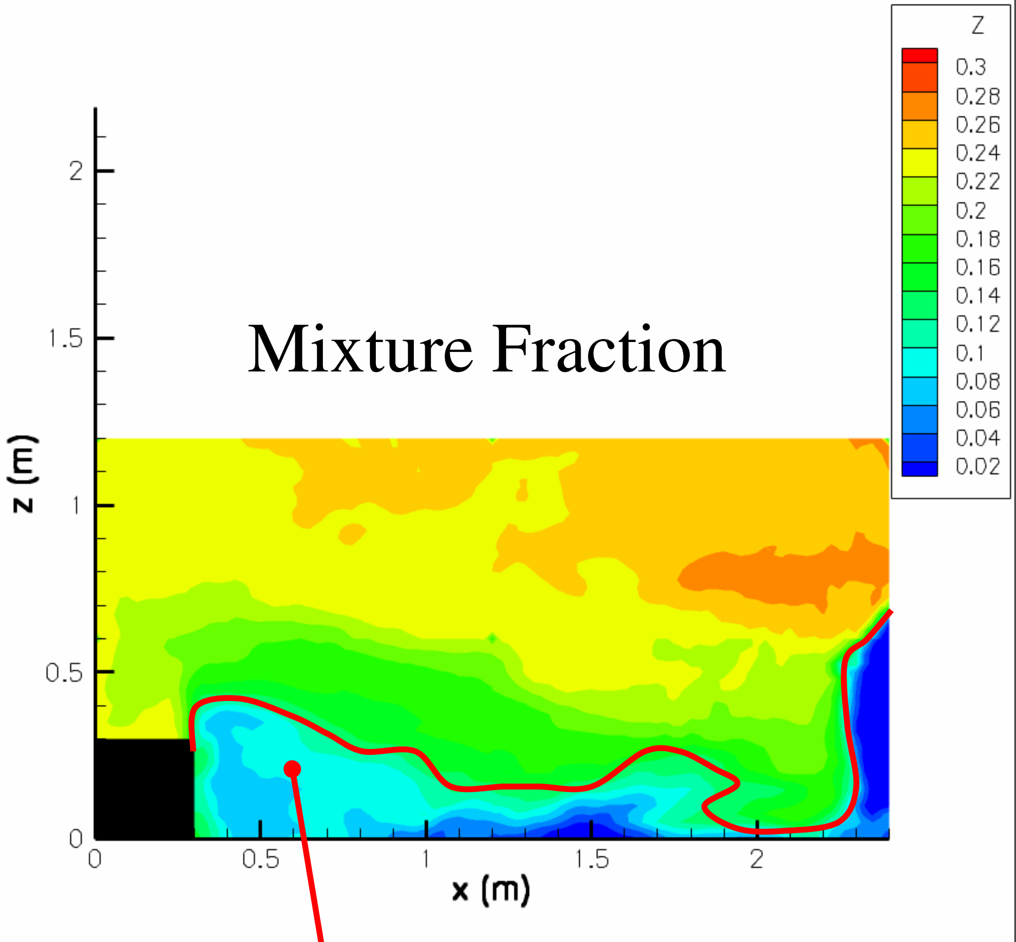




flammable region

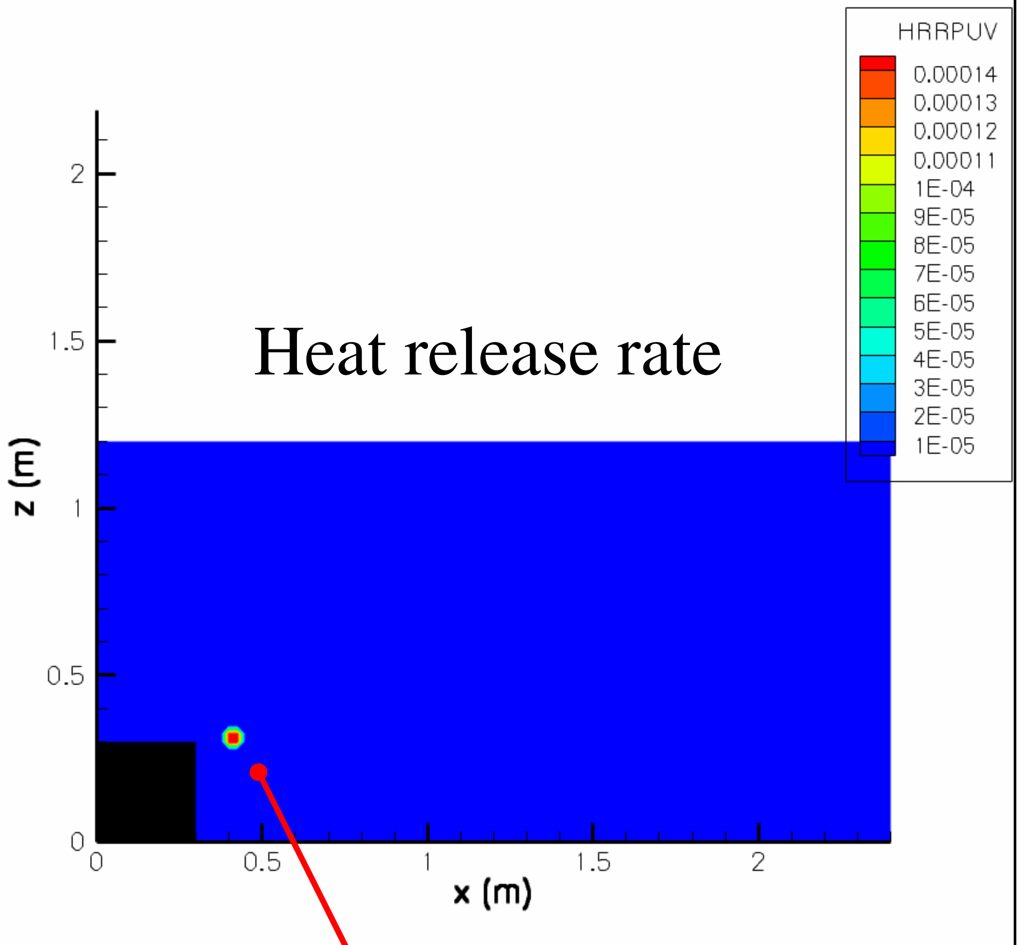
Validation Tests: Simulation of Backdraft

- Phase 2: ignition at time $t = 3.7$ s after hatch opening (Experiment: ignition delay is 6.7 s)



Mixture Fraction

growth of flammable region (gravity current)

