Radiation-Driven Flame Extinction in Fires

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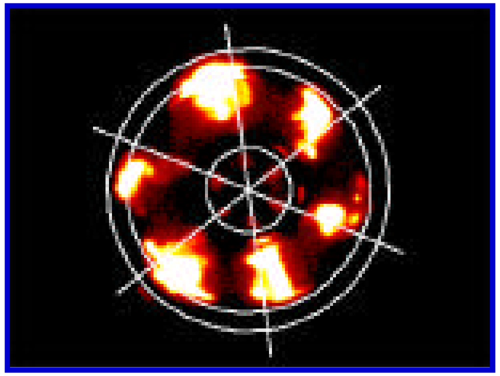
Diffusion Flame Extinction

- Motivation:
  - *Combustion science*
    - Flame extinction has a significant impact on the performance of non-premixed combustion systems. It determines in part the turbulent flame structure and the levels of pollutant emission (*NOx*, *CO*, soot).
  - **Engine applications**
    - Extinction due to high turbulence intensities in IC- or gas-turbine engines (momentum-driven, high-Reynolds number flames)

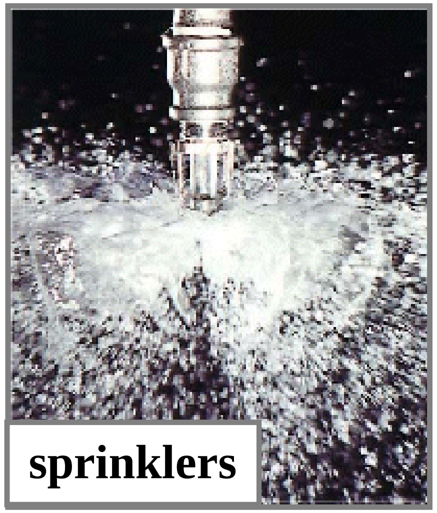


Diesel engine

Diffusion Flame Extinction

- Motivation:
  - **Fire applications**
    - Extinction due to air vitiation in under-ventilated compartment fires or large-scale pool fires (buoyancy-driven, moderate-Reynolds number flames)
    - Extinction due to inert gaseous agents or water sprays in fire suppression applications

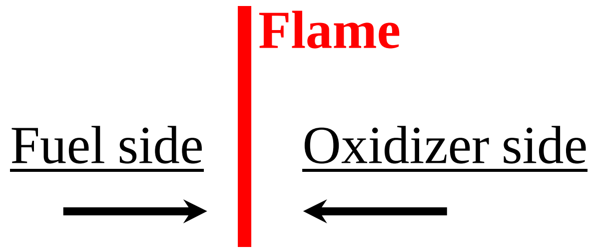
pool fire



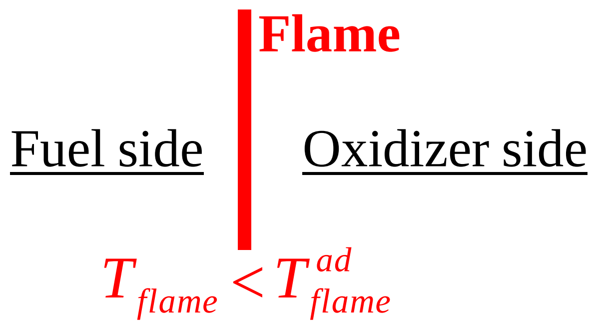
sprinklers

Diffusion Flame Extinction

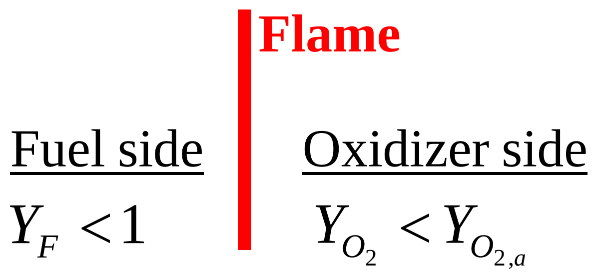
- Different flame extinction phenomena:
  - *Aerodynamic quenching*: flame weakening due to flow-induced perturbations (*i.e.* decrease in flame residence time)



  - *Thermal quenching*: flame weakening due to heat losses (*e.g.* heat losses by convection/conduction to walls, by thermal radiation, by water evaporative cooling in fire suppression applications)



  - *Quenching by dilution*: flame weakening due to changes in fuel stream or oxidizer stream composition (*e.g.* air vitiation in under-ventilated fires)



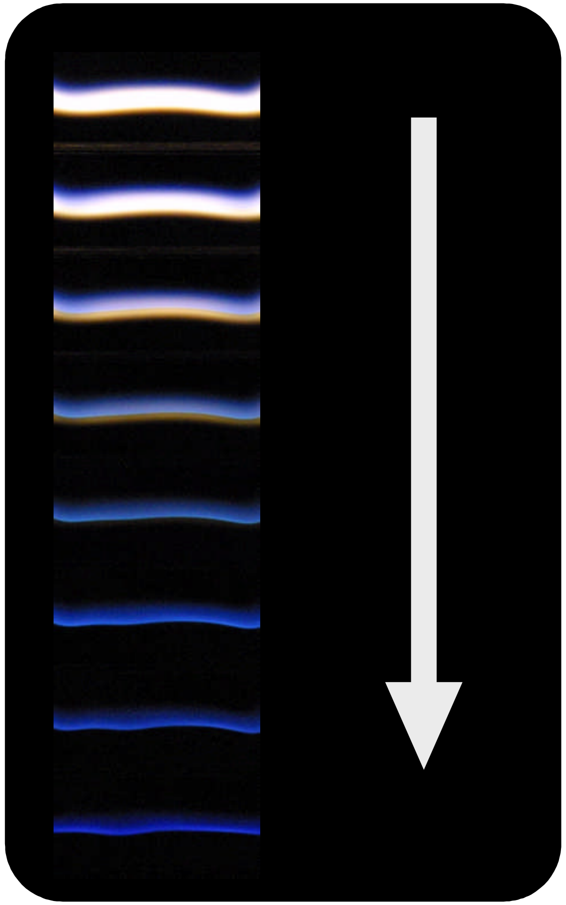
Diffusion Flame Extinction

- Different flame extinction phenomena:
  - ➢ Single criterion to predict extinction (laminar flame theory):

$$\boxed{Da = \frac{\tau_{mixing}}{\tau_{chemical}} \leq Da_{critical}}$$

$$Da = \frac{\tau_{mixing}}{\tau_{chemical}} \sim \frac{(1/\chi_{st})}{\exp(T_a/T_{st})}$$

  - ➢ Two fundamental limits:
    - **Fast mixing limit**: Da is small because χ_{st} is large (*e.g.*, aerodynamic quenching)
    - **Slow mixing limit**: Da is small because T_{st} is small (*e.g.*, thermal or dilution quenching)

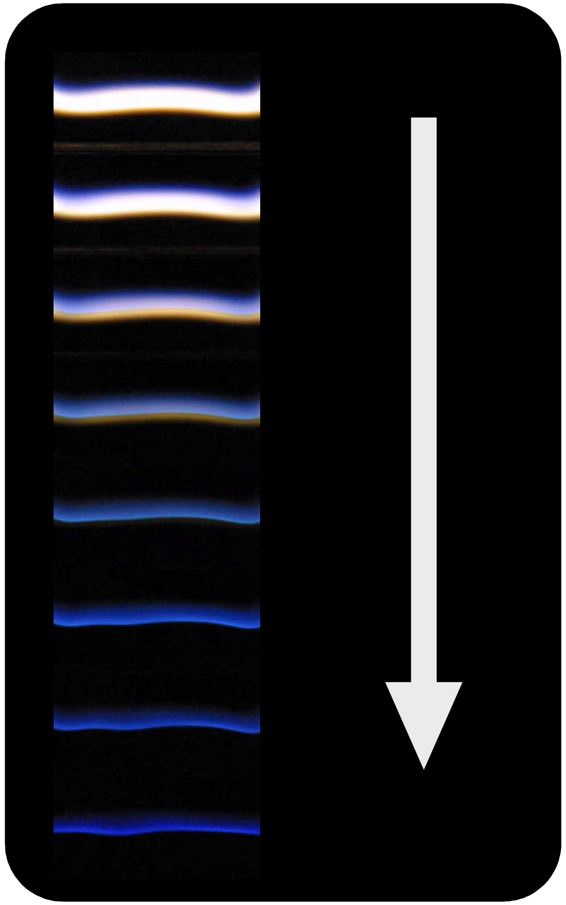


Diffusion Flame Extinction

- Different flame extinction phenomena:
  - **Fast mixing limit**: also called *kinetic* extinction
  - Criterion for extinction:

$$\boxed{\chi_{st} \geq \chi_{critical}}$$

  - Sources: aerodynamic quenching
    - Liñán (1974) *Acta Astronautica*
    - Williams (1985) "*Combustion Theory*"
    - Peters (2000) "*Turbulent Combustion*"

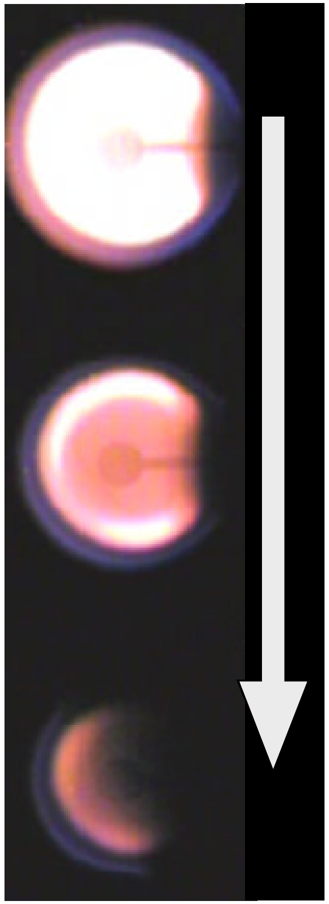


Diffusion Flame Extinction

- Different flame extinction phenomena:
  - **Slow mixing limit**: also called *radiation* extinction
  - Criterion for extinction:

