Analysis of Reaction–Advection–Diffusion Spectrum of Laminar Premixed Flames

Ashraf N. Al-Khateeb *Joseph M. Powers*

DEPARTMENT OF AEROSPACE AND MECHANICAL ENGINEERING

UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA

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Diffusion

For a continuous random walk in 2-D, a particle must make

$$N = \left(\frac{d}{l}\right)^2 \tag{1}$$

steps to travel a distance d, where l is the mean free path. The time required is then

$$t = N\frac{l}{v_s} = \frac{d^2}{l^2}\frac{l}{v_s} = \frac{d^2}{l v_s}, \tag{2}$$

where v_s is the sound speed. Defining a diffusion coefficient

$$\kappa \equiv l v_s, \tag{3}$$

yields

$$t = \frac{d^2}{\kappa}. \tag{4}$$

SEE ALSO: Diffusion Coefficient, Diffusion Equation, Eddy Diffusion, Effusion, Graham's Law of

DIffusion length vs. reaction time: $\ell = \sqrt{D\tau}$

Outline

- Introduction
- Simple one species reaction–advection–diffusion problem.
- Simple two species reaction–diffusion problem.
- Laminar premixed hydrogen–air flame.
- Summary

Introduction

Motivation and background

- Combustion is often unsteady and spatially inhomogeneous.
- Most realistic reactive flow systems have multi-scale character.
- Severe stiffness, temporal and spatial, arises in detailed gas-phase kinetics modeling.
- As the scales' range widens, more stringent demands arise to assure the accuracy of the results.
- Proper numerical resolution of all scales is critical to draw correct conclusions and achieve a mathematically verified solution.

- Segregation of chemical dynamics from transport dynamics is a prevalent notion in combustion modeling, *e.g.* operator splitting.
- However, reaction, advection, and diffusion scales are coupled in reactive flows.
- The interplay between chemistry and transport needs to be captured for accurate modeling.
- Spectral analysis is a tool to understand the coupling between transport and chemistry.
- All relevant scales have to be brought into simultaneous focus *a priori* for DNS.

General objective

To identify the scales associated with each Fourier mode of a variety of wavelengths for unsteady spatially inhomogenous reactive flow problems.

Particular objective

To calculate the time scale spectrum of a one-dimensional atmospheric pressure hydrogen–air system.

Model problem I

A linear one species model for reaction, advection, and diffusion:

$$\frac{\partial \psi(x,t)}{\partial t} + u\frac{\partial \psi(x,t)}{\partial x} = D\frac{\partial^2 \psi(x,t)}{\partial x^2} - a\psi(x,t),$$

$$\psi(0,t) = \psi_u, \quad \left.\frac{\partial \psi}{\partial x}\right|_{x=L} = 0, \qquad \psi(x,0) = \psi_u.$$

Time scale spectrum

For the spatially homogenous version: $\psi(t) = \psi_u \exp\left(-at\right),$

$$\tau = \frac{1}{a} \;\Rightarrow\; \Delta t < \frac{1}{a}.$$

Length scale spectrum

- The steady structure:

$$\psi_s(x) = \psi_u \left(\frac{\exp(\mu_1 x) - \exp(\mu_2 x)}{1 - \frac{\mu_1}{\mu_2} \exp(L(\mu_1 - \mu_2))} + \exp(\mu_2 x) \right),$$

$$\mu_1 = \frac{u}{2D} \left(1 + \sqrt{1 + \frac{4aD}{u^2}} \right), \qquad \mu_2 = \frac{u}{2D} \left(1 - \sqrt{1 + \frac{4aD}{u^2}} \right),$$

$$\ell_i = \left| \frac{1}{\mu_i} \right|.$$

- For fast reaction ($a >> u^2/D$):

$$\ell_1 = \ell_2 = \sqrt{\frac{D}{a}} \Rightarrow \Delta x < \sqrt{\frac{D}{a}}.$$