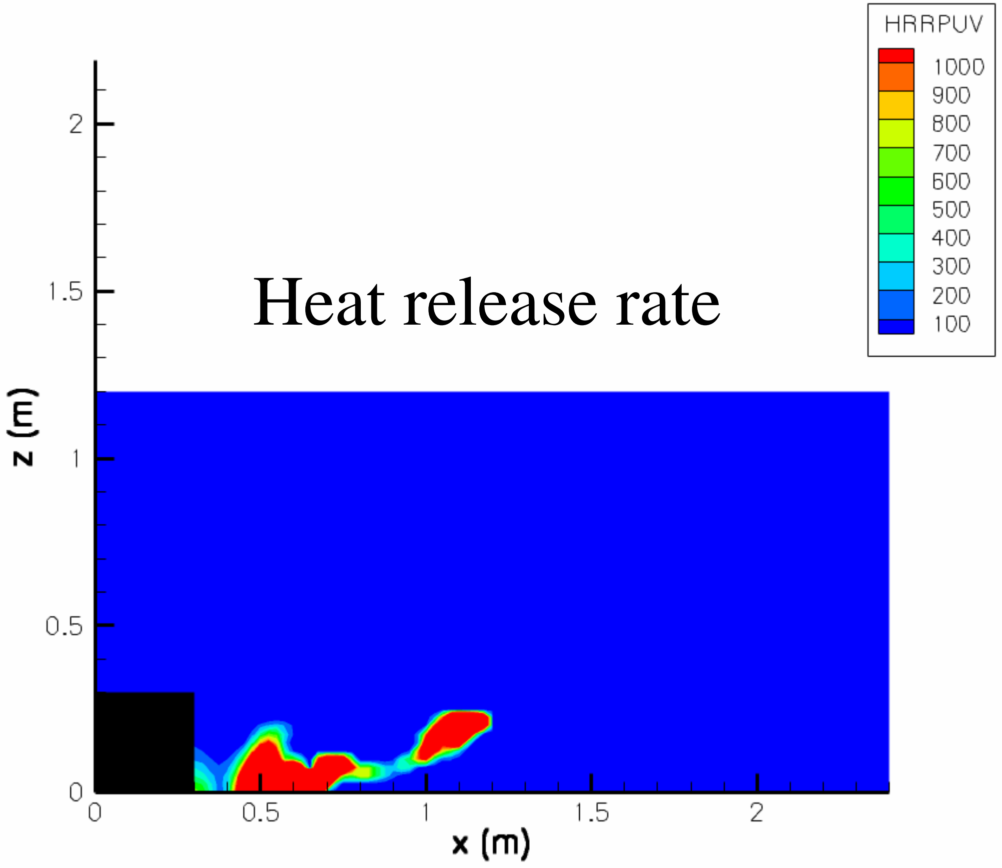


Heat release rate

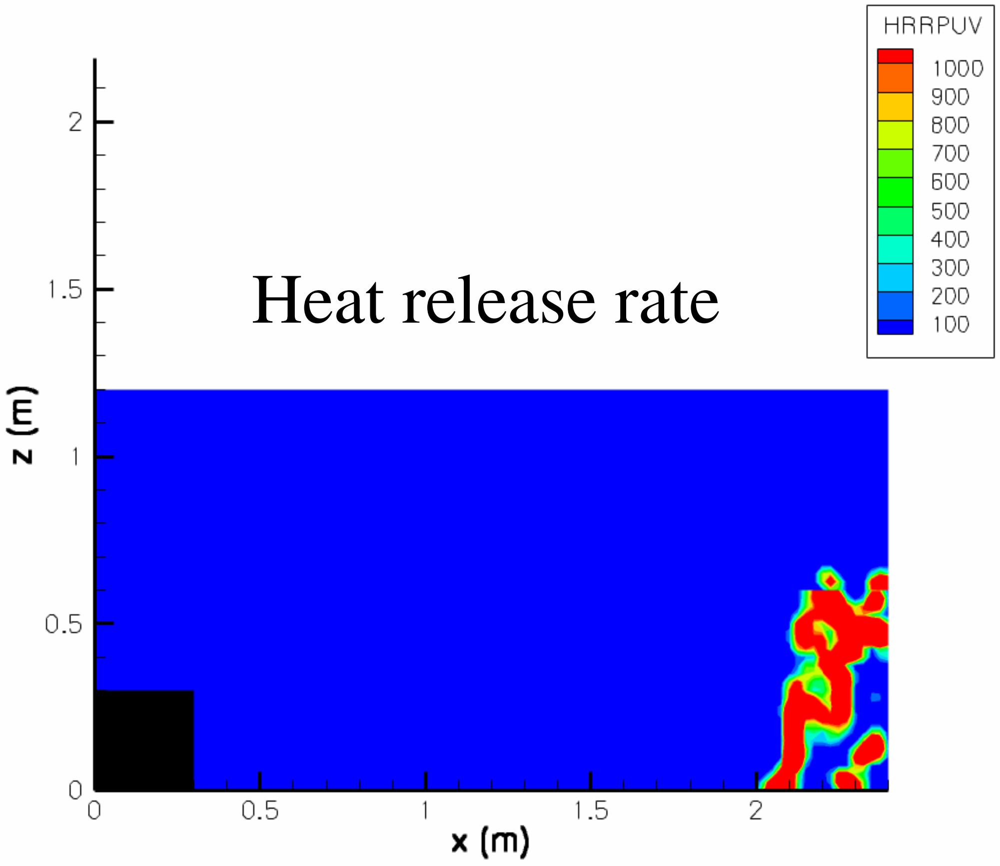
Ignition at the spark ignitor

Validation Tests: Simulation of Backdraft

- Phase 2: flame propagation across compartment (duration ~ 3.8 s)



