Direct Numerical Simulations of Nonpremixed Flame Quenching by Fine Water Droplets

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Diffusion Flame Extinction

- **Extinction Mechanisms:**
  - ***Aerodynamic quenching*: flame weakening due to attenuation of reactivity as a result of reduced flame residence time**

$$\chi_{st} \geq \chi_{st,ext}^{ref}$$

  - ***Thermal quenching*: flame weakening due to heat losses**
    - **Convection/conduction to the walls**
    - **Radiative heat loss**
    - **Dilution (e.g. air vitiation)**
    - **Water evaporation**

$$\chi_{st} \geq \underbrace{\chi_{st,ext}}_{\text{critical value}} = \underbrace{\chi_{st,ext}^{ref}}_{\text{critical value at reference conditions}} \times \exp\left(-T_a\left(\frac{1}{T_{st}} - \frac{1}{T_{st,ext}^{ref}}\right)\right)$$

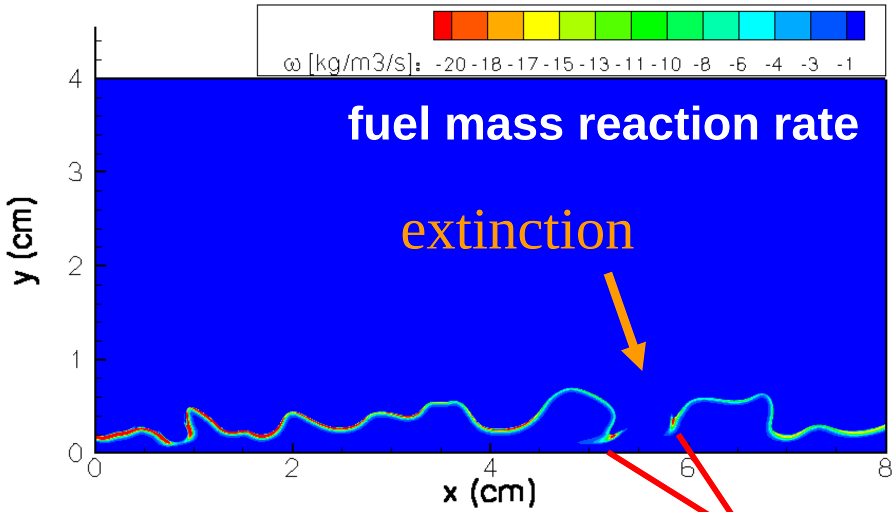
: Wang & Trouvé (2006) *Combustion and Flame*

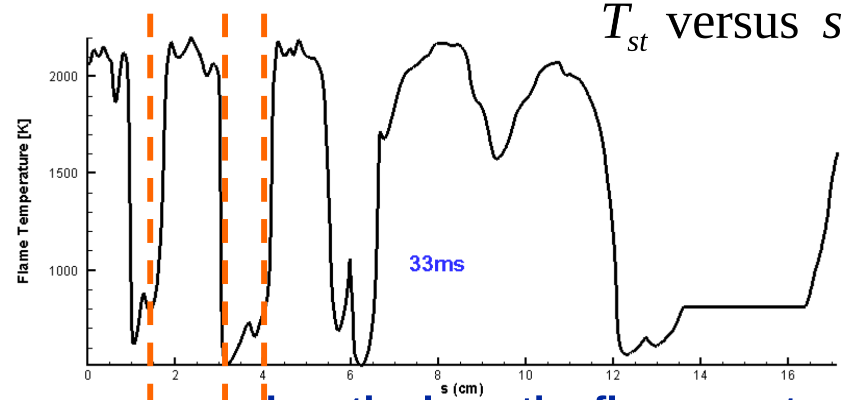
Modified extinction criterion for flame-wall interaction

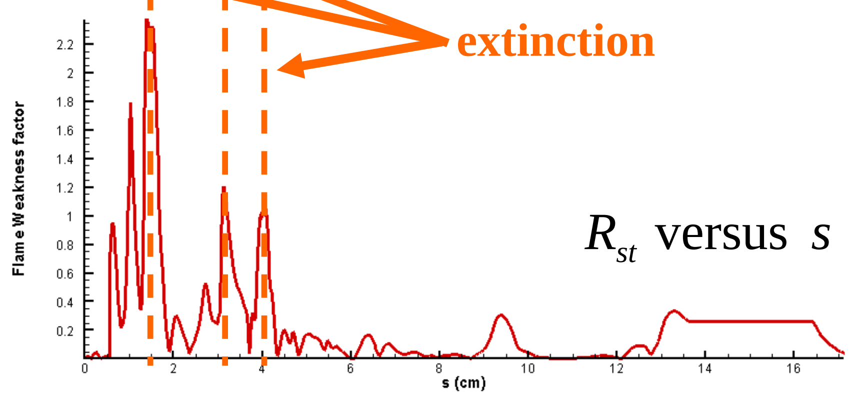
Flame-Wall Interaction

Narayanan & Trouve (2007) – See also CP11 "Soot and Radiation"

- Non-premixed C_2H_4-air turbulent jet diffusion flame near a wall







Extinction criterion

$$R = \frac{\chi_{st}}{\chi_{st,ext}} = \frac{\chi_{st}}{\chi_{st,ext}^{ad}\exp(\beta H)} \geq 1$$

Flame weakness factor — **Wall cooling factor**

$$\beta = \frac{T_a(T_{st}^{ad} - T^{\infty})}{(T_{st}^{ad})^2}$$ **Zeldovich number**

$$H = \frac{c_p(T - T^{\infty})}{\Delta H_f}\left(\frac{1}{Y_F^{\infty}} + \frac{1}{(Y_{O_2}^{\infty}/r_s)}\right) + \frac{Y_F}{Y_F^{\infty}} + \frac{Y_{O_2}}{Y_{O_2}^{\infty}} - 1$$