Spatio-temporal spectrum

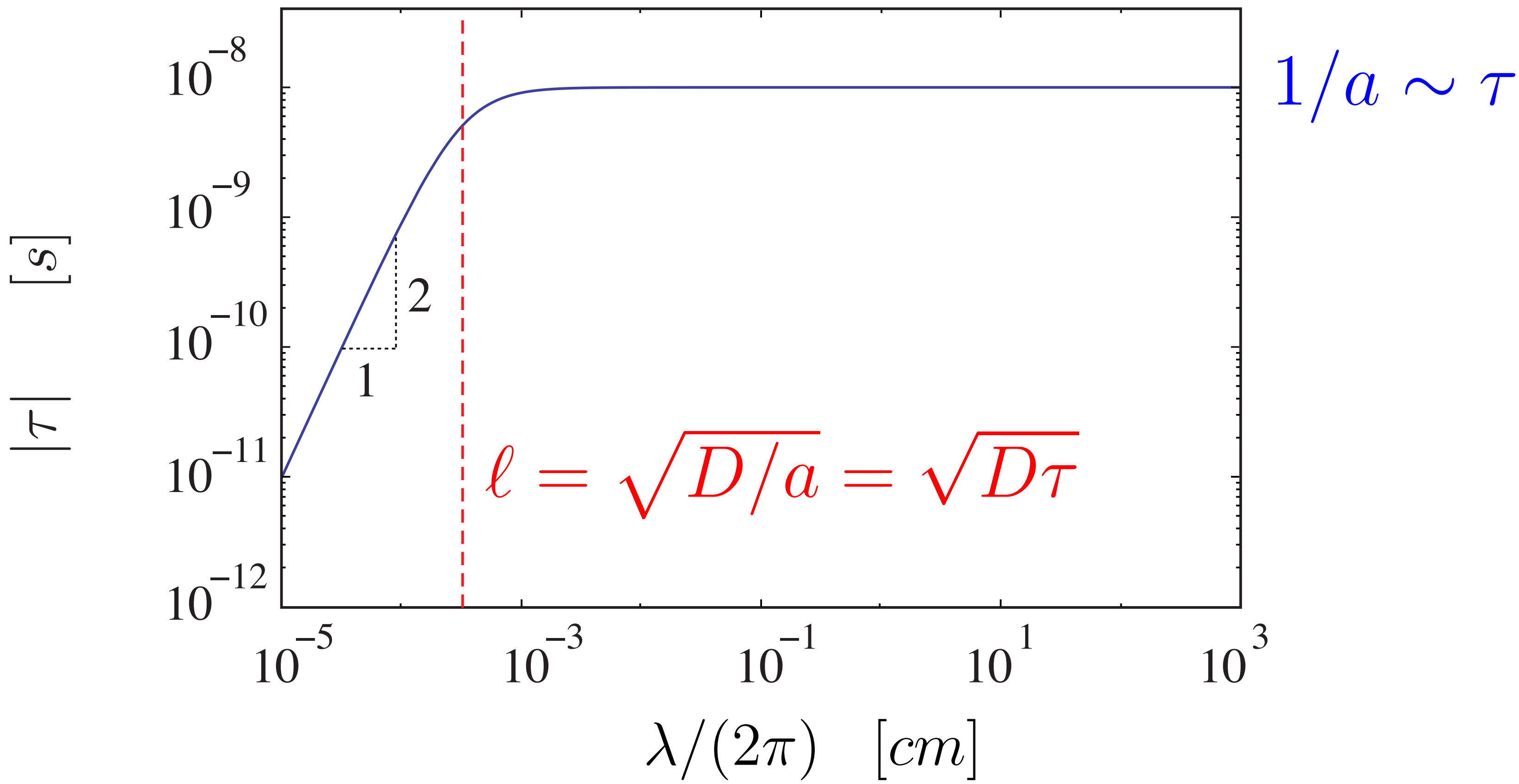
$1)$ continuous spectrum:

$$\psi(x,t) = \Psi(t) e^{\mathbf{i}kx} \quad \Rightarrow \quad \Psi(t) = C \exp\left(-a\left(1 + \frac{\mathbf{i}ku}{a} + \frac{Dk^2}{a}\right) t\right).$$

$$\left.\begin{array}{l} \bullet \text{ long wavelength: } \lim_{k\to 0} \tau = \lim_{\lambda\to\infty} \tau = \frac{1}{a}, \\ \bullet \text{ short wavelength: } \lim_{k\to\infty} \tau = \lim_{\lambda\to 0} \tau = \frac{\lambda^2}{4\pi^2}\frac{1}{D}, \end{array}\right\} \quad \mathcal{S}_t = \left(\frac{2\pi}{\lambda}\sqrt{\frac{D}{a}}\right)^2.$$

- Balance between reaction and diffusion at $k \equiv \frac{2\pi}{\lambda} = \sqrt{\frac{a}{D}} = 1/\ell$,
- Using Taylor expansion:

$$|\tau| = \frac{1}{a}\left(1 - \frac{D}{a\left(\frac{\lambda}{2\pi}\right)^2} - \frac{u^2}{2a^2\left(\frac{\lambda}{2\pi}\right)^2}\right) + \mathcal{O}\left(\frac{1}{\lambda^4}\right).$$



- Similar to $H_2 - air : \tau \sim 1/a = 10^{-8}\ s$, $D = 10\ cm^2/s$,
- $\ell = \sqrt{\frac{D}{a}} = 3.2 \times 10^{-4}\ cm$.

$2)$ Spatially discretized spectrum: $\psi(x,t) \rightarrow \psi_i(t), \quad i = 1, \ldots, \mathcal{N}.$

- Original boundary conditions:

$$\mathbf{A} \cdot \frac{d\boldsymbol{\psi}}{dt} = \mathbf{B} \cdot \boldsymbol{\psi} \;\; \Rightarrow \;\; (\mu\mathbf{A} - \mathbf{B}) \cdot \boldsymbol{v} = \mathbf{0}.$$

- Dirichlet boundary condition modification:

$$\tau_j = \frac{1}{a + \frac{2D(\mathcal{N}+1)^2}{L^2}\left(1 - \sqrt{1 - \frac{u^2L^2}{4D^2(\mathcal{N}+1)^2}}\cos\left(\frac{j\pi}{\mathcal{N}-1}\right)\right)}, j = 1, ..., \mathcal{N}-2,$$

Effects of advection and diffusion: $\tau_1 \sim \frac{1}{a}\left(1 - \frac{D}{a(L/\pi)^2} - \frac{1}{4}\frac{u^2}{aD}\right),$

For small $\mathcal{N}$: $\lim_{\Delta x \rightarrow \infty} \tau_j \rightarrow 1/a,$