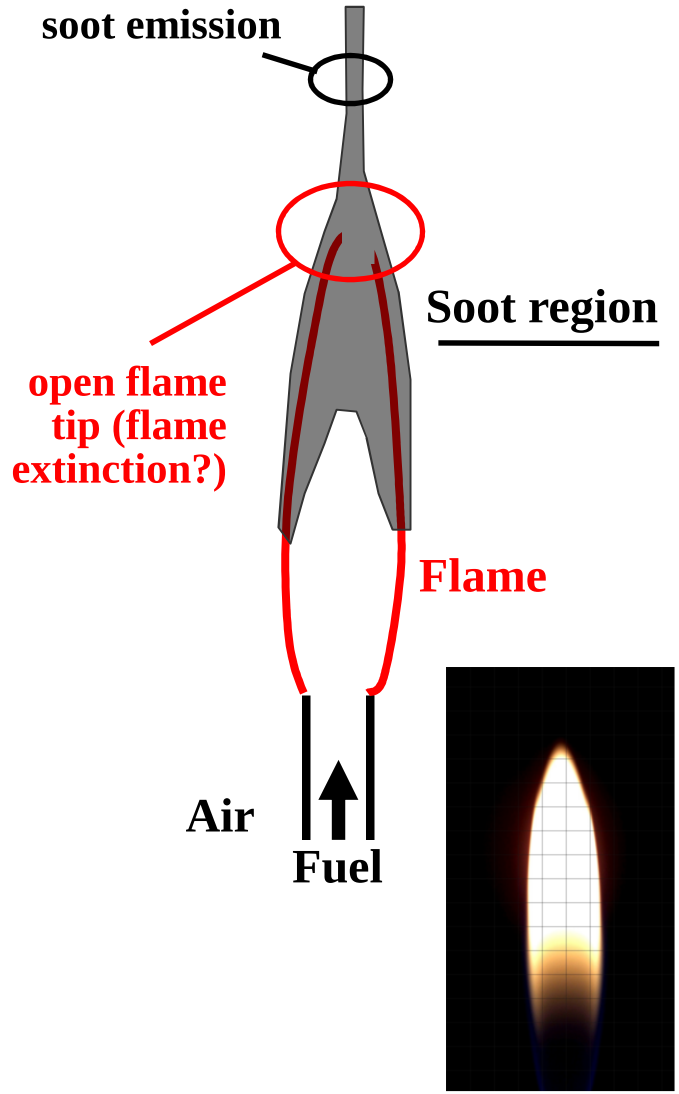
$$\boxed{\Gamma_{rad} \geq \Gamma_{critical}} \qquad \boxed{\chi_{st} \leq \chi^{*}_{critical}}$$

  - <u>Sources</u>: thermal quenching in microgravity combustion
    - Sohrab, Liñán & Williams (1982) *Combustion Science and Technology*
    - T'ien (1986) *Combustion and Flame*
    - Chao, Law & T'ien (1990) *Proceedings Combustion Institute* **23**
    - Bedir & T'ien (1998) *Combustion and Flame*



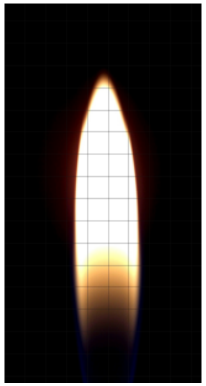
Diffusion Flame Extinction

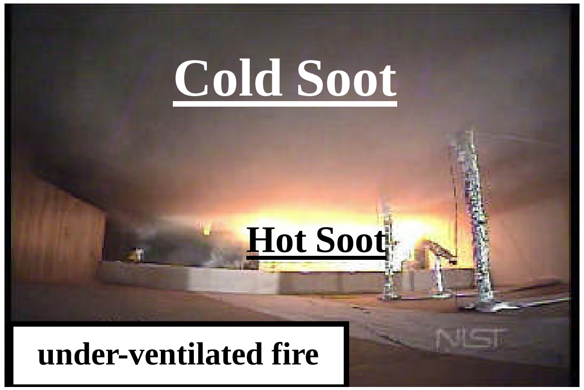
- Relation between radiation extinction and soot emission/smoke point studies:
  - *Unclear*: many recent studies of radiation extinction correspond to one-dimensional flames that are soot-free at the extinction limit
  - *But*: past studies of the smoke point (SP) of laminar jet diffusion flames suggest that SP is controlled by the flame luminosity; hence, SP may be interpreted as a radiation extinction event
  - Source:
    - Markstein, de Ris (1984) *Proceedings Combustion Symposium*



Objectives

- Study mechanisms responsible for diffusion flame extinction in laminar and turbulent flames (focus on conditions relevant to fire applications)
  - ➢ Establish flame extinction criterion; construct flammability map(s)
- Tools:
  - ➢ Asymptotic analysis of extinction limits of laminar counter-flow diffusion flames exposed to different levels of radiant losses
  - ➢ Direct Numerical Simulations (DNS) of laminar counter-flow and co-flow diffusion flames, and of turbulent diffusion flames
- Explore relationship between flame extinction and soot emission





Numerical approach

- Use direct numerical simulation (DNS)
  - Leverage DOE-sponsored SciDAC collaboration on DNS solver called S3D – *Sandia Ntl. Laboratories* (J.H. Chen), *Univ. Michigan* (H.G. Im)

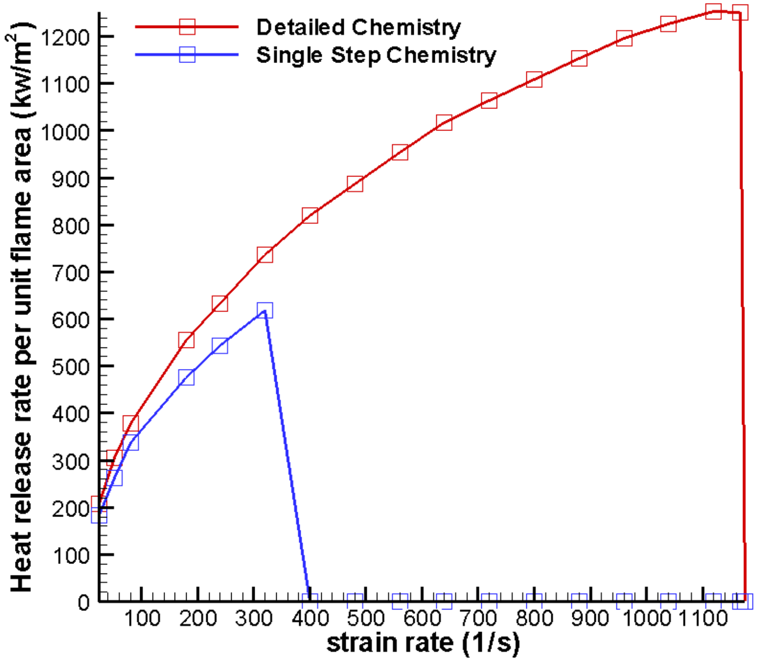
- DNS solver S3D
  - Navier-Stokes solver; fully compressible flow formulation
  - High-order methods: 8th order finite difference; 4th order explicit Runge-Kutta time integrator
  - Characteristic-based boundary condition treatment (NSCBC)
  - Structured Cartesian grids
  - Parallel (MPI-based, excellent scalability)
  - <u>Flame modeling</u>: detailed fuel-air chemistry (CHEMKIN-compatible); simplified soot formation model; thermal radiation model (Discrete Ordinate/Discrete Transfer Methods); Lagrangian particle model to describe dilute liquid sprays

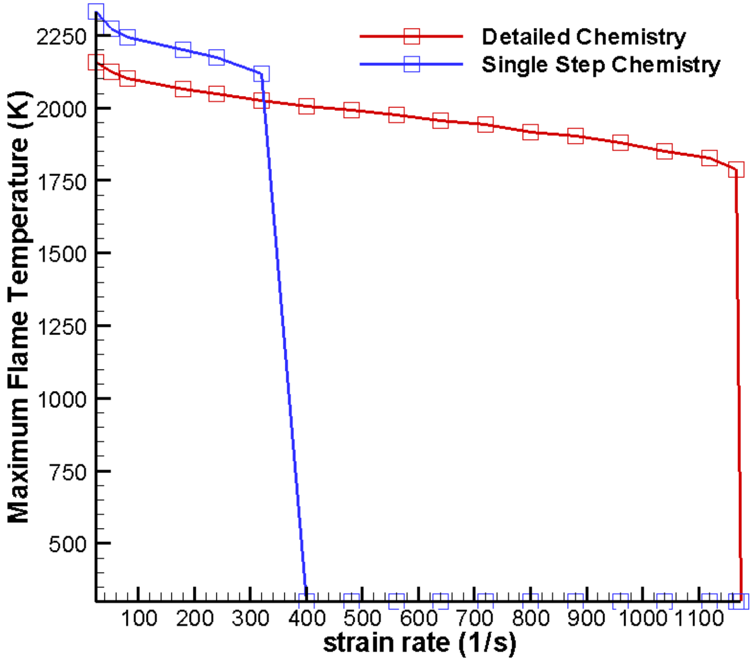
Flame Modeling

- **Combustion model:** single-step chemistry, ethylene-air combustion (Westbrook & Dryer, 1981)

$$\dot{\omega}_F = B_{RR}\left(\frac{\rho Y_F}{M_F}\right)^p \left(\frac{\rho Y_{O_2}}{M_F}\right)^q \exp\left(-\frac{T_a}{T}\right)$$

  - Counter-flow flame: comparison of laminar flame response to changes in strain rate for single-step and detailed chemistry





Flame Modeling

- **Soot formation model:** a phenomenological approach (Moss *et al.*, Lindstedt *et al.*)
  - Two-variable model; empirical description of fundamental soot formation processes (nucleation, surface growth, coagulation, oxidation)
  - Model parameters are fuel-dependent
  - No PAH chemistry
  - Monodispersed soot particle size distribution

$$\frac{\partial}{\partial t}(\rho Y_{soot}) + \frac{\partial}{\partial x_i}(\rho u_i Y_{soot}) = -\frac{\partial}{\partial x_i}(\rho Y_{soot} V_{t,i}) + \frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc}\frac{\partial Y_{soot}}{\partial x_j}\right) + \dot{\omega}'''_{s,nucleation} + \dot{\omega}'''_{s,\substack{surface\\growth}} - \dot{\omega}'''_{s,oxidation}$$

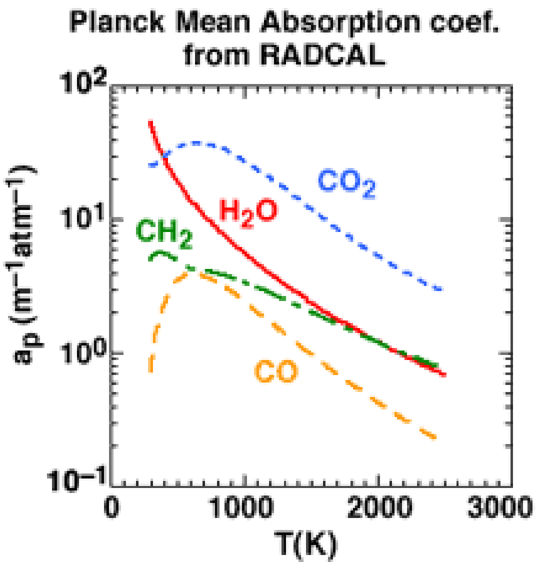
$$\frac{\partial}{\partial t}\left(\frac{n_{soot}}{N_A}\right) + \frac{\partial}{\partial x_i}\left(u_i \frac{n_{soot}}{N_A}\right) = -\frac{\partial}{\partial x_i}\left(\frac{n_{soot}}{N_A} V_{t,i}\right) + \frac{\partial}{\partial x_j}\left(\frac{\mu}{\rho Sc}\frac{\partial}{\partial x_j}\left(\frac{n_{soot}}{N_A}\right)\right) + \dot{\omega}'''_{n,nucleation} - \dot{\omega}'''_{n,coagulation}$$

Flame Modeling

- **Thermal radiation transport model:** non-scattering, gray gas assumption; Discrete Transfer Method (Lockwood & Shah, 1981)