Excess enthalpy (< 0)

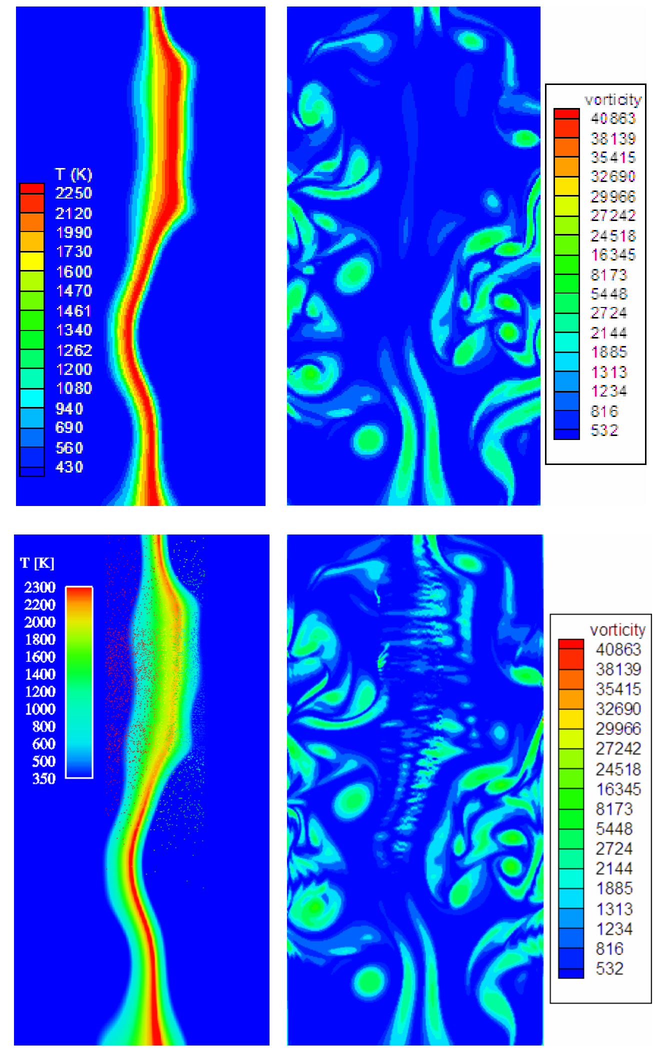
Objectives

Laminar/Turbulent Nonpremixed Flame Extinction by Water Spray

DOE INCITE 2007 (U. Michigan, U. Maryland, U. Wisconsin)

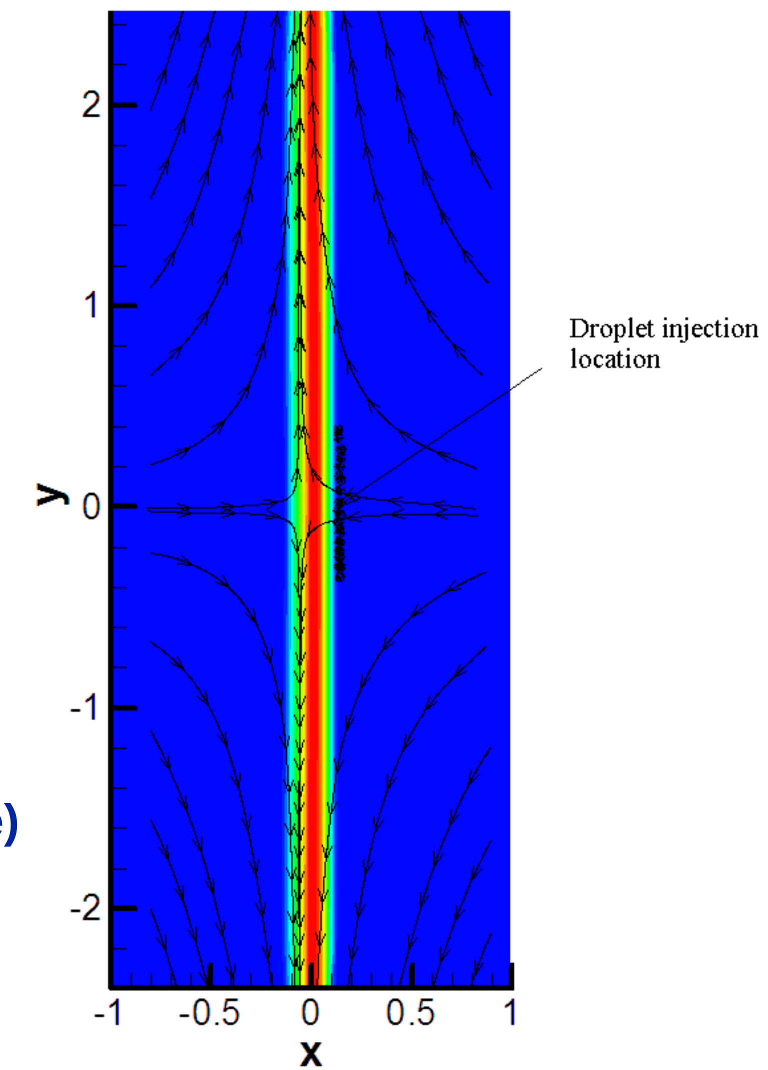
(Innovative and Novel Computational Impact on Theory and Experiment)

- **Science Issues**
  - **Extinction by flame cooling due to spray**
  - **Strain- & spray-induced quenching**
  - ***Unified extinction criteria accounting for heat/radical losses due to water spray evaporation***
- **High-fidelity simulation to demonstrate advanced physical submodels**
  - **Optically thick gas and soot radiation**
  - **Lagrangian spray model**
  - **Improved characteristic boundary conditions**
- **Three-dimensional counterflow simulation (in progress)**
  - **Rectangular Cartesian coordinate**
  - **Domain size ≈ 10cm^3, 10 million grid points, physical time ≈ 20ms**
  - **Re ≈ 100, Da ≈ 3-4, strain rate ≈ 1000s^{-1}**