For large $\mathcal{N}$: $\lim_{\Delta x \rightarrow 0} \tau_j \rightarrow \frac{L^2}{(4D(\mathcal{N}+1)^2)},$

$$\left.\right\} \mathcal{S}_t = \left(\frac{2(\mathcal{N}+1)}{L}\sqrt{\frac{D}{a}}\right)^2.$$

Model problem II

An uncoupled reaction-diffusion system with chemical stiffness:

$$\frac{\partial \psi_i(x,t)}{\partial t} = D\frac{\partial^2 \psi_i(x,t)}{\partial x^2} - a_i \psi_i(x,t),$$

$$\psi_i(0,t) = \psi_{iu}, \quad \frac{\partial \psi_i}{\partial x}(L,t) = 0, \qquad \psi_i(x,0) = \psi_{iu}.$$

Time scale spectrum

For the spatially homogenous version: $\psi_i(t) = \psi_{iu} \exp\left(-a_i t\right),$

$$\tau_i = \frac{1}{a_i} \quad \Rightarrow \quad \mathcal{S}_t = \frac{a_{largest}}{a_{smallest}} \quad \Rightarrow \quad \Delta t < \frac{1}{a_{largest}}.$$

Length scale spectrum

- The steady structure: $\psi_{is}(x) = \frac{\psi_{iu}}{\cosh\left(L/\sqrt{\frac{D}{a_i}}\right)} \cosh\left(\frac{L-x}{\sqrt{\frac{D}{a_i}}}\right),$

$$\ell_i = \sqrt{\frac{D}{a_i}} \quad \Rightarrow \quad \mathcal{S}_t = \sqrt{\frac{a_{largest}}{a_{smallest}}}, \quad \Delta x < \sqrt{\frac{D}{a_{largest}}}.$$

Spatio-temporal spectrum

1) Continuous spectrum:

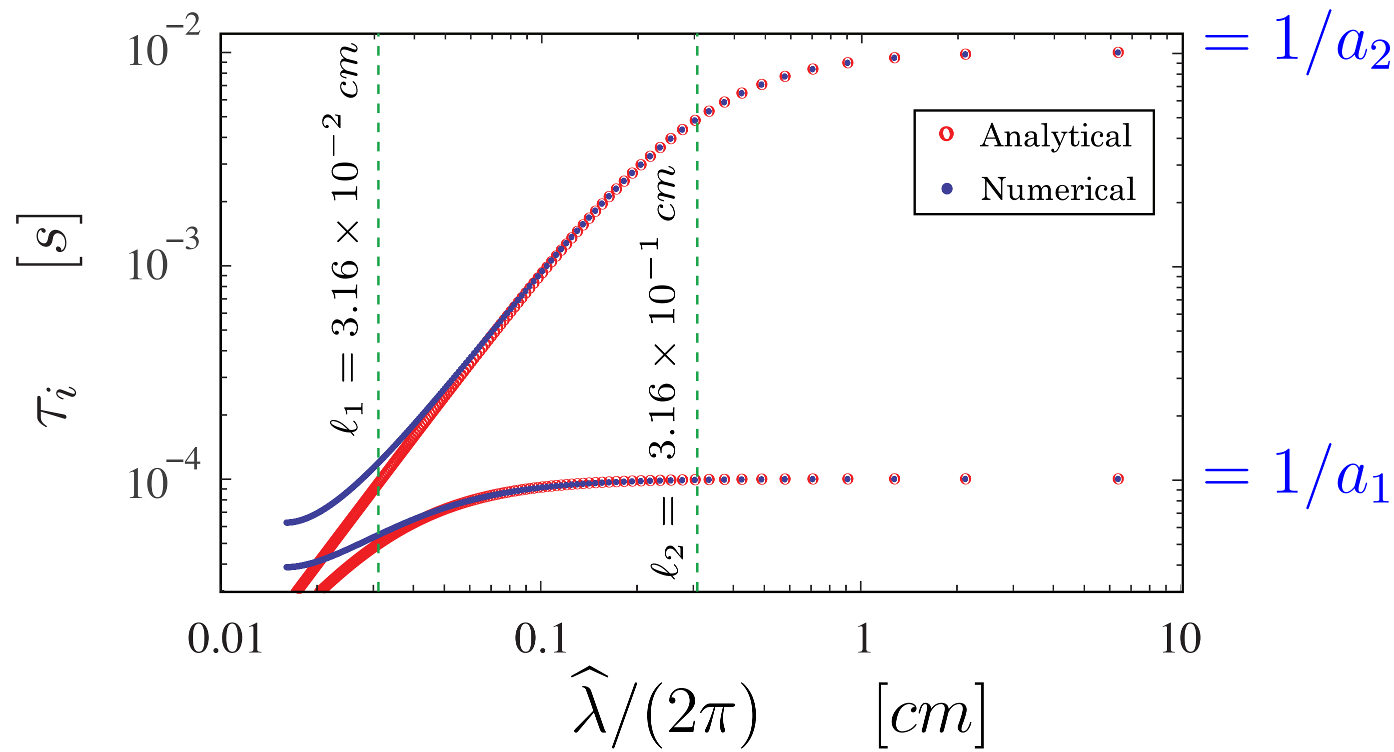
$$\psi_i(x,t) = \Psi_i(t)e^{\mathbf{i}kx} \quad \Rightarrow \quad \Psi_i(t) = C\exp\left(-a_i\left(1+\frac{Dk^2}{a_i}\right)t\right).$$