  - Radiative transfer equation

$$\frac{dI}{ds} = \underbrace{\kappa(\sigma T^4/\pi)}_{\text{Emission}} - \underbrace{\kappa I}_{\text{Absorption}}$$



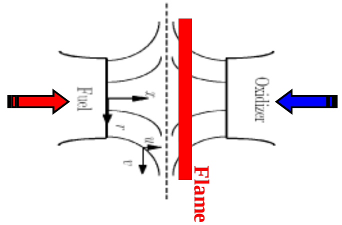
  - Mean absorption coefficient [m^{-1}]

$$\kappa = p(x_{H_2O}a_{H_2O} + x_{CO_2}a_{CO_2}) + \kappa_{soot}$$

    - $a_{p,i}$ is the Planck mean absorption coefficient for species i [m^{-1} atm^{-1}] and is obtained from tabulated data (TNF Workshop web site)
    - κ_{soot} is the soot mean absorption coefficient [m^{-1}]

$$\kappa_{soot} = C_{soot} \times f_v T = C_{soot} \times (\rho Y_{soot}/\rho_{soot})T \longrightarrow C_{soot} = 1817\ \mathrm{m^{-1}K^{-1}}$$

AEA Analysis



- Classical activation energy asymptotic (AEA) analysis
  - Mass density variations handled with Howarth transformation

$$\xi = \int_0^x (\rho / \rho_2) dx$$

  - Mixture fraction equation and solution (α is strain rate)

$$-\alpha\xi \frac{dZ}{d\xi} = D_2 \frac{d^2 Z}{d\xi^2}$$

$$\Rightarrow \; Z = \frac{1}{2} - \frac{1}{2} \mathrm{erf}\left(\frac{\xi}{\sqrt{2D_2/\alpha}}\right)$$

  - Flame structure given by flamelet equations (in mixture fraction space)

$$-\frac{\chi_{st}}{2} \frac{d^2 T}{dZ^2} = \left(\frac{\Delta H_F}{c_p}\right) \frac{\dot{\omega}_F}{\rho_{st}}$$

AEA Analysis

- Classical decomposition into inner/outer layers
  - Perform asymptotic expansion in terms of small parameter ε

$$\varepsilon = \frac{1}{Ze} = \frac{(T_{st})^2}{T_a}\left(\frac{c_p}{\Delta H_F Y_{F,1}}\right)$$

  - Inner layer problem

$$T = T_{st} - \varepsilon\theta\left(\frac{\Delta H_F Y_{F,1}}{c_p}\right) + O(\varepsilon^2)\ ;\ Z = Z_{st} + \varepsilon\varsigma + O(\varepsilon^2)$$

$$\boxed{\frac{d^2\theta}{d\varsigma^2} = \delta[\theta + \varsigma]^p[\theta - \frac{Z_{st}\varsigma}{(1-Z_{st})}]^q \exp(-\theta)}$$

(δ is a reduced Damkohler number)

$$(d\theta / d\zeta)_{\zeta\to-\infty} = -1\ ;\ (d\theta / d\zeta)_{\zeta\to+\infty} = Z_{st}/(1-Z_{st})$$

AEA Analysis

- AEA flame structure with thermal radiation
  - Temperature decomposition (outer layer problem)

$$T = T_{BS}^{ad} - \Delta T$$

  - Governing equation for temperature deficit due to radiant cooling

$$\alpha \xi \frac{d}{d\xi}(\Delta T) = -D_2 \frac{d^2}{d\xi^2}(\Delta T) - \frac{\dot{q}_{rad}}{\rho c_p}$$

  - Green's function solution

$$\boxed{\Delta T(\xi) = \int_{-\infty}^{+\infty} \frac{\dot{q}_{rad}}{\rho c_p}(\xi^*)\, g(\xi, \xi^*) d\xi^*}$$

  - Consider that chemical reaction zone is thin compared to characteristic radiation length scale ($(\kappa \delta_{reaction}) << 1$): inner layer problem is essentially unchanged

AEA Analysis

- AEA flame structure with thermal radiation
  - Green's function solution

$$\Delta T(\xi) = \int_{-\infty}^{+\infty} \frac{\dot{q}_{rad}}{\rho c_p}(\xi^*)\, g(\xi,\xi^*)\, d\xi^*$$

  - Emitting/absorbing medium (spectrally-averaged gray)

$$\boxed{\dot{q}_{rad} = \kappa(4\sigma T^4 - G)}$$

Planck mean aborption coefficient:

$$\kappa = p(x_{CO_2} a_{CO_2} + x_{H_2O} a_{H_2O}) + C_{soot} \times f_v T$$

Analytical expression for G (as a function of optical depth τ):

$$\boxed{\begin{aligned} G = {} & 2\pi[I_{b,1}E_2(\tau) + I_{b,2}E_2(\tau_R - \tau) \\ & + \int_0^{\tau} I_b(\tau')E_1(\tau - \tau')d\tau' + \int_{\tau}^{\tau_R} I_b(\tau')E_1(\tau' - \tau)d\tau'] \end{aligned}}$$

AEA Analysis

- AEA flame structure with soot
  - Two-equations model for ssot mass fraction and soot number density (Moss *et al.*, Lindstedt *et al.*)

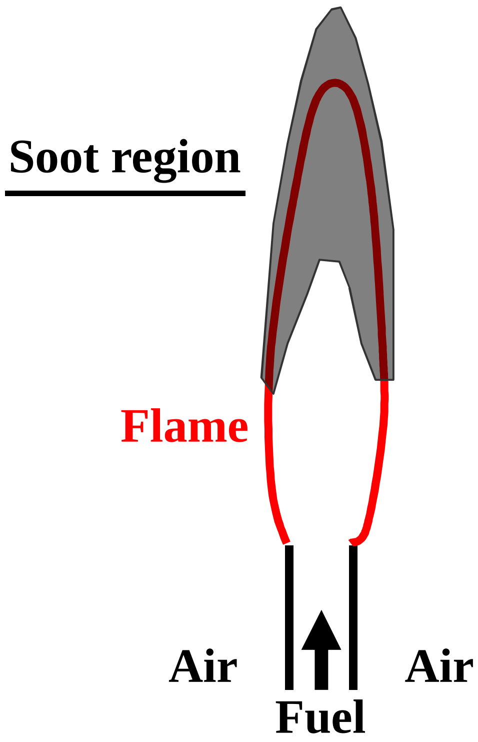
$$\boxed{\begin{aligned}(-\alpha\xi+\bar{V}_t)\frac{dY_{soot}}{d\xi}+\frac{d\bar{V}_t}{d\xi}Y_{soot}&=\frac{\dot{\omega}_{Y_{soot}}}{\rho}\\(-\alpha\xi+\bar{V}_t)\frac{d}{d\xi}\left(\frac{n_{soot}}{\rho N_A}\right)+\frac{d\bar{V}_t}{d\xi}\left(\frac{n_{soot}}{\rho N_A}\right)&=\frac{\dot{\omega}_{n_{soot}}}{\rho}\end{aligned}}$$

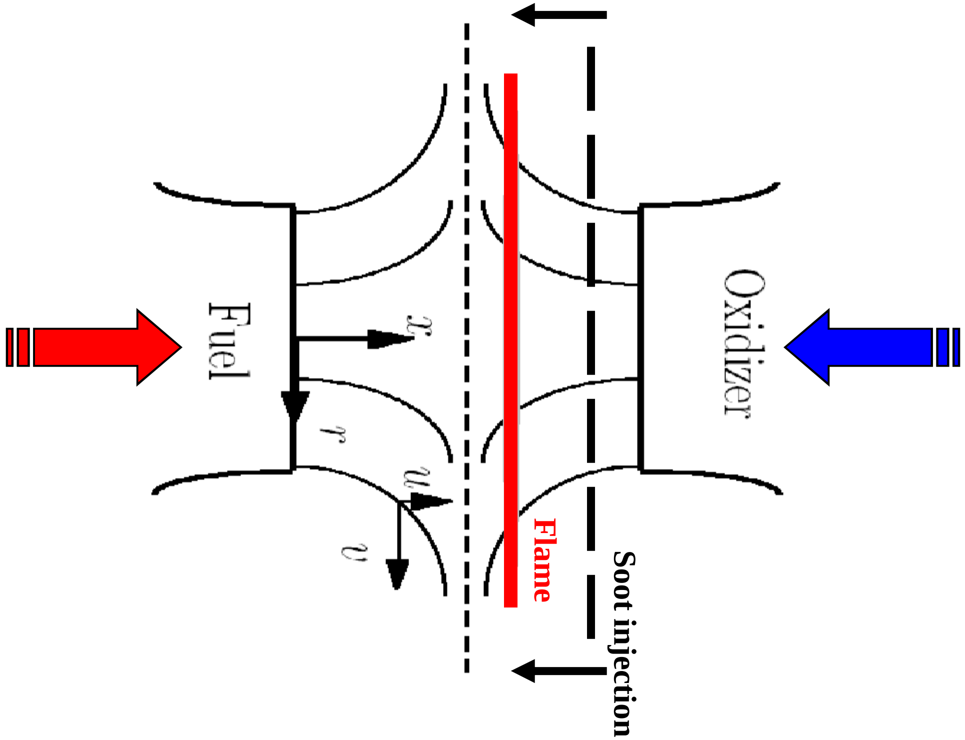
  - Soot formation and oxidation rates (C_2H_2-air combustion)

$$\begin{aligned}\dot{\omega}_{Y_{soot}}&=c_\alpha(\rho^2\sqrt{T}X_F)\exp\left(-\frac{T_\alpha}{T}\right)+c_\gamma(\rho\sqrt{T}X_F)\exp\left(-\frac{T_\gamma}{T}\right)\times n_{soot}\\&\quad-c_O\left(\frac{X_{O_2}}{\sqrt{T}}\right)\exp\left(-\frac{T_O}{T}\right)\times(\rho Y_{soot})^{2/3}n_{soot}^{1/3}\\\dot{\omega}_{n_{soot}}&=c_\delta c_\alpha(\rho^2\sqrt{T}X_F)\exp\left(-\frac{T_\alpha}{T}\right)-c_\beta\sqrt{T}\times\left(\frac{n_{soot}}{N_A}\right)^2\end{aligned}$$

AEA Analysis

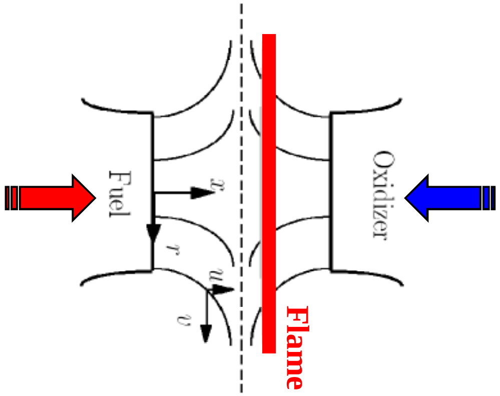
- AEA flame structure with soot
  - External soot loading: a mechanism to simulate non-local effects observed in multi-dimensional flames in a one-dimensional framework
  - Soot loading from the flame air side