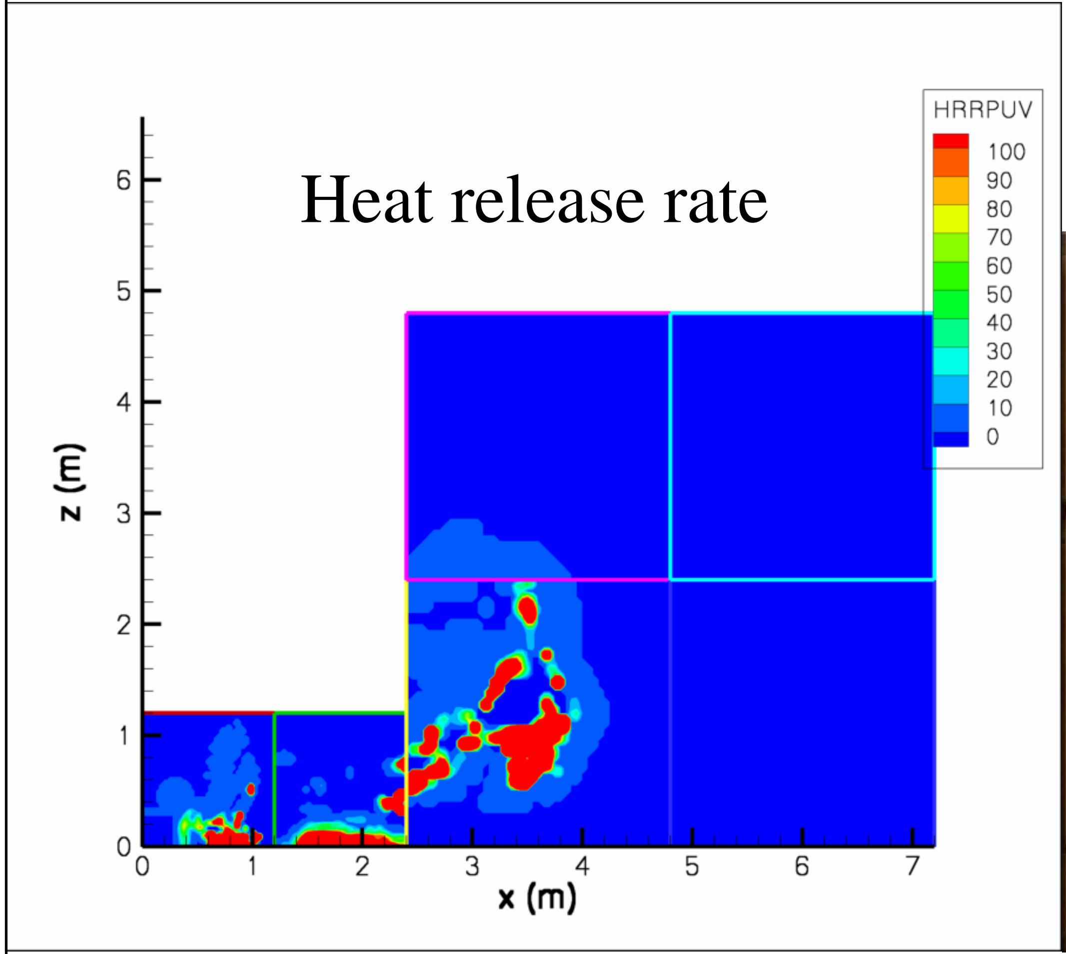
time t = 5.5 s after hatch opening



time t = 7.5 s after hatch opening

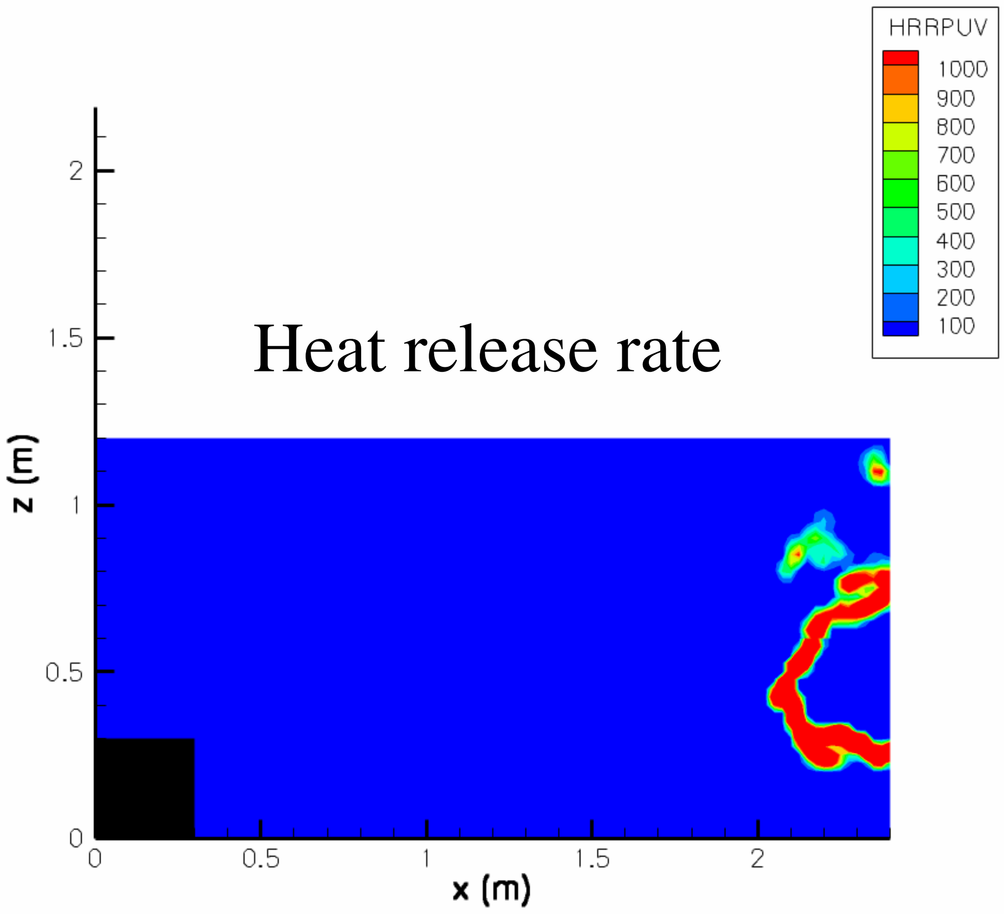
Validation Tests: Simulation of Backdraft