Model Configuration

- 2-D Counterflow Nonpremixed flame
  - High-order finite-difference (S3D)
  - Modified NSCBC at inflow/outflow boundaries
  - Lagrangian spray model (Rutland)
  - Ethylene vs. air (DRG mechanism, Lu & Law)
  - Gray gas radiation, discrete ordinate method
- Computational Parameters
  - Domain size: 5cmx2cm (800^2 grid points)
  - $\chi_{st} = 20\ s^{-1} \sim 0.4\chi_{st,ext}$
  - Homogeneous turbulence injected at the inlet ($u'/U = 2.0$, $L_{11} = 1.25$cm)
- Spray parameters
  - Spherical, monodisperse (d=40 μm,mist regime)
  - Injected 1.4mm from the flame at the local gas velocity
  - Loading: 15%/32% /80% of local heat release



Unified Extinction Criterion

- Excess enthalpy for multi-component systems

$$H = \frac{\Delta h_{th}(T, Y_k)}{h_F^0 \times Z_{st} + h_O^0 \times (1 - Z_{st}) - (\sum_k h_k^0 Y_k^{eq}(Z_{st}))}$$

$$\Delta h_{th}(T, Y_k) = (\int_{T_0}^{T} c_p dT) - \underbrace{[(\int_{T_0}^{T_F} c_{p,F} dT) \times Z + (\int_{T_0}^{T_O} c_{p,O} dT) \times (1 - Z)]}_{\text{mixing}} - \underbrace{[h_F^0 \times Z + h_O^0 \times (1 - Z) - h^0]}_{\text{heat release}}$$

$$c_p = (\sum_k c_{p,k} Y_k) \; ; \; c_{p,F} = (\sum_k c_{p,k} Y_{k,F}) \; ; \; c_{p,O} = (\sum_k c_{p,k} Y_{k,O})$$

$$h^0 = (\sum_k h_k^0 Y_k) \; ; \; h_F^0 = (\sum_k h_k^0 Y_{k,F}) \; ; \; h_O^0 = (\sum_k h_k^0 Y_{k,O})$$

  - ***H* = 0 accounts for effects of heat loss and differential diffusion**

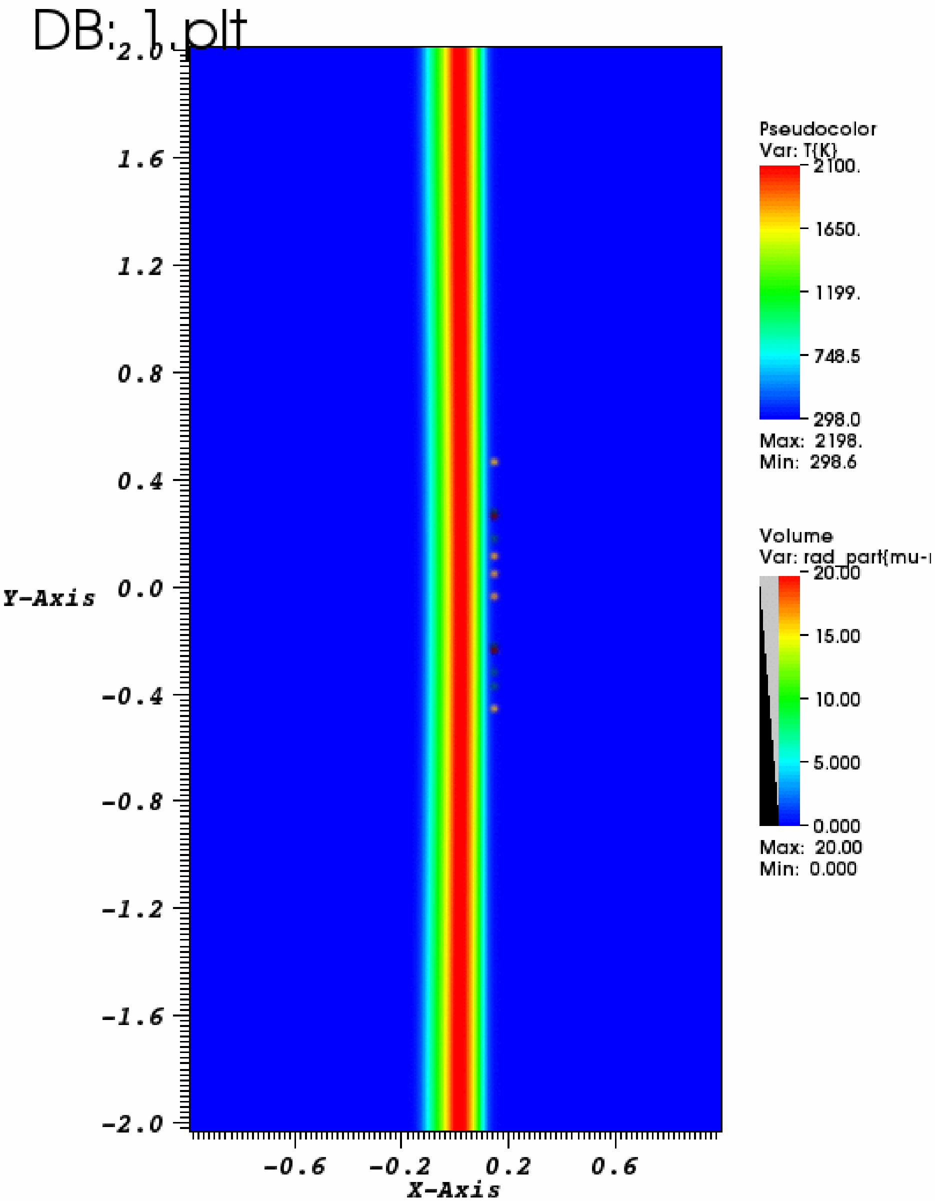
- Extinction Criterion:

$$R = \frac{\chi_{st}}{\chi_{st,ext}} = \frac{\chi_{st}}{\chi_{st,ext}^{ad} \exp(\beta H)} \geq 1$$