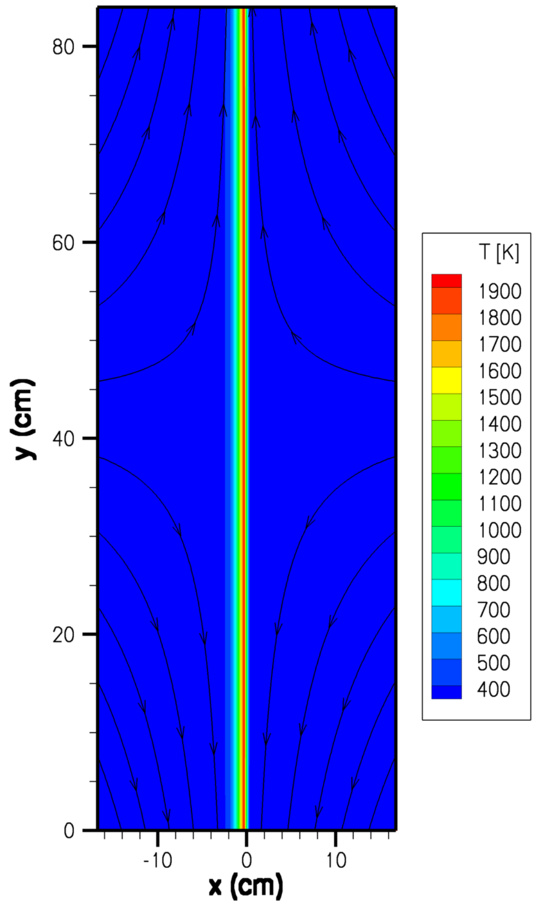




Laminar Counter-Flow Flames

- Reference counter-flow diffusion flame configuration
  - Flamelet perspective: steady flame structure obtained as a function of flame stretch, ranging from ultra-high to ultra-low values



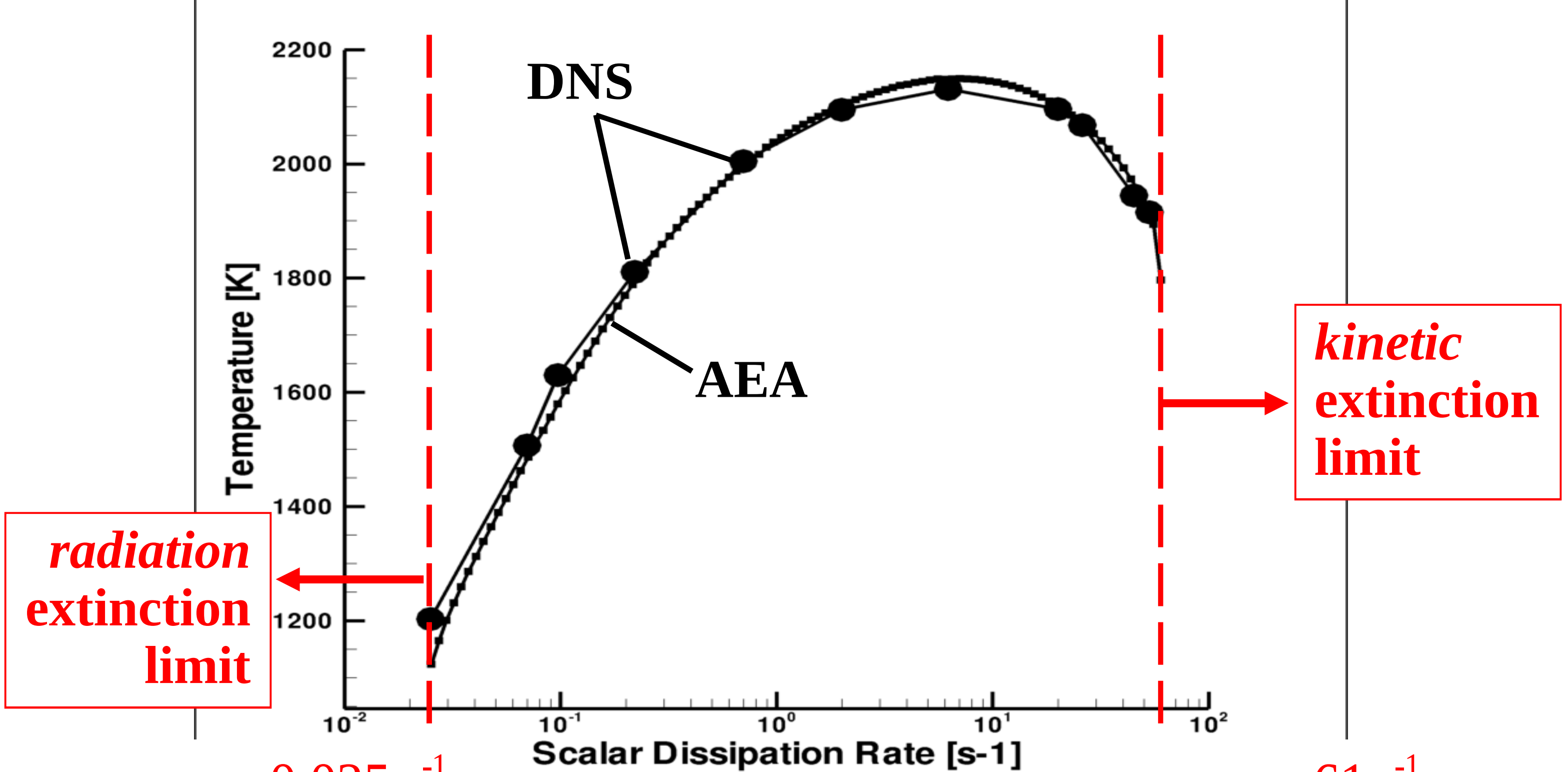


$\Delta x = 60\ \mu\text{m}$
variable Δy

Laminar Counter-Flow Flames

- Reference counter-flow flame configuration
  - Flamelet database: steady flame structure obtained as a function of flame stretch, ranging from ultra-high to ultra-low values

T_{st} versus χ_{st}



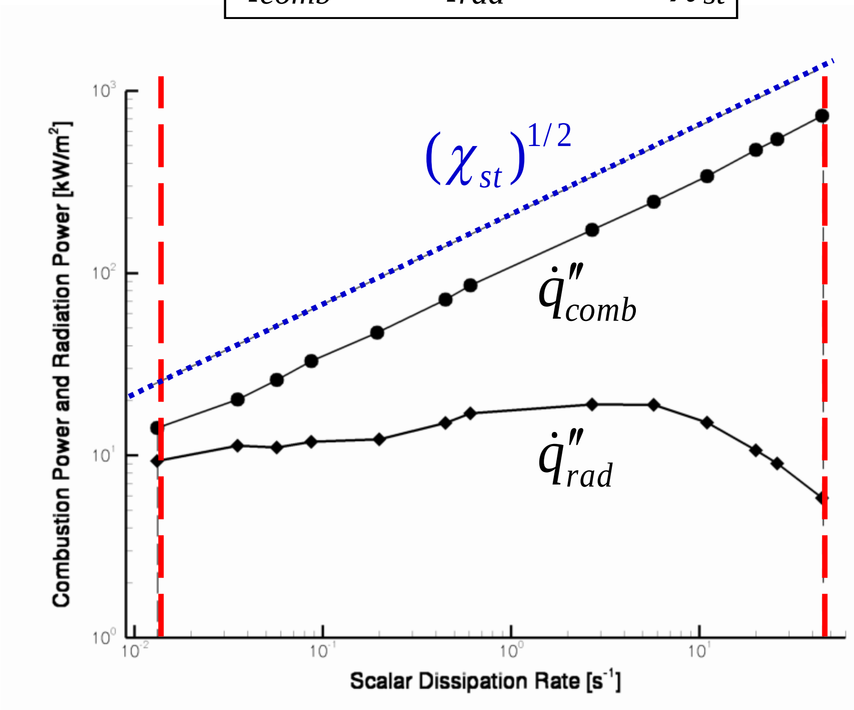
$\chi_{ext,LL} \approx 0.025\,\mathrm{s}^{-1}$ $\chi_{ext,UL} \approx 61\,\mathrm{s}^{-1}$

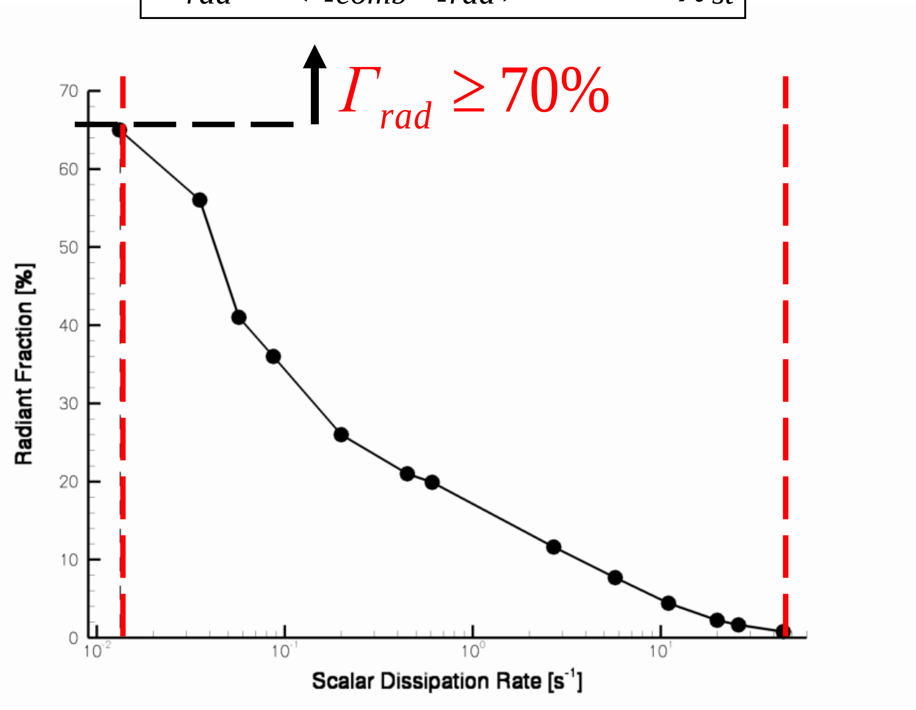
Laminar Counter-Flow Flames

- Reference counter-flow flame configuration
  - Flamelet database: steady flame structure obtained as a function of flame stretch, ranging from ultra-high to ultra-low values