2) Discrete spectrum:

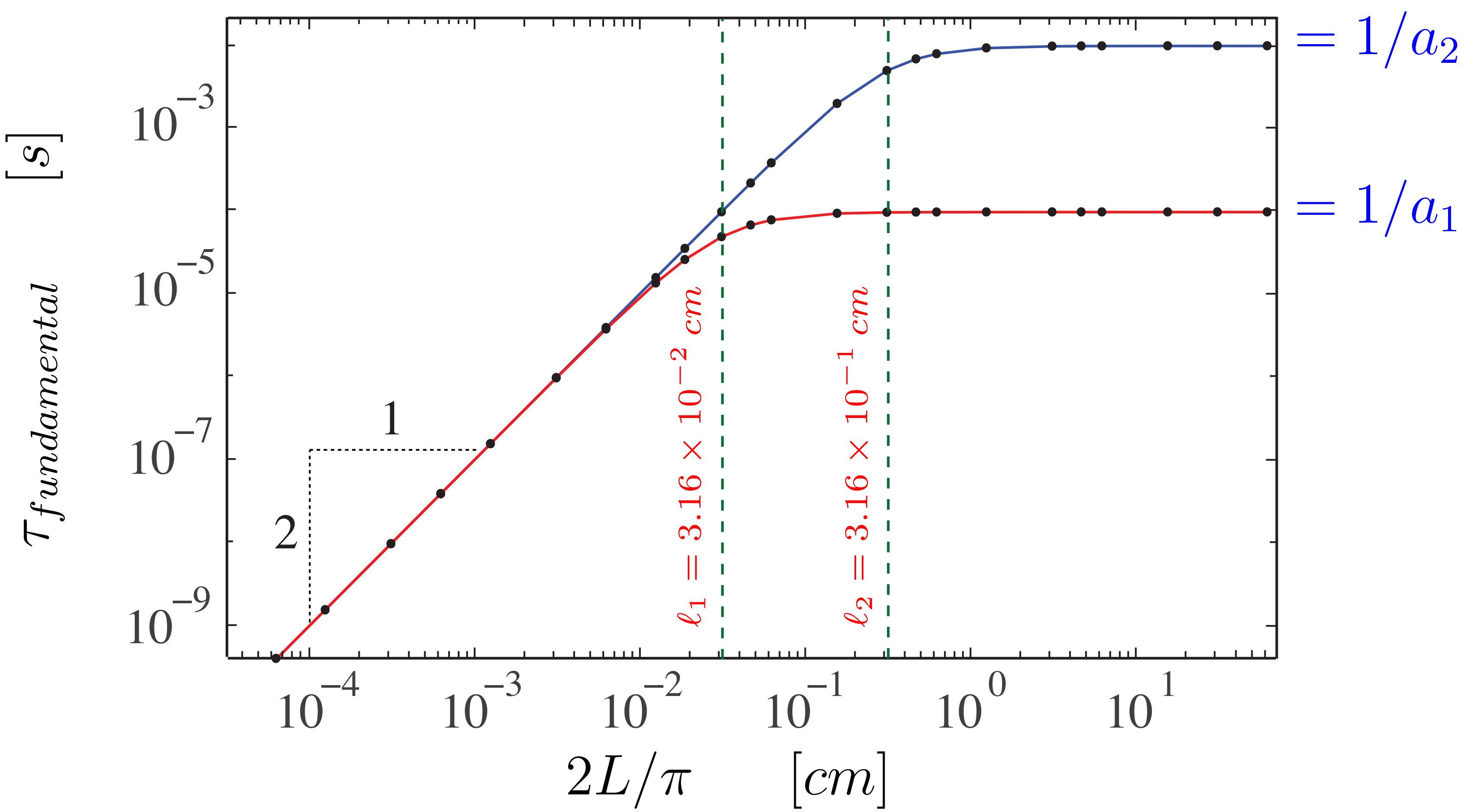
$$\psi_i = \psi_{is} + \sum_{\kappa=1}^{\infty} A_\kappa \exp\left(-a_i\left[1+\left(\frac{(2\kappa-1)\pi}{2L}\sqrt{\frac{D}{a_i}}\right)^2\right]t\right)\sin\left(\frac{(2\kappa-1)\pi}{2L}x\right).$$

$3)$ Spatially discretized spectrum:

- for $a_1 = 10^4\ s, a_2 = 10^2\ s, D = 10\ cm^2/s$, and $L = 10\ cm$,
- modified wavelength: $\widehat{\lambda} = 4L/(2\mathfrak{n} - 1)$,
- associated length scale: $\ell = \widehat{\lambda}/(2\pi) \;\Rightarrow\; \ell = \frac{2L}{(2\mathfrak{n}-1)\pi}$,
- prediction from length scale spectrum: $\ell_i = \sqrt{D/a_i}$,