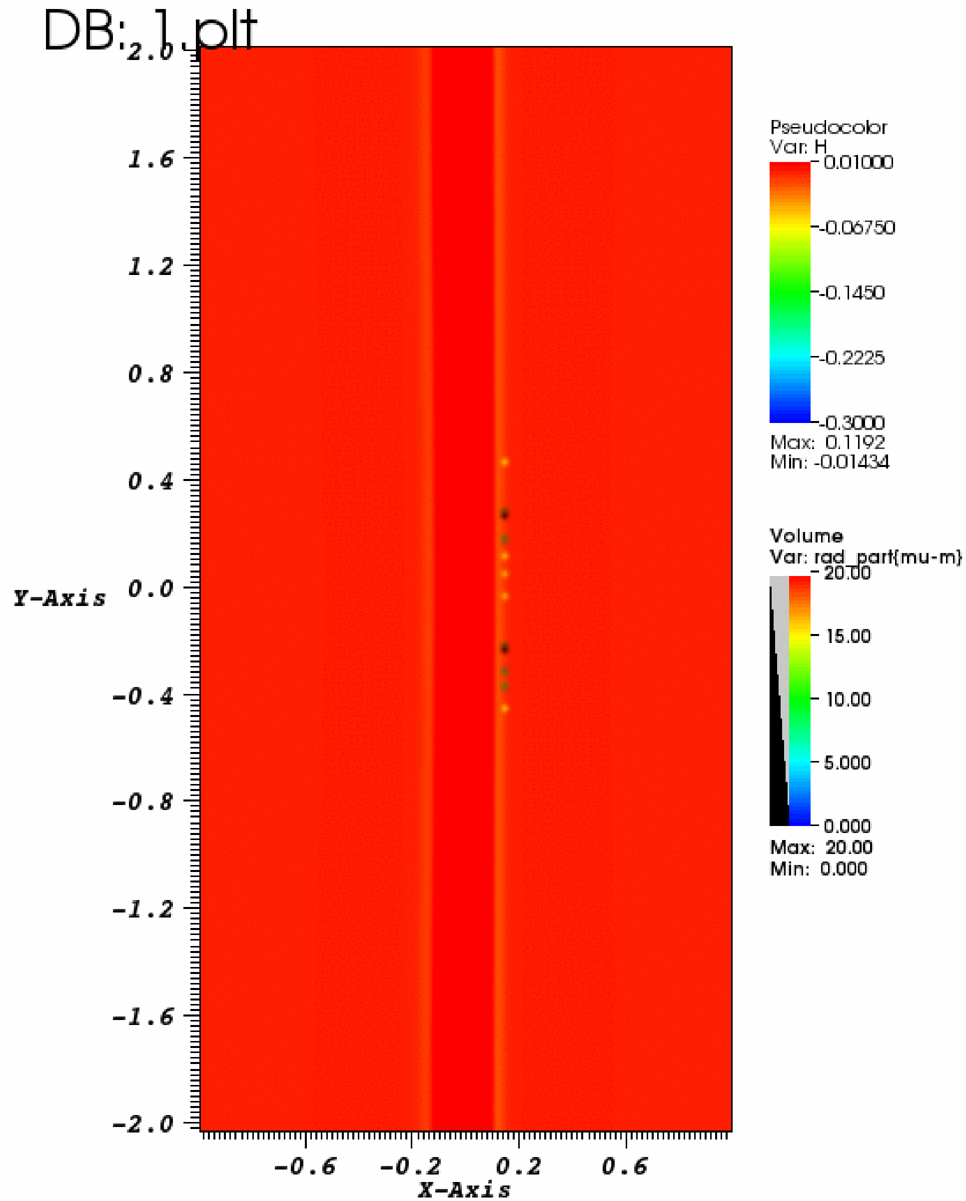
where the Zeldovich number (β) is determined based on Law *et al.*

$$T_a = \frac{E_a}{R^0} = -2 \frac{\partial \ln f^\circ}{\partial (1/T_b^\circ)} \quad (f^\circ = \rho_u S_L)$$

Laminar Flame Results (32% loading)