$\dot{q}''_{comb}$ and $\dot{q}''_{rad}$ versus χ_{st}

$\Gamma_{rad} = (\dot{q}''_{comb}/\dot{q}''_{rad})$ versus χ_{st}





$\dot{q}''_{comb} \sim (\chi_{st})^{1/2}$ and $\dot{q}''_{rad} \sim$ constant

Laminar Counter-Flow Flames

- Extinction limits: correspond to critical value of Damköhler number

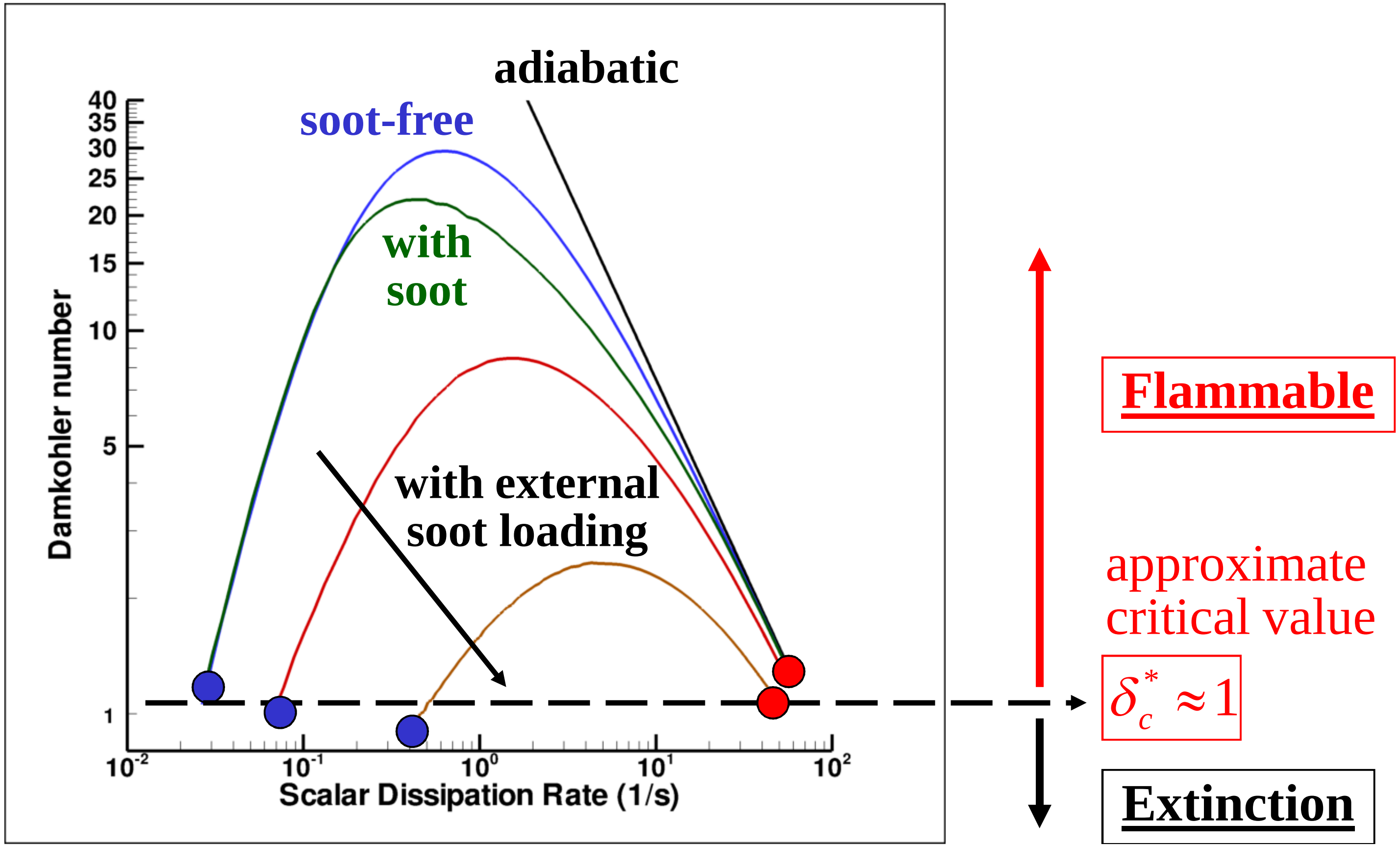
$$\delta^* = \frac{8\rho_{st}^{(p+q-1)} Y_{F,1}^{(p+q-1)} r_s^{\ q} A \exp(-T_a/T_{st})}{(1+b)^2 (10^6)^{p+q-1} M_F^{\ (p-1)} M_{O_2}^{\ q} \chi_{st} Ze^{(p+q+1)}} \le \delta_c^*$$

Laminar Counter-Flow Flames

- Extinction limits: correspond to critical value of Damköhler number

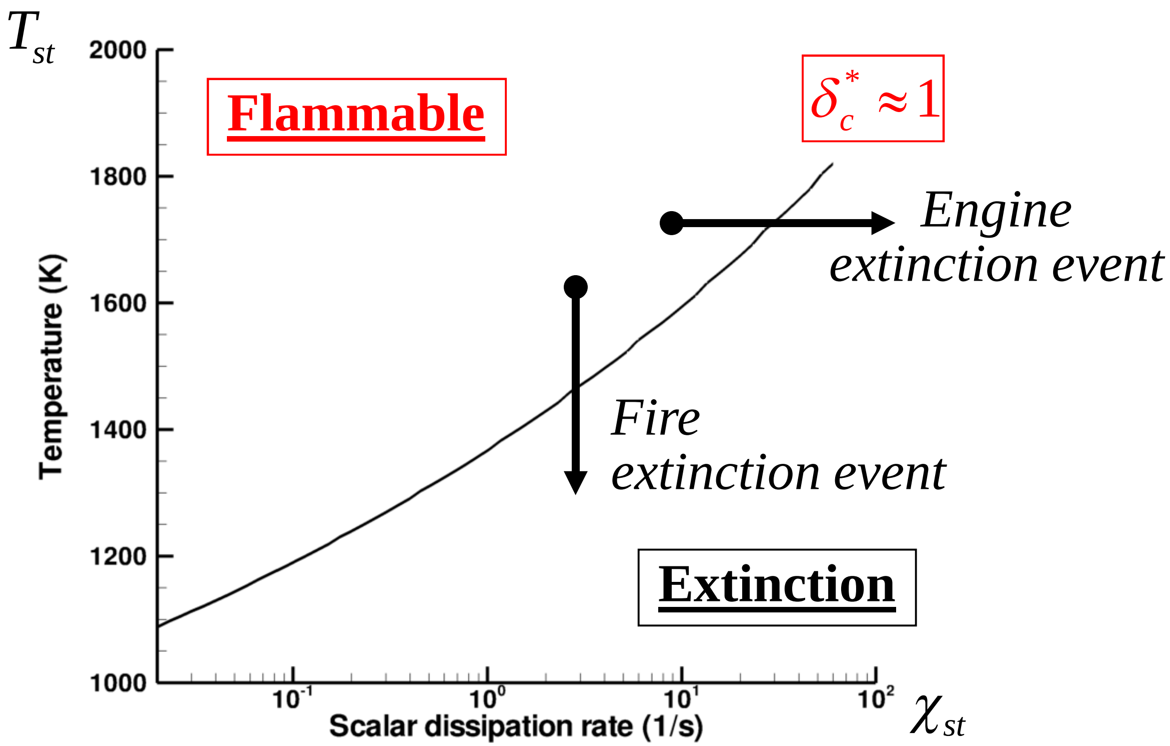
$$\delta^* = \frac{8\rho_{st}^{(p+q-1)} Y_{F,1}^{(p+q-1)} r_s^{\,q} A \exp(-T_a / T_{st})}{(1+b)^2 (10^6)^{p+q-1} M_F^{(p-1)} M_{O_2}^{\,q} \chi_{st} Ze^{(p+q+1)}} \le \delta_c^*$$

δ^* versus χ_{st}



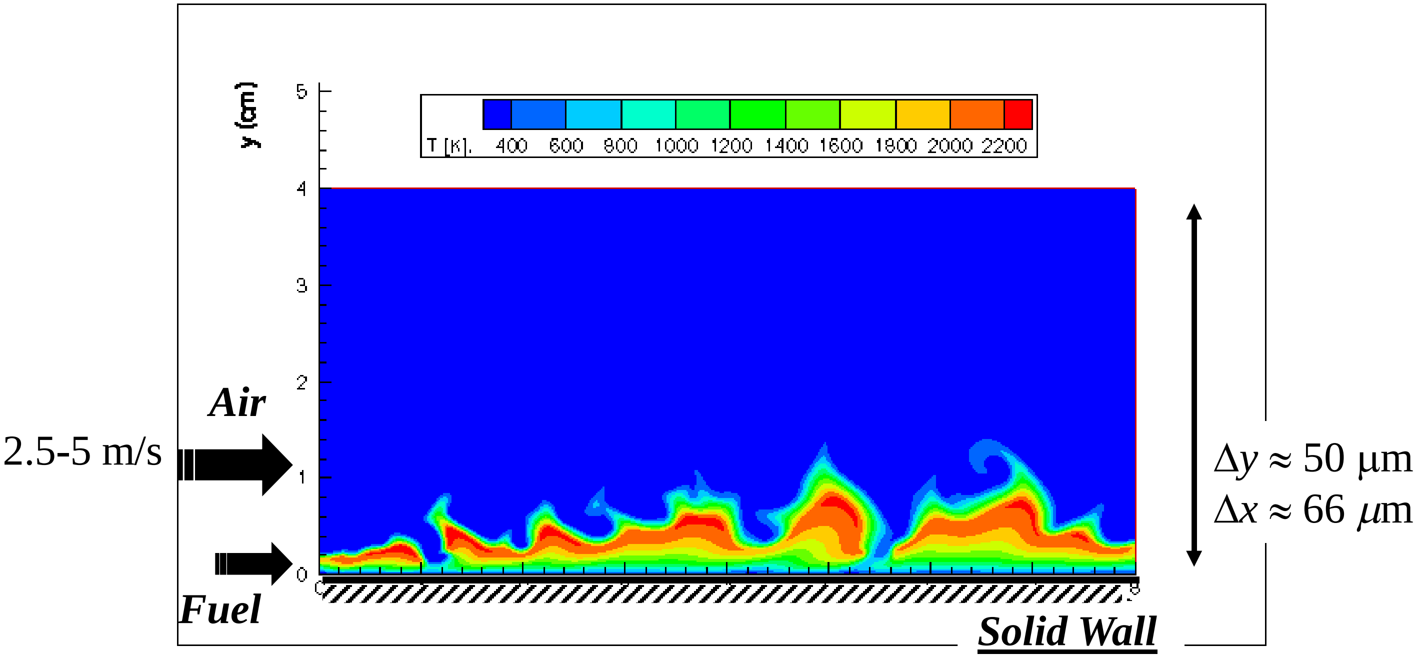
Laminar Counter-Flow Flames

- Extinction limits
  - Flammability map with mixing rate and fuel-air flame temperature as coordinates