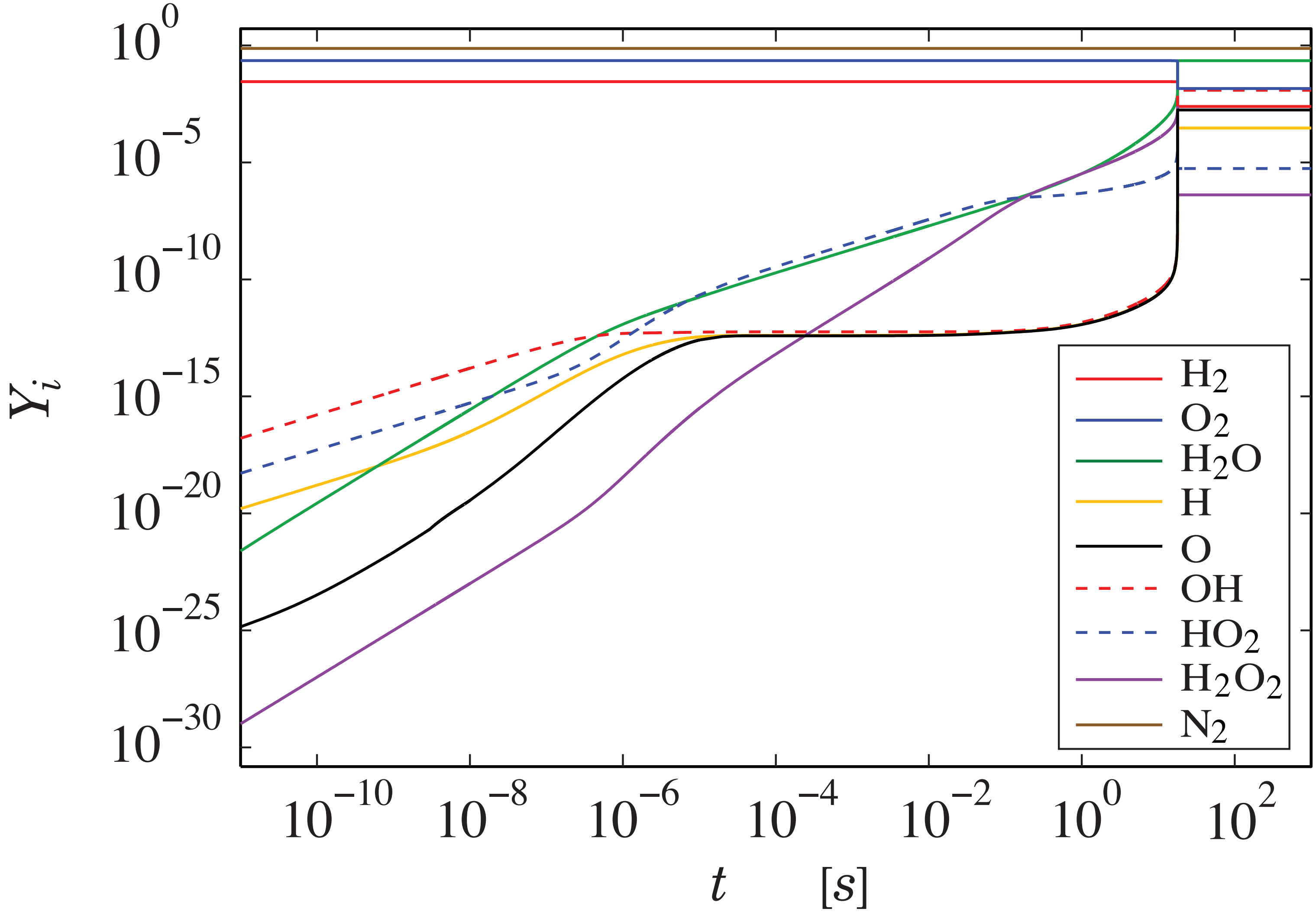
- Prediction from length scale spectrum: $\ell_i = \sqrt{D/a_i}$,