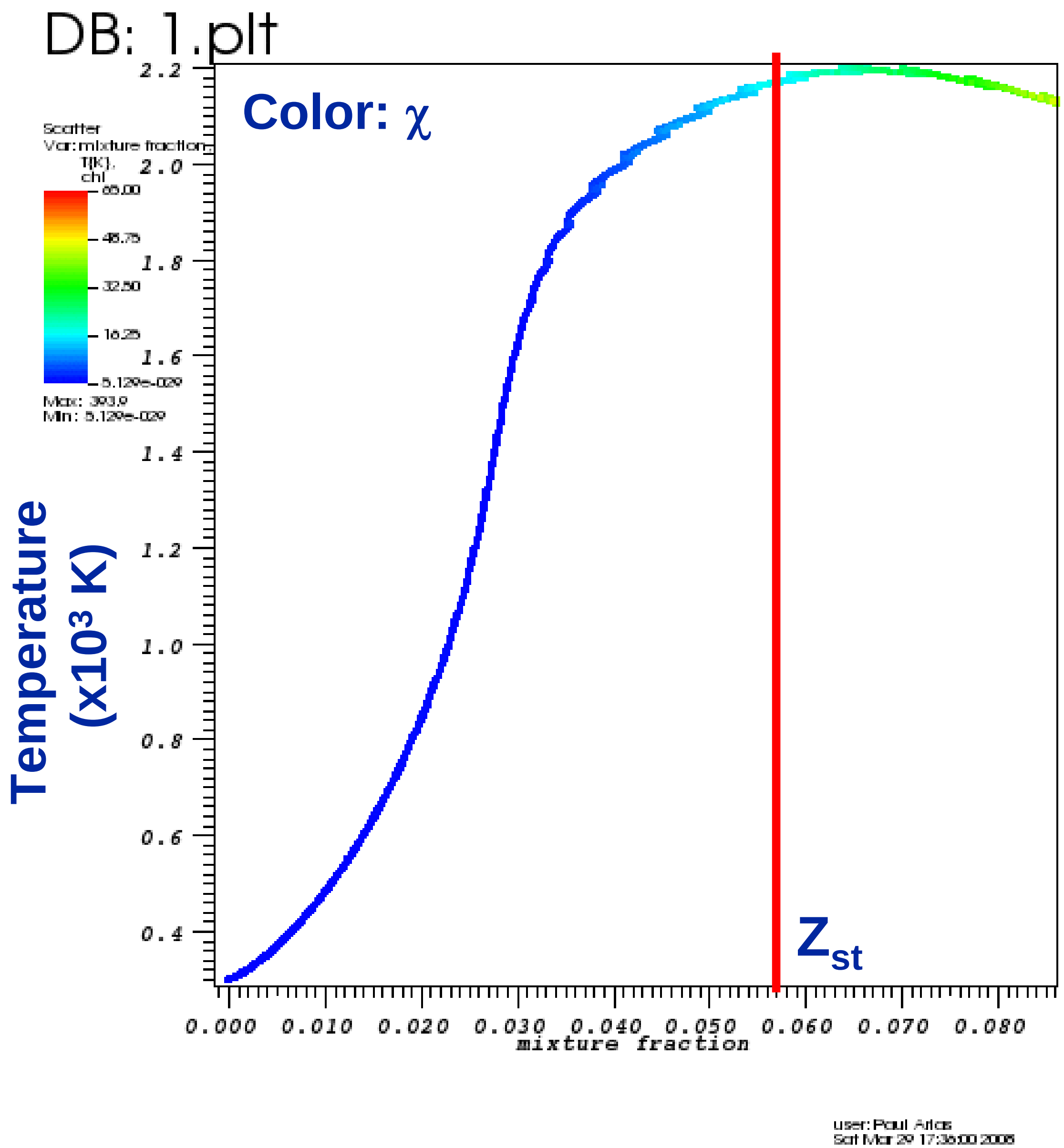


Temperature

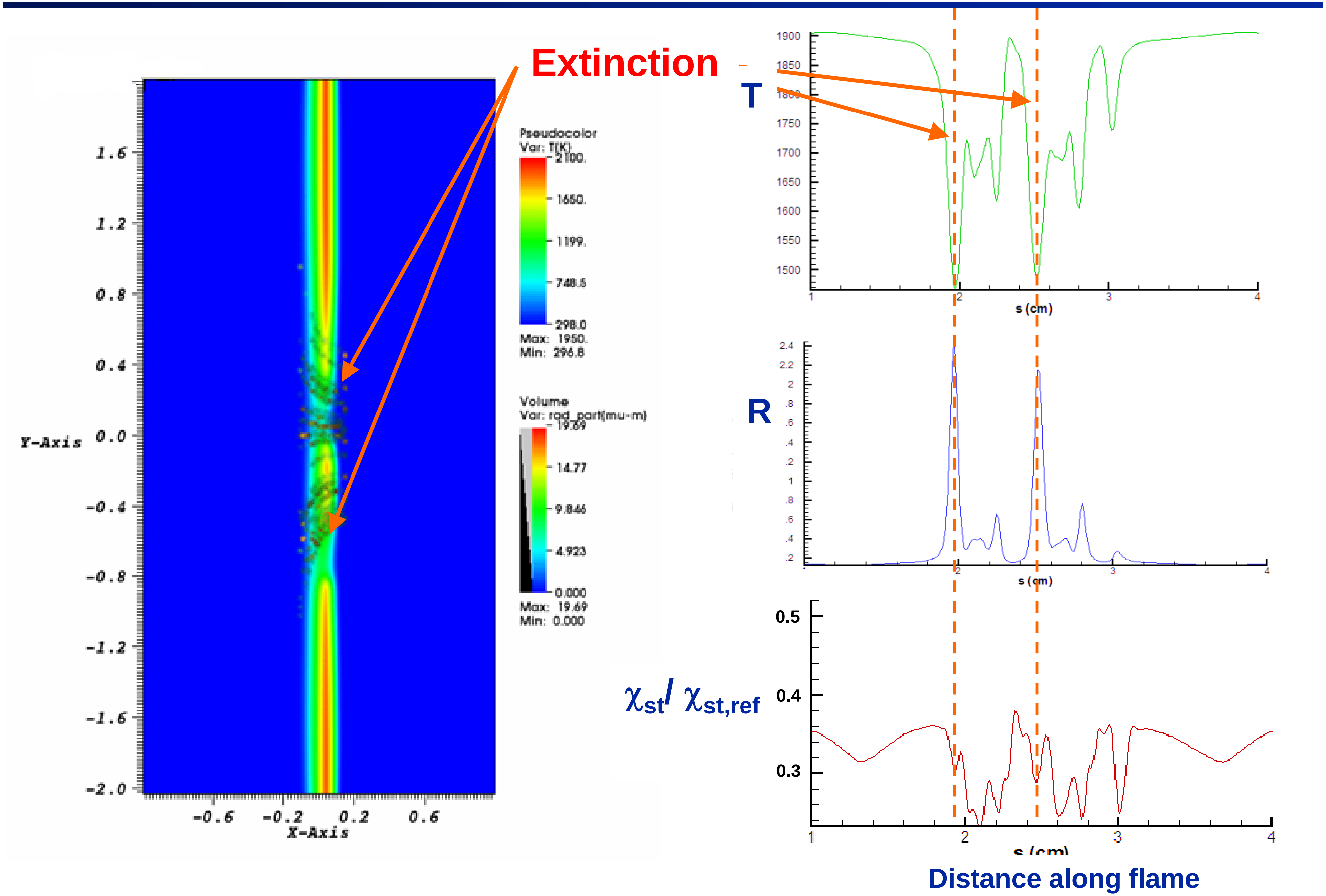


Excess enthalpy variable

Laminar Flame Results (32% loading)