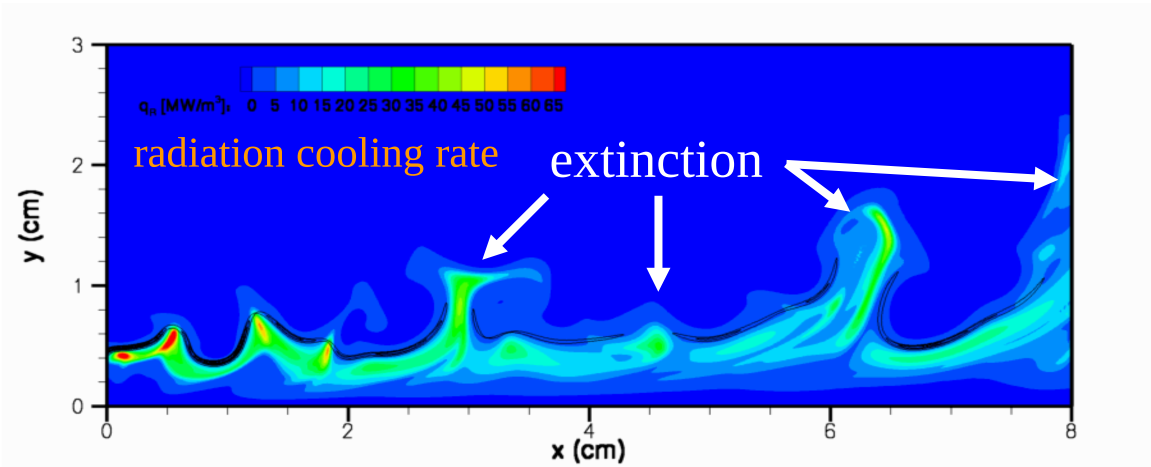
Turbulent Wall-Jet Flames

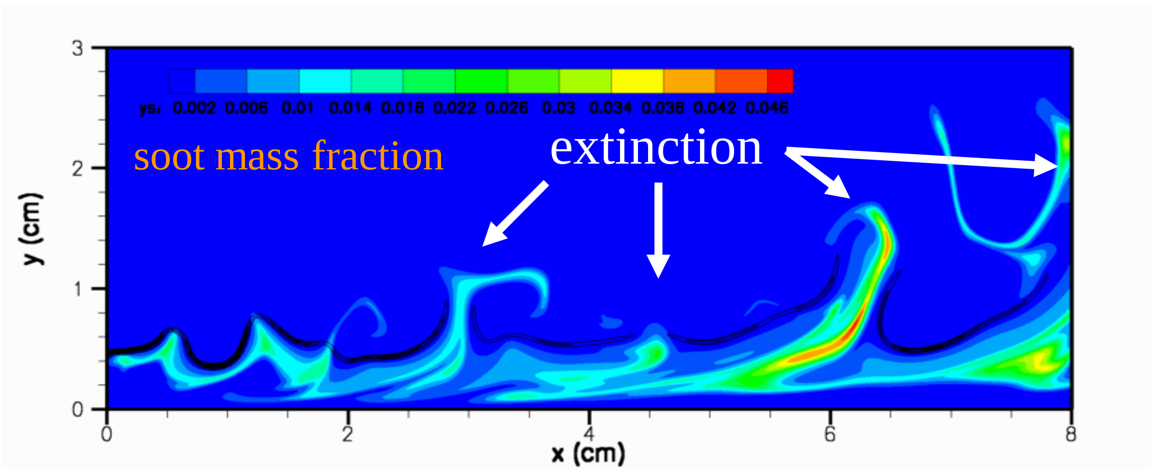
- Simplified turbulent flame configuration
  - *Two-dimensional* (8×4 cm^2); grid size: 1216×376 (uniform×stretched); prescribed inflow turbulent fluctuations (u' = 1-2.5 m/s; L_t = 1.7 mm)



Turbulent Wall-Jet Flames

- Analysis of flame structure (case: T_w = 300 K; δ = 0.5 cm; with soot/radiation; C_{soot} = 7000 $m^{-1}K^{-1}$)





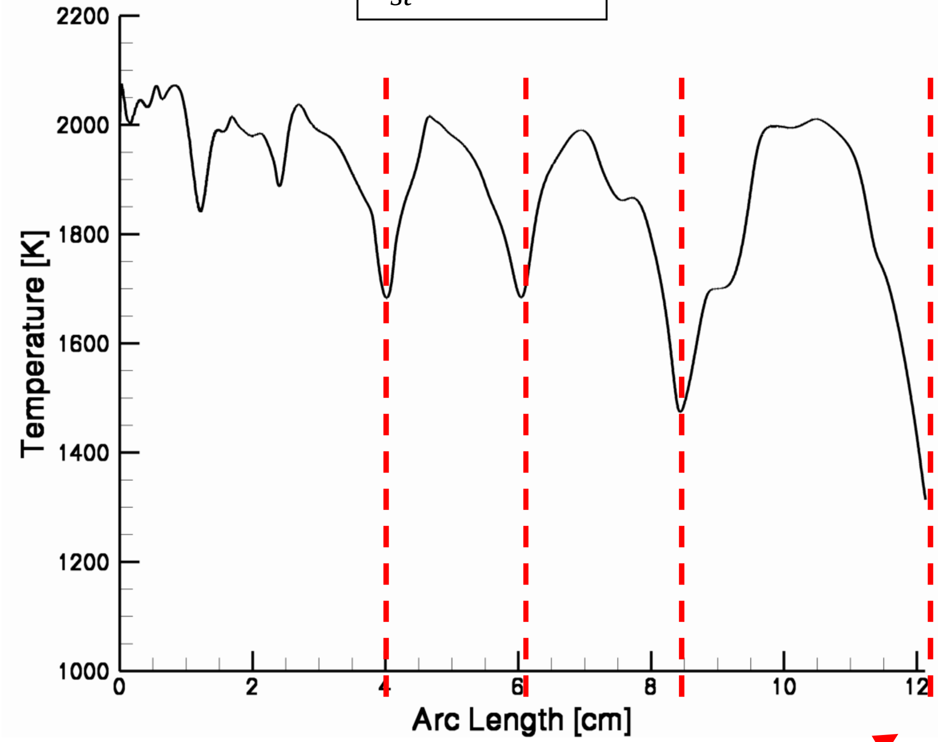
Observations:

- radiative cooling region is not thin
- soot region is not thin
- Weak flame events correlated with soot mass leakage across the flame

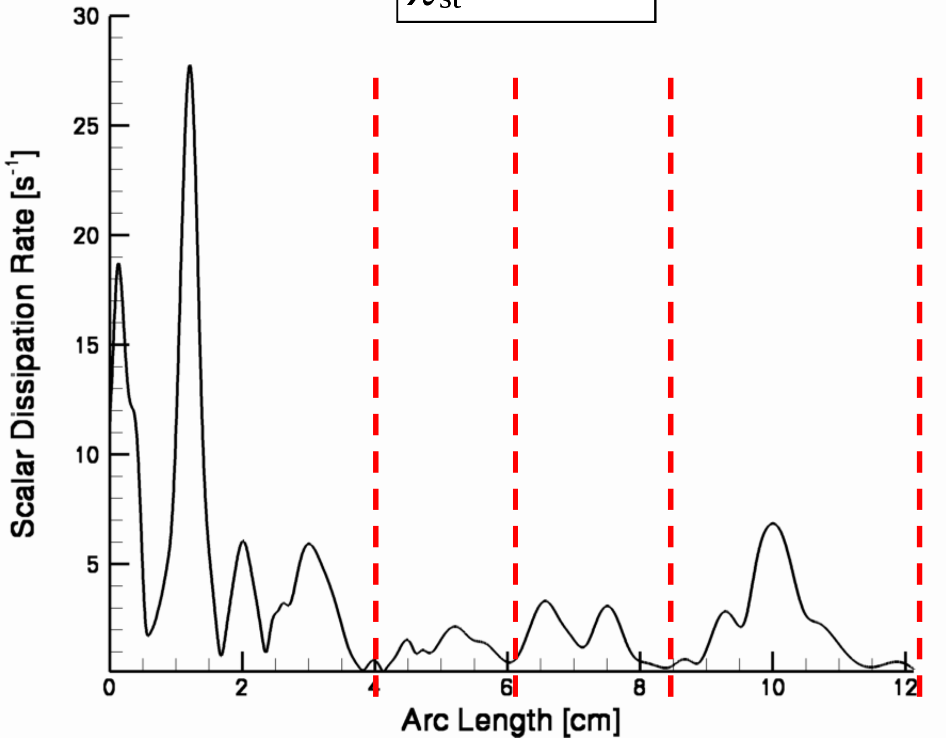
Turbulent Wall-Jet Flames

- Analysis of flame structure (case: T_w = 300 K; δ = 0.5 cm; with soot/radiation; C_{soot} = 7000 m^{-1}K^{-1})

T_{st} versuss



χ_{st} versuss

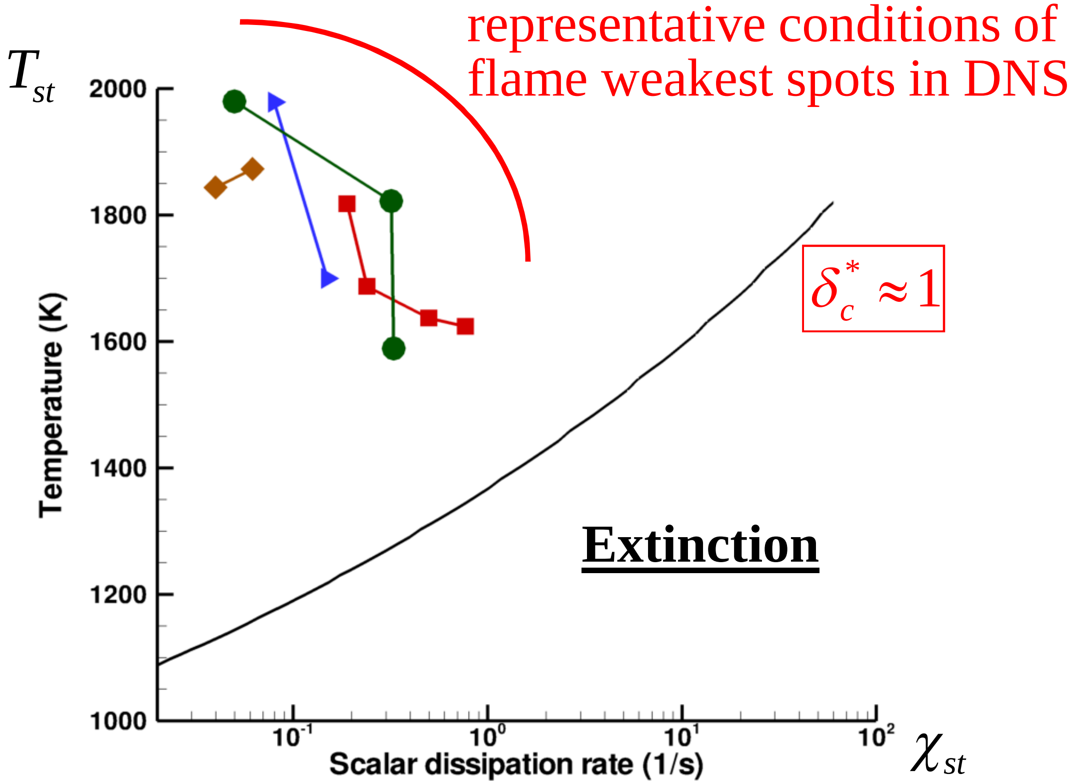


weak spots

weak flame events occur at low values of flame stretch (slow mixing limit)