Laminar Premixed Hydrogen–Air Flame

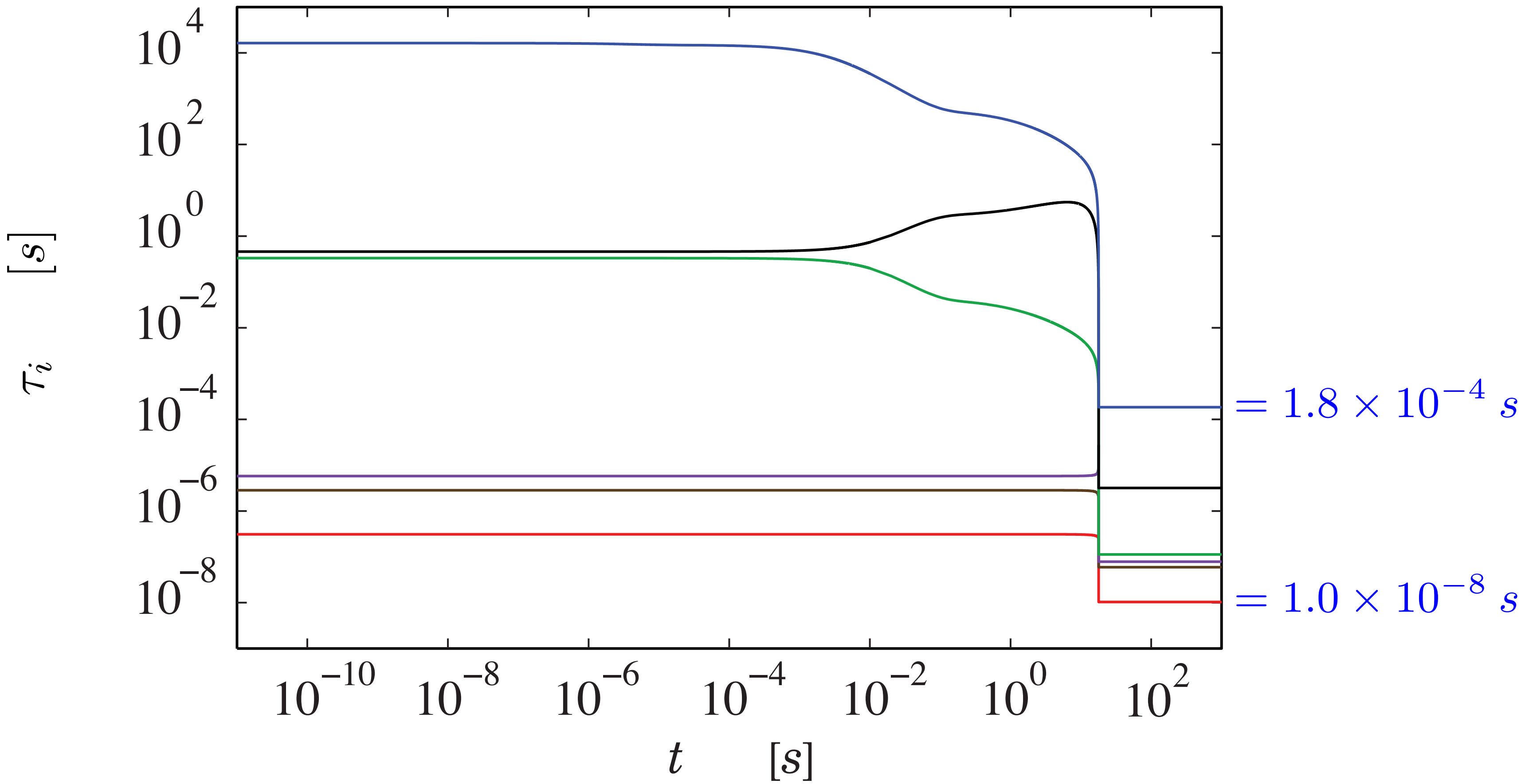
- $N = 9$ species, $\mathrm{L} = 3$ atomic elements, and $J = 19$ reversible reactions,
- $Y_u =$ stoichiometric Hydrogen-Air: $2H_2 + (O_2 + 3.76N_2)$,
- $T_u = 800\ K$,
- $p_o = 1\ atm$,
- neglect Soret effect, Dufour effect, and body forces,
- CHEMKIN and IMSL are employed.