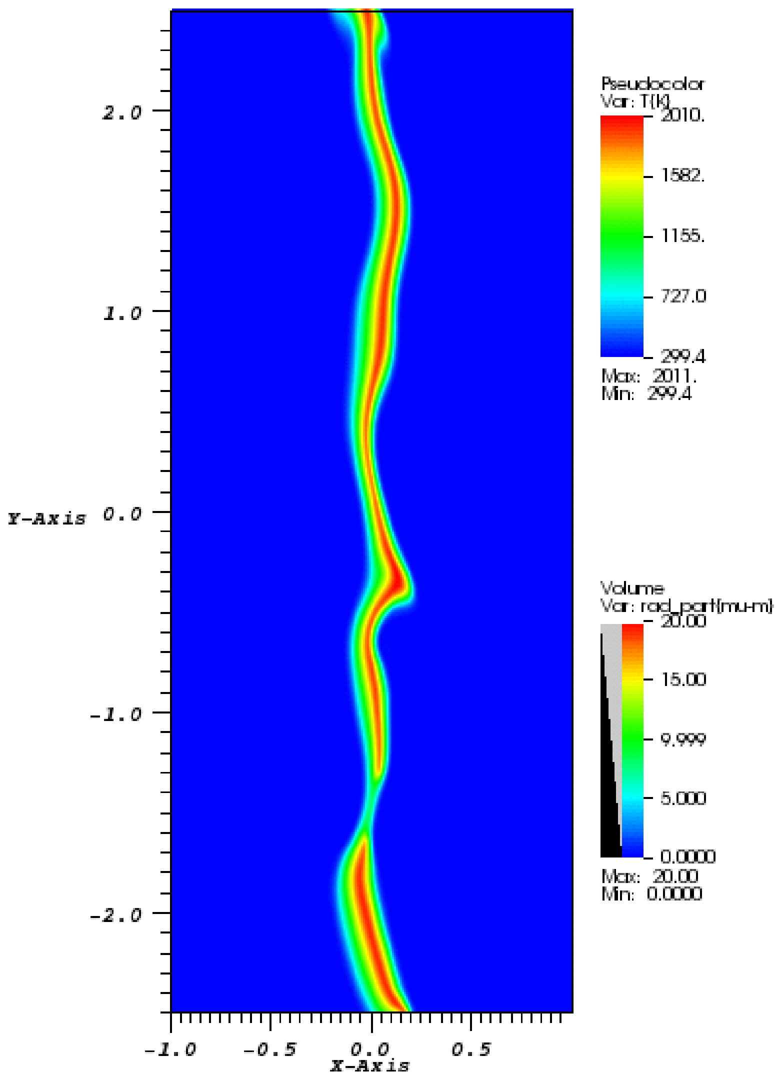


Extinction Analysis

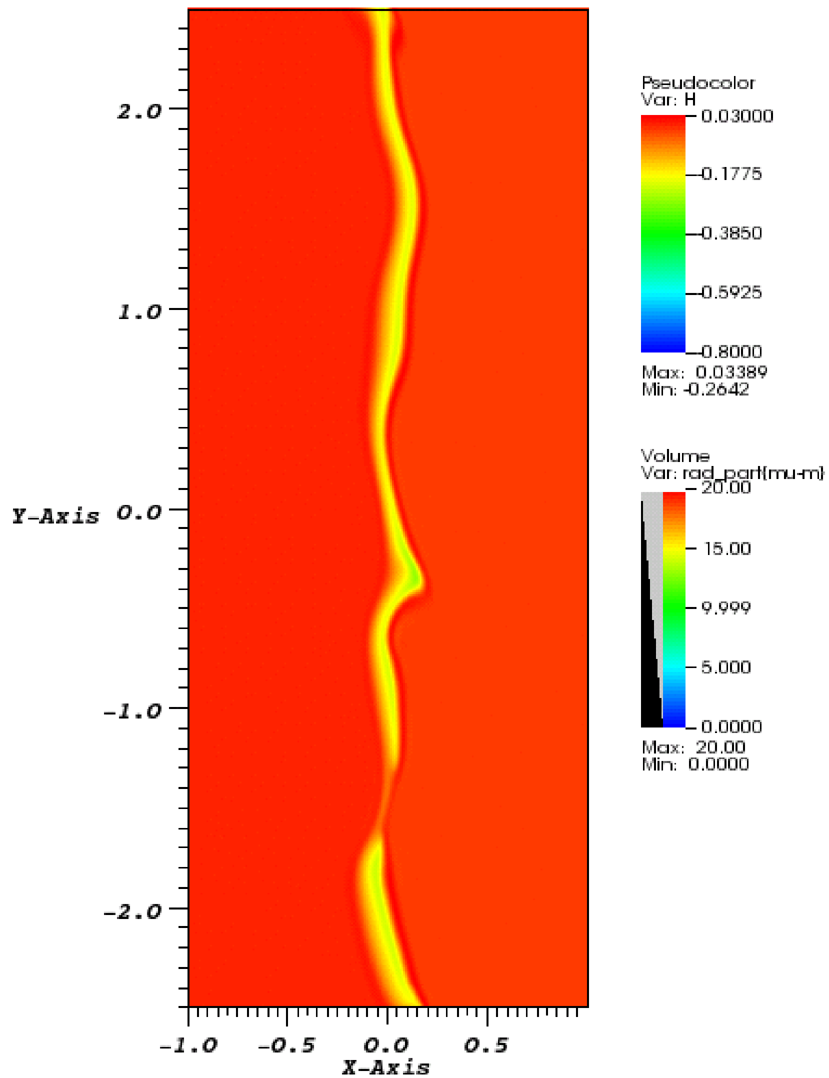


Turbulent Flames with Spray

Temperature

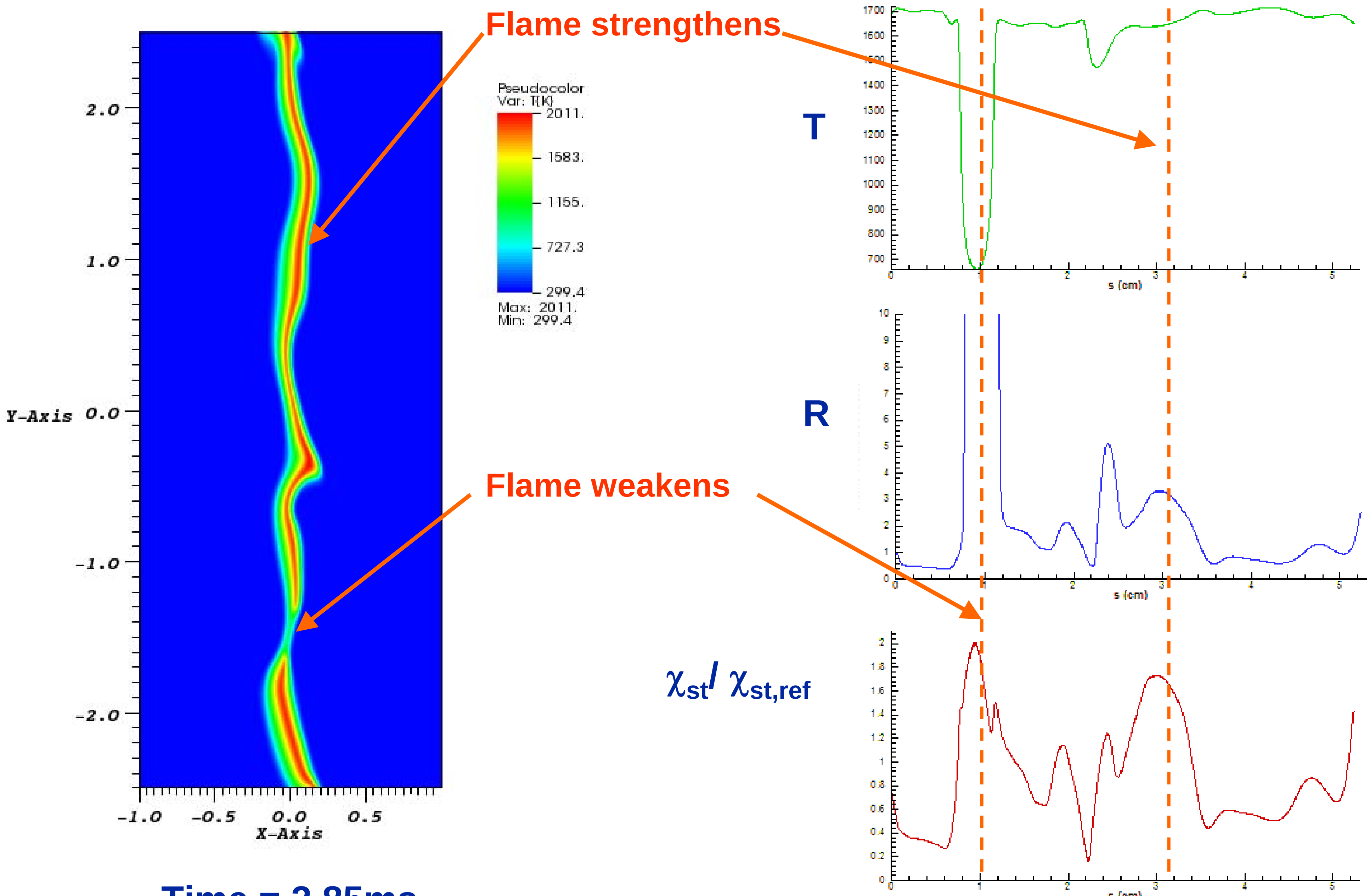


Temperature



Time duration 2.85ms-4.54ms

Turbulence without spray

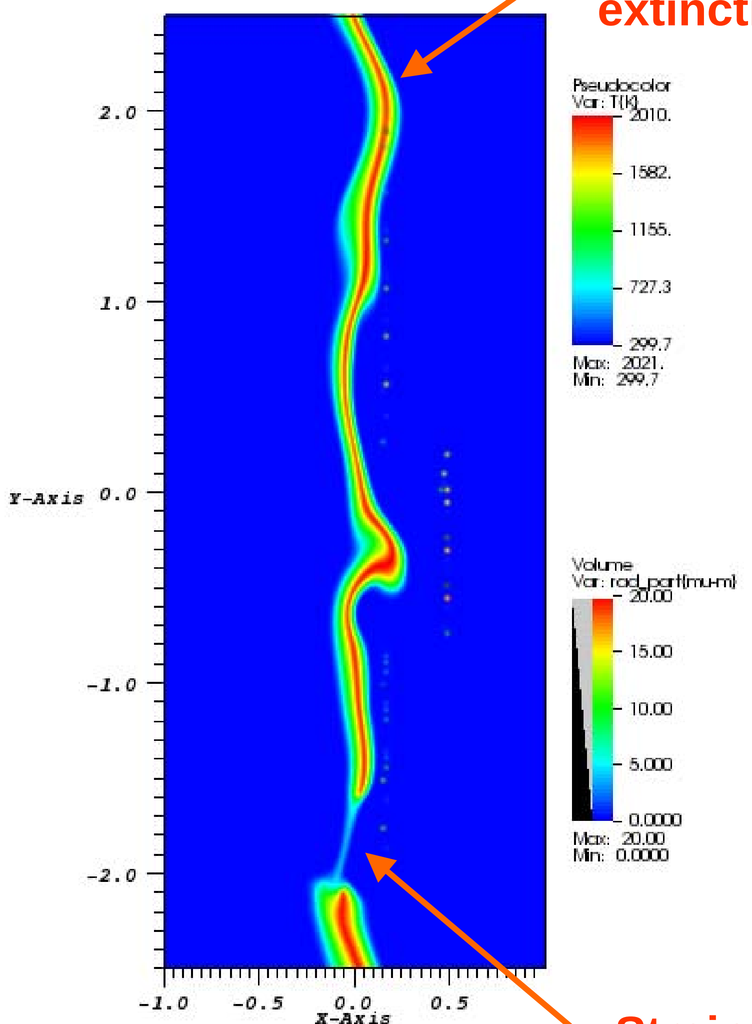


Time = 2.85ms

Distance along flame

Turbulence with spray