Laminar Counter-Flow Flames

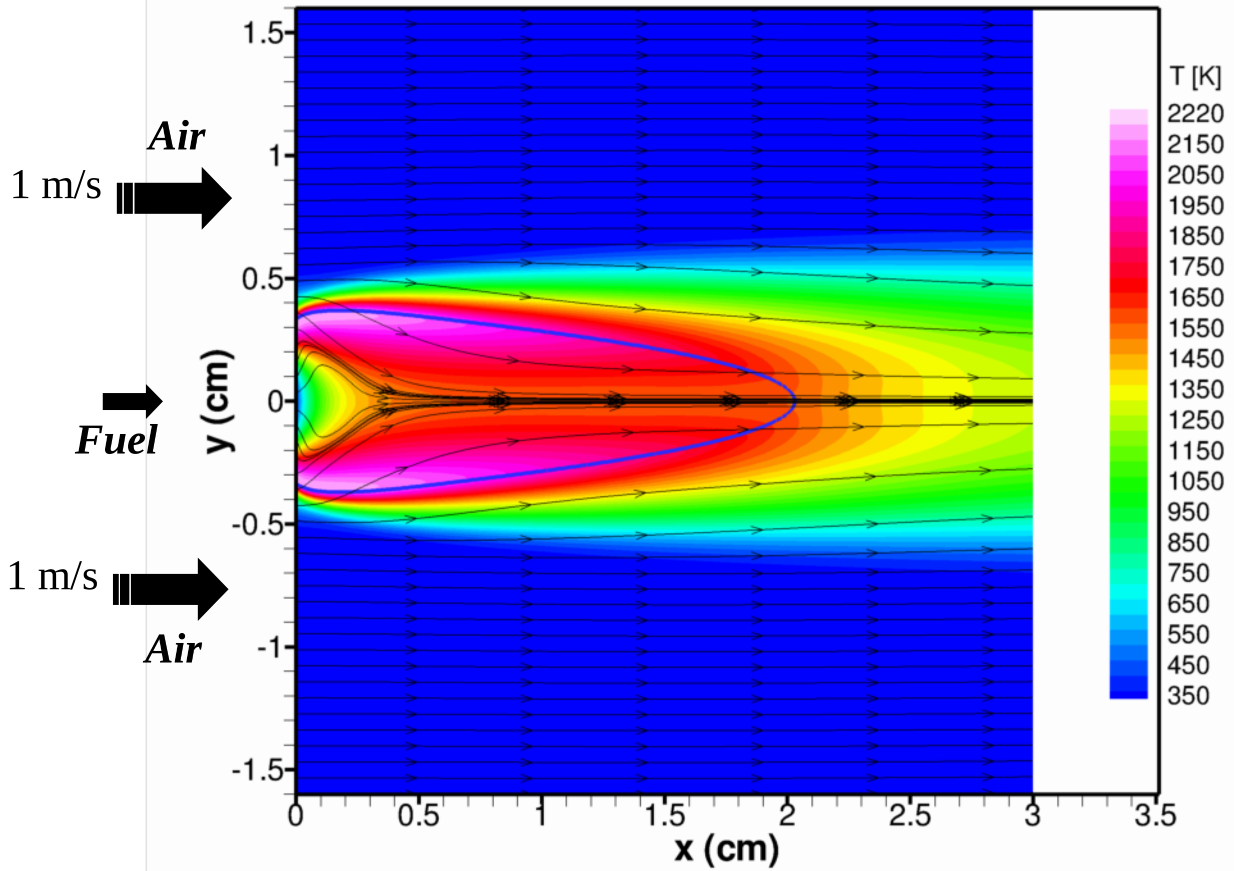
- Extinction limits
  - Flammability map with mixing rate and fuel-air flame temperature as coordinates



Flame weakest spots (*e.g.*, locations that show soot mass leakage) correspond to weak burning conditions, not flame extinction

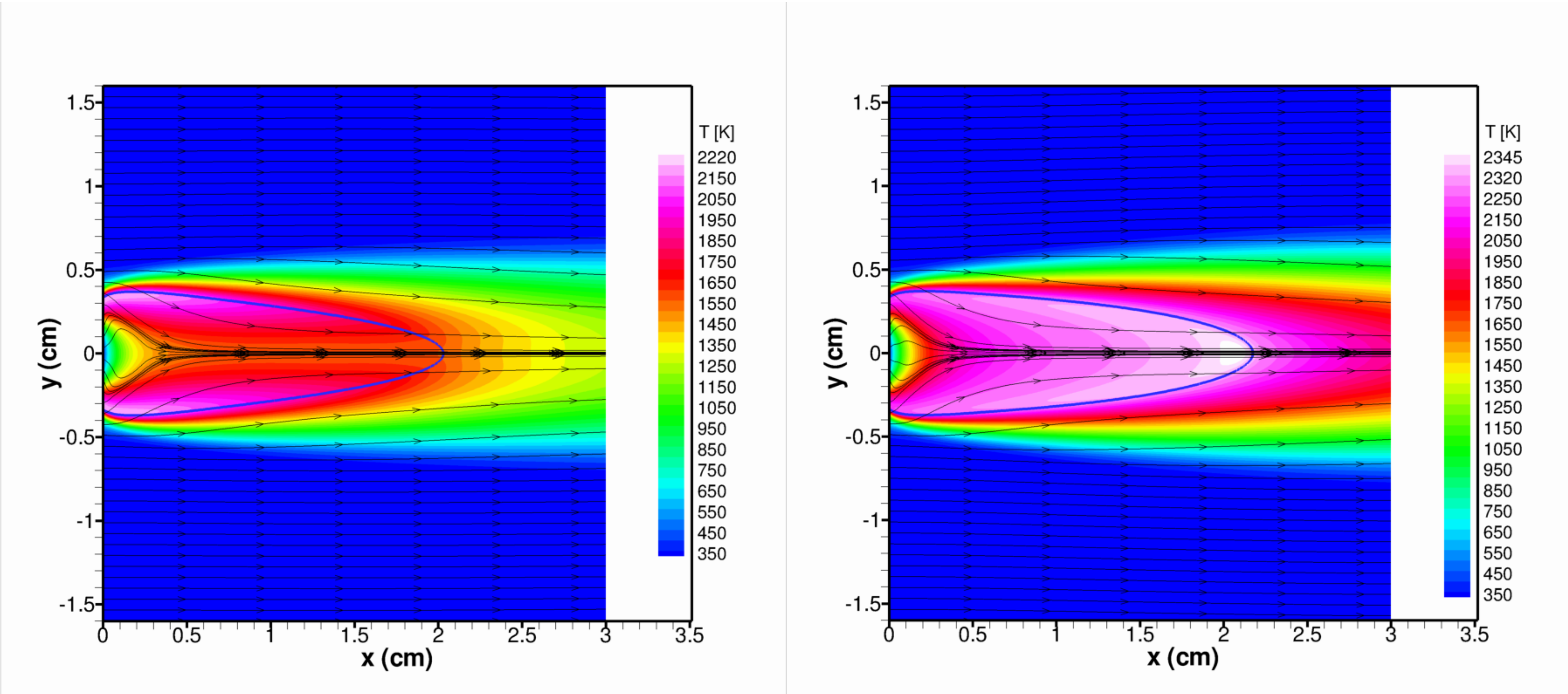
Laminar Co-Flow Flames

- Simplified laminar flame configuration
  - High air co-flow velocity, diffusive-driven incoming fuel stream, zero-*g*
  - Recirculation zone close to fuel surface, long residence times



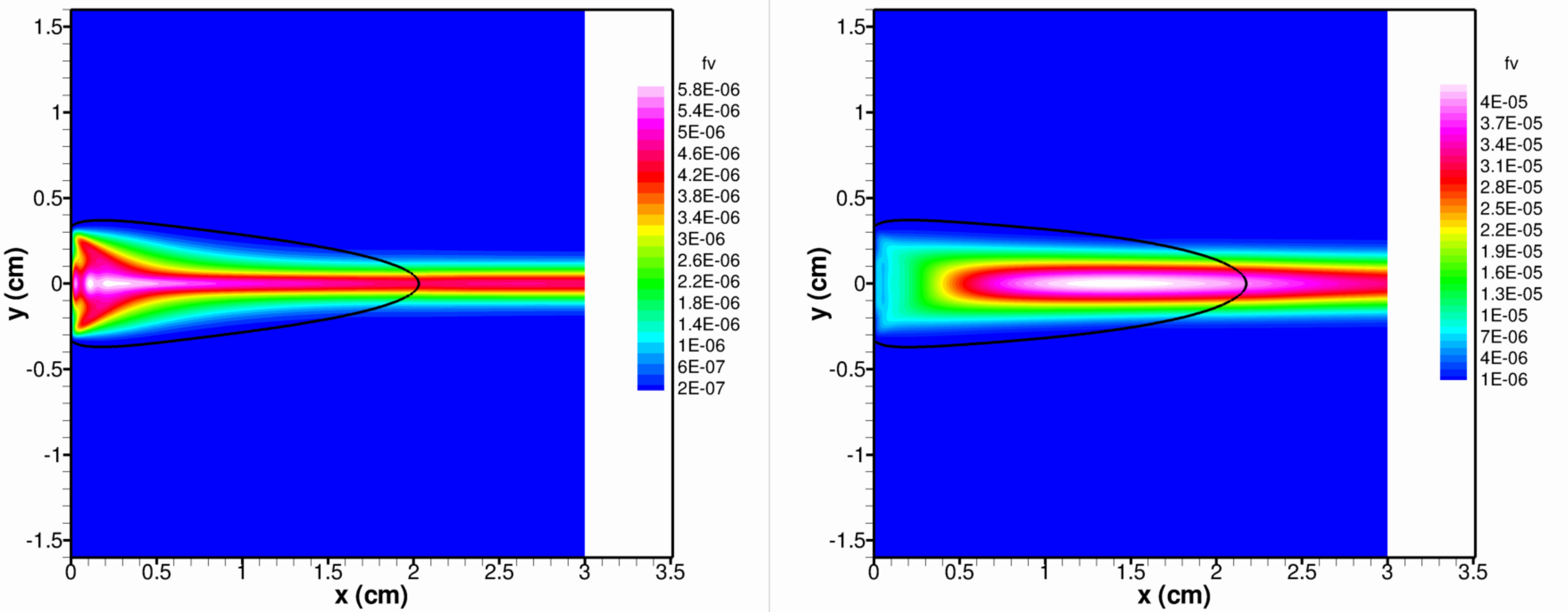
Laminar Co-Flow Flames

- Simplified laminar flame configuration
  - Comparison between solutions with (left) and without radiation (right)
  - Flame tip temperatures differ by more than 700 K