TIme evolution of the spatially homogenous version

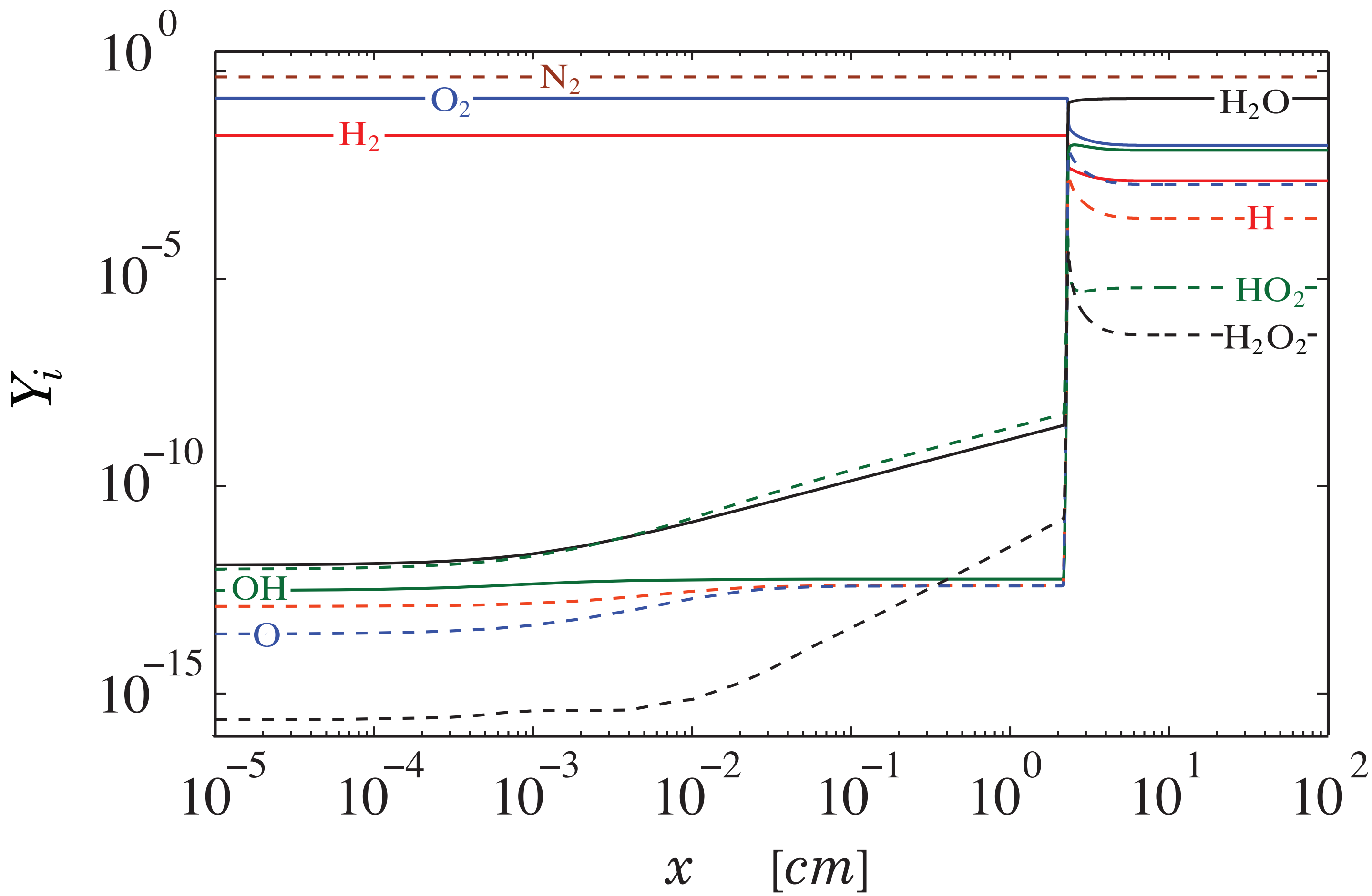


Time scale spectrum

- $\mathcal{S}_t \sim \mathcal{O}\left(10^4\right)$,
- $\Delta t < \tau_{fastest} = 1.03 \times 10^{-8}\ s,$



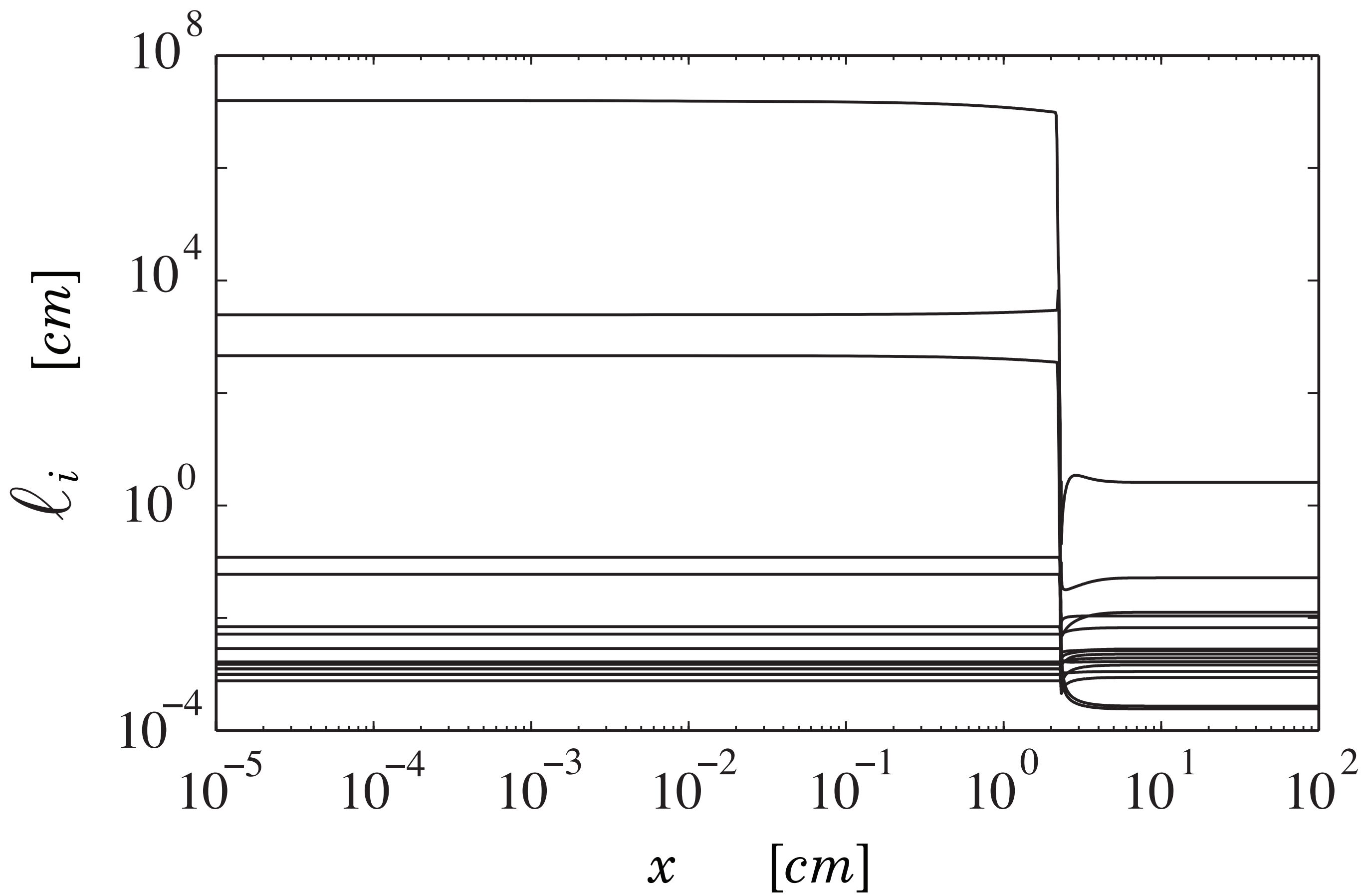
Fully resolved steady structure[a]



[a] Al-Khateeb, Powers, and Paolucci, *Communications in Computational Physics,* to appear.

Length scale spectrum

- $\mathcal{S}_x \sim \mathcal{O}\left(10^4\right)$,
- $\Delta x < \ell_{finest} = 2.41 \times 10^{-4}\ cm$,



Spatio-temporal spectrum

- PDEs $\longrightarrow$ $2N + 2$ PDAEs,

$$\mathbf{A}(\mathbf{z}) \cdot \frac{\partial \mathbf{z}}{\partial t} + \mathbf{B}(\mathbf{z}) \cdot \frac{\partial \mathbf{z}}{\partial x} = \mathbf{f}(\mathbf{z}).$$

- Spatially homogeneous system at chemical equilibrium subjected to a spatially inhomogeneous perturbation, $\mathbf{z}' = \mathbf{z} - \mathbf{z}^e$,

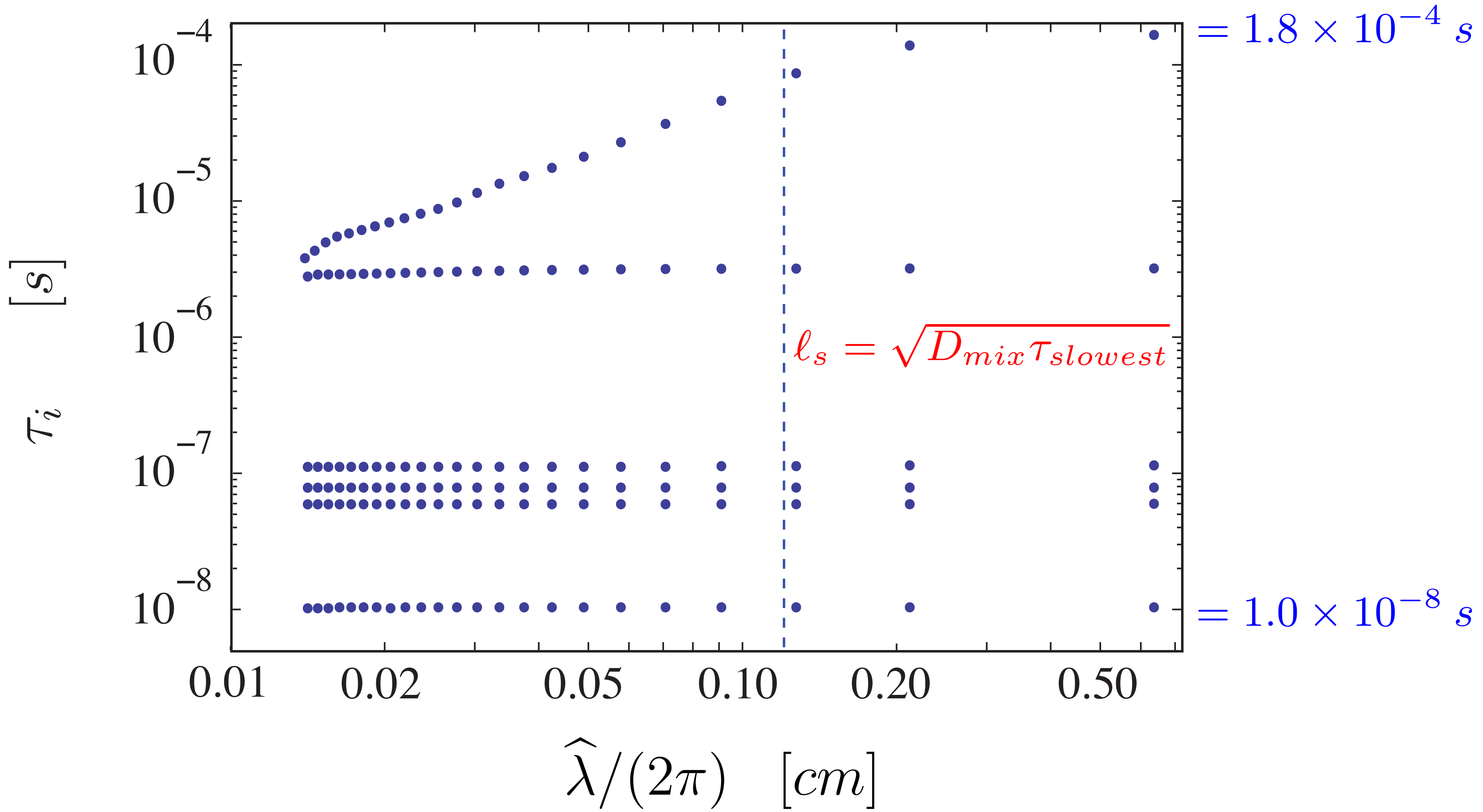
$$\mathbf{A}^e \cdot \frac{\partial \mathbf{z}'}{\partial t} + \mathbf{B}^e \cdot \frac{\partial \mathbf{z}'}{\partial x} = \mathbf{J}^e \cdot \mathbf{z}'.$$

- Spatially discretized spectrum,