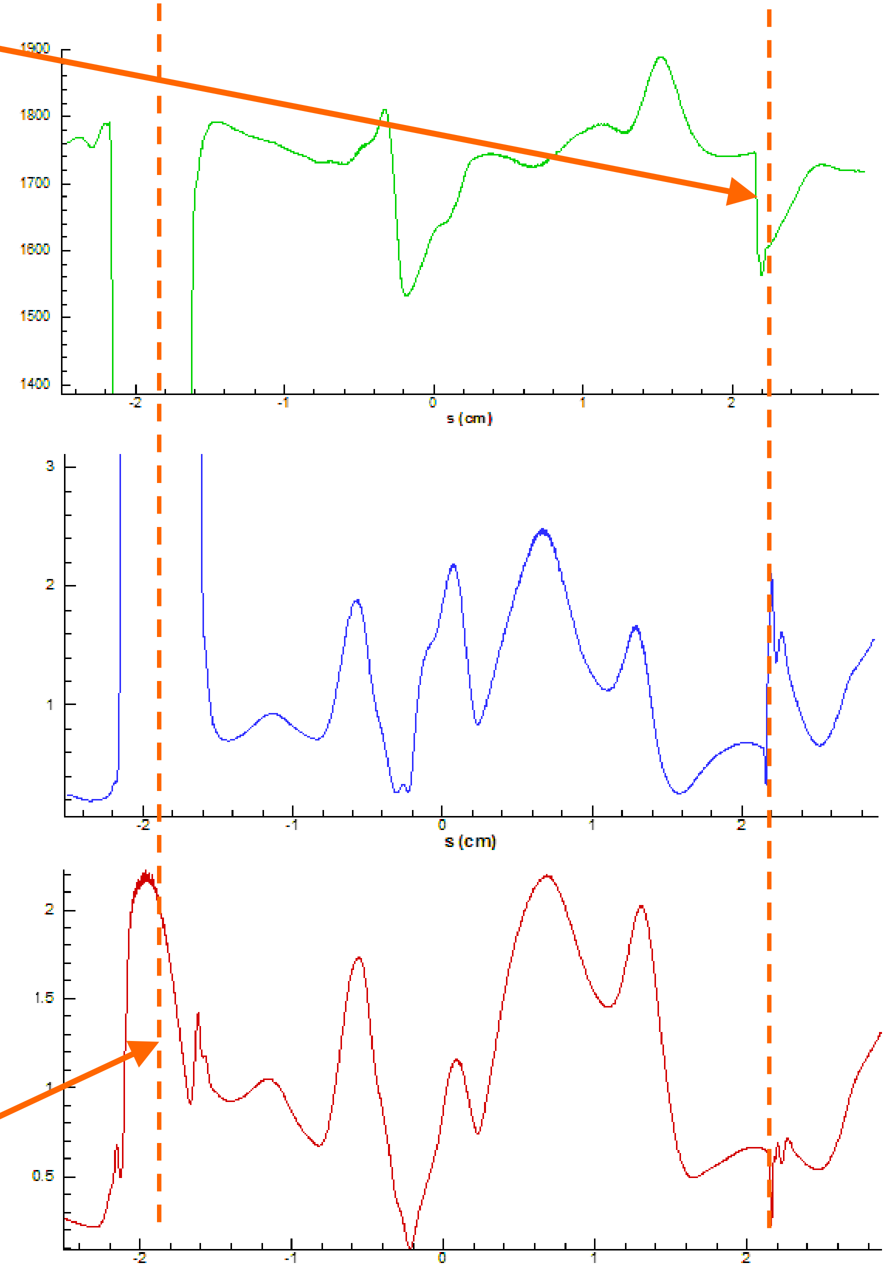
Spray-induced extinction



T

R

$\chi_{st} / \chi_{st,ref}$



Strain-induced extinction

Time = 4.1ms

Distance along flame

Summary & Future Work

- Modified extinction criterion was defined based on excess enthalpy variable.
- The criterion was extended for multi-component, detailed chemistry system by using the effective activation energy.
- Preliminary results suggested that the excess enthalpy variable properly accounts for the flame extinction caused by various flame weakening mechanisms.
- Additional parametric studies are needed to assess the effects of
  - Spray loading, size distribution, injection velocity
  - Strong transients
  - Differential diffusion