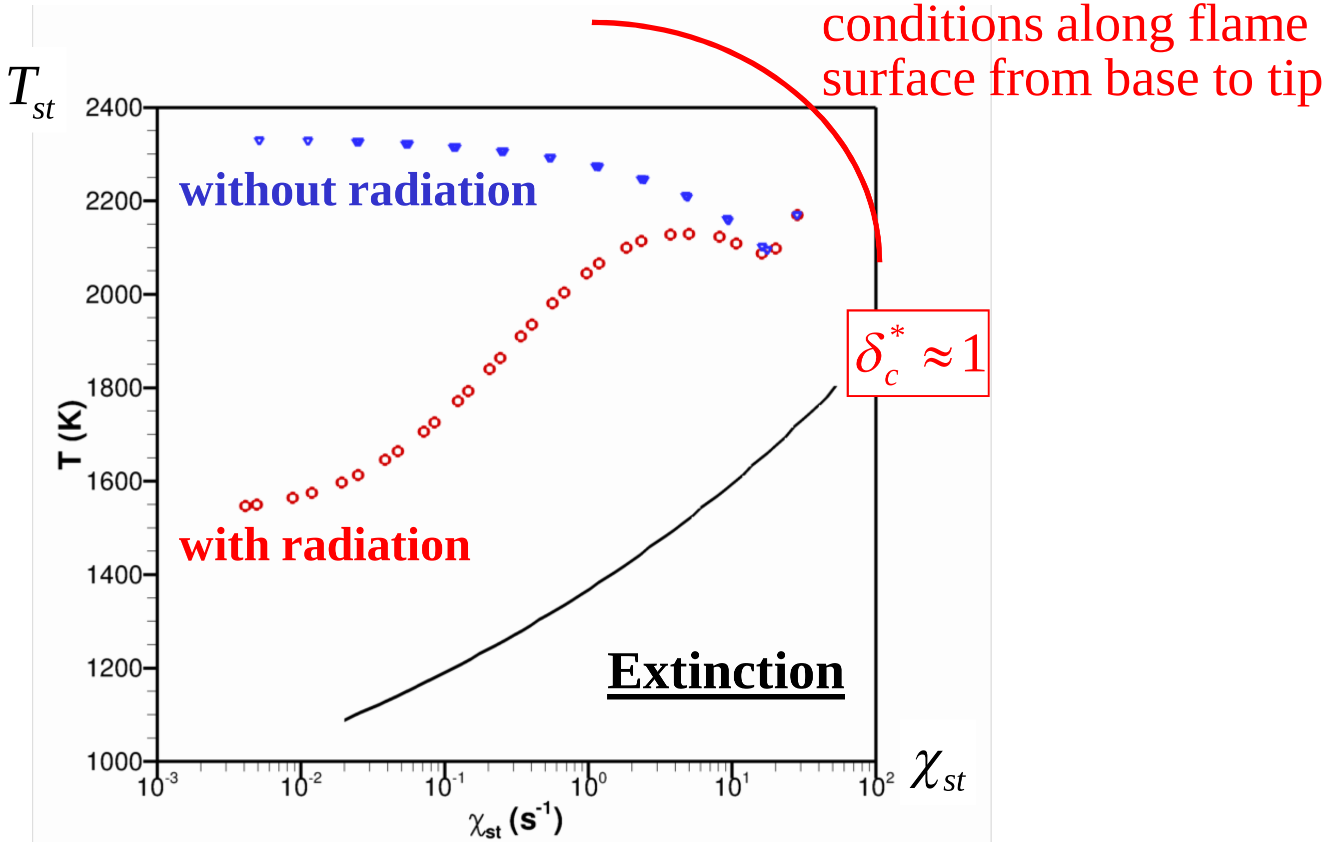
Laminar Co-Flow Flames

- Simplified laminar flame configuration
  - Comparison between solutions with (left) and without radiation (right)
  - Both flames feature both large amounts of soot within the flame envelope and soot mass leakage across the flame tip



Laminar Counter-Flow Flames

- Extinction limits
  - Flammability map with flame temperature and mixing rate as coordinates



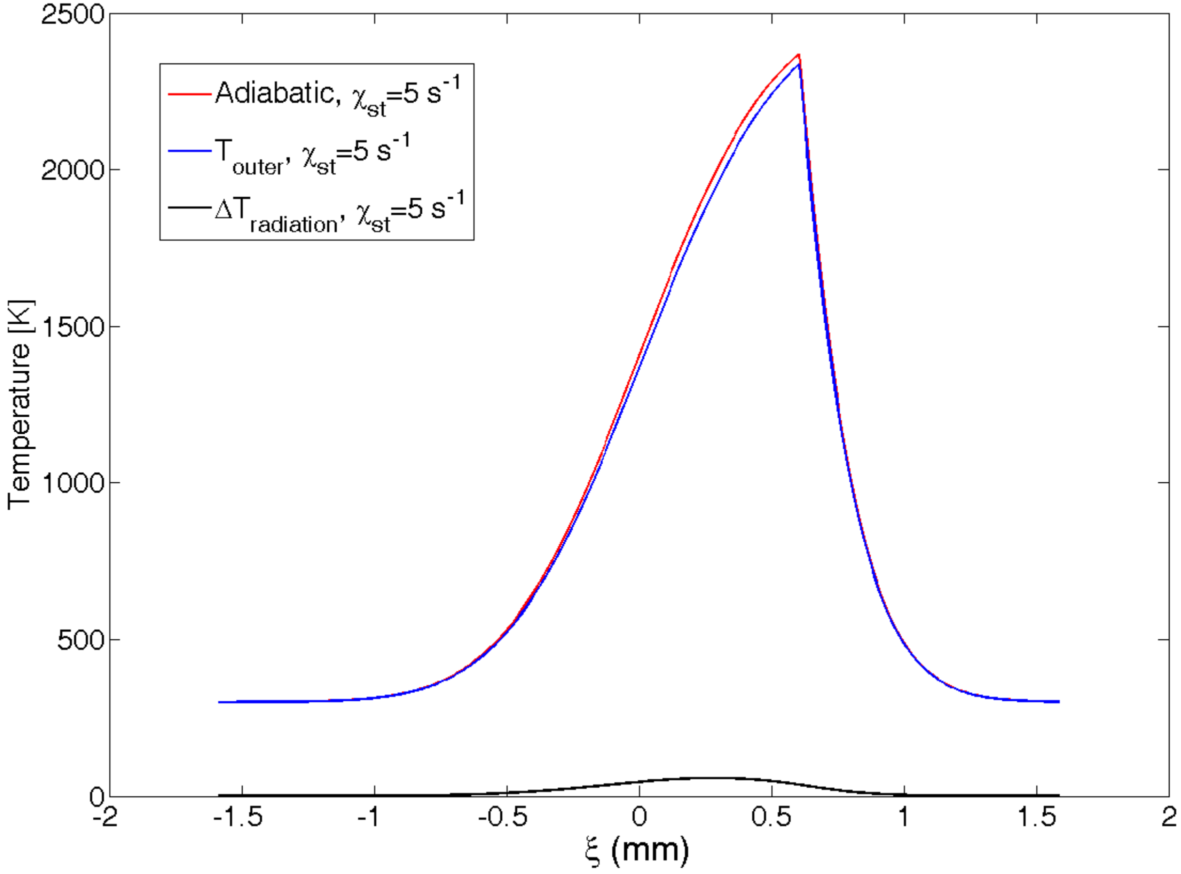
Flame tip (*e.g.*, location that show soot mass leakage) corresponds to weak burning conditions, not flame extinction

Conclusions

- AEA theory and DNS are used to make fundamental observations of extinction phenomena in non-adiabatic turbulent diffusion flames
- In laminar counter-flow flames, two different sets of flame extinction conditions are observed:
  - *Kinetic* extinction occurring under fast mixing conditions
  - *Radiation* extinction occurring under slow mixing conditions
- These 2 different modes correspond to the same extinction limit:
  - AEA analysis suggests that all extinction limits may be described by a single criterion corresponding to a critical value of the Damköhler number
  - Soot has a significant impact on the extinction limit
- In laminar co-flow flames and in turbulent flames, it is found that soot mass leakage events do not correspond to radiation extinction events

Laminar Counter-Flow Flames

- Intermediate stretch rate: $\chi_{st} = 5\ s^{-1}$
  - Flame temperature versus distance normal to the flame

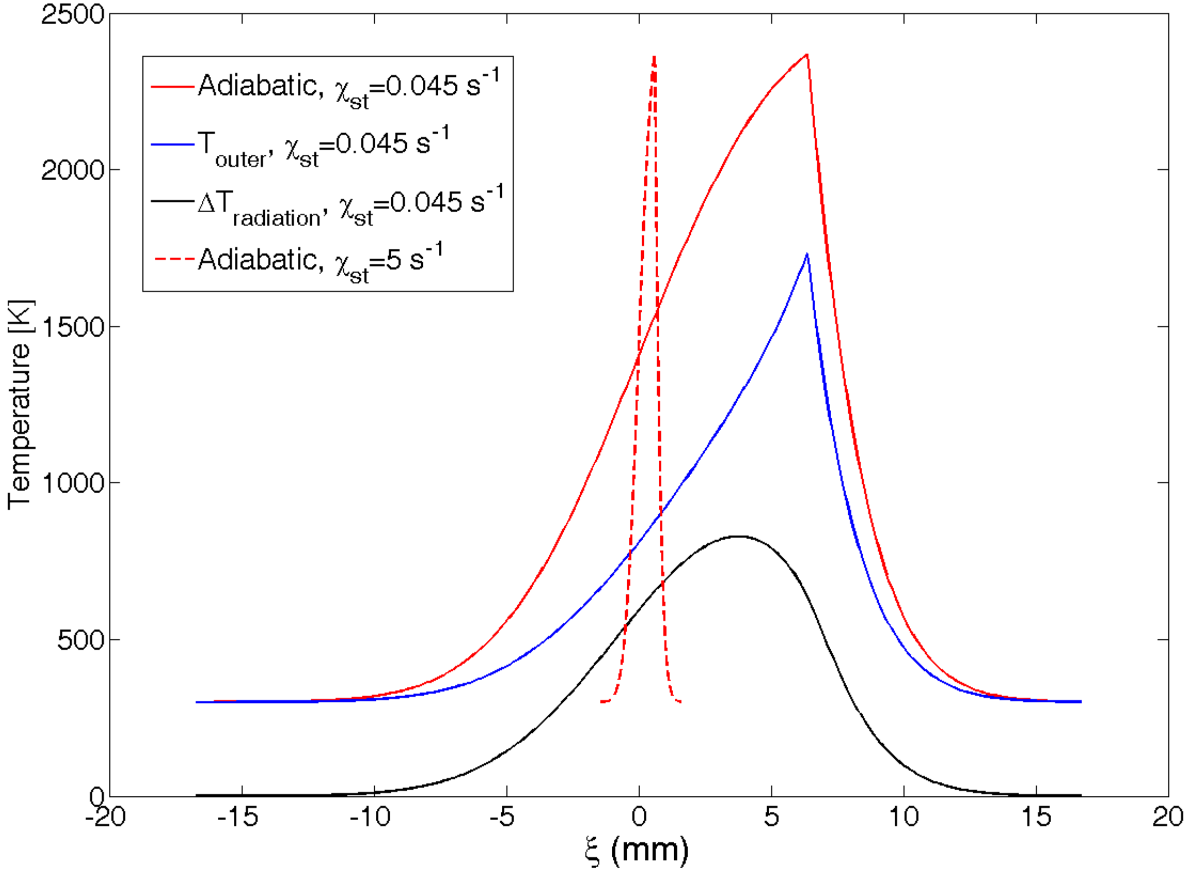


- Weak radiation effects

$$(\kappa \delta_{outer}) << 1$$

Laminar Counter-Flow Flames

- Low stretch rate: $\chi_{st} = 0.045\ s^{-1}$
  - Flame temperature versus distance normal to the flame



- Strong radiation effects

$$(\kappa\delta_{outer}) = O(1)$$