- Phase 2: fireball outside of the compartment (time *t* ~ 7.5 s)

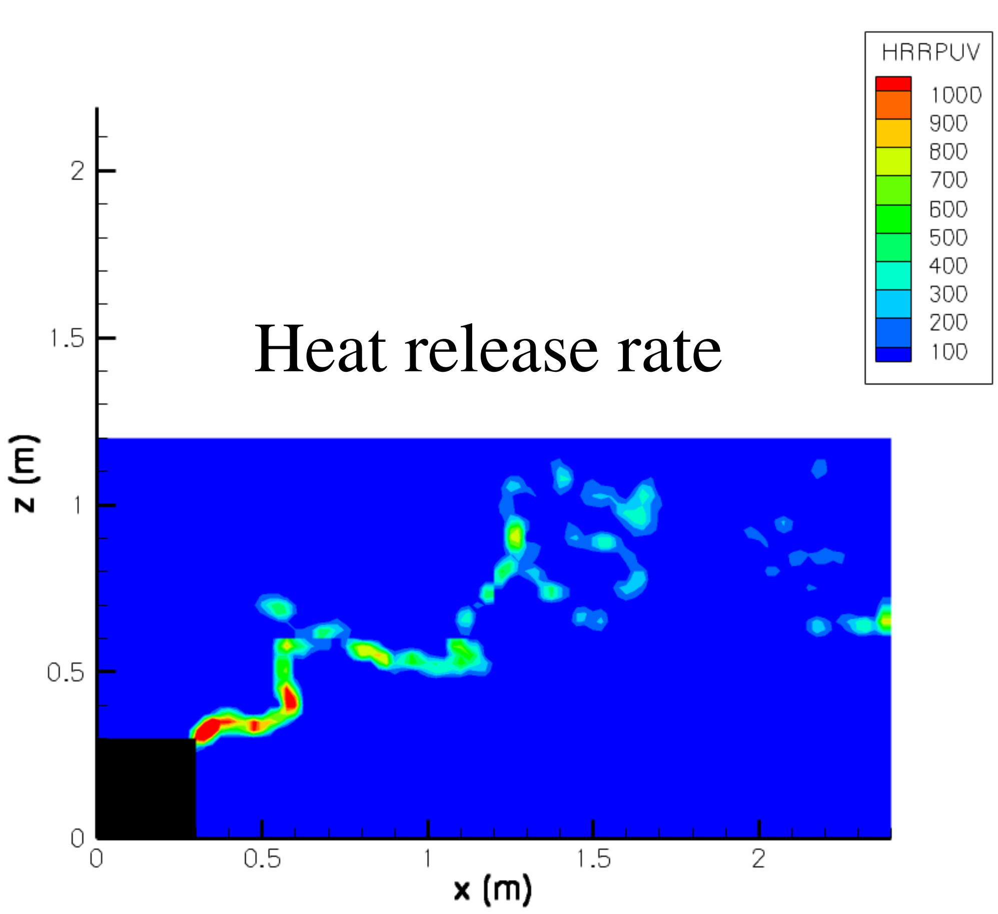


Validation Tests: Simulation of Backdraft

- Phase 2: diffusion flame at the vent (duration ~ 40s)



time t = 31 s after hatch opening



time t = 40 s after hatch opening
(extinction due to fuel depletion)

Conclusion

- A partially-premixed combustion (PPC) model has been implemented into FDS. The PPC formulation is based on:
    - A mixture fraction model (featuring a vitiated air flame extinction capability) to describe non-premixed combustion
    - A reaction progress variable model to describe premixed combustion
    - A coupling interface based on the concept of a flame index
- The performance of the PPC model has been evaluated in a series of verification tests (*e.g.* laminar flame propagation in homogeneous/inhomogeneous fuel-air mixtures; transient ignition followed by a deflagration/diffusion-flame sequence inside a closed compartment)
- *Current work*: validation tests based on comparisons with experimental data (indoor backdraft events; large-scale outdoor LNG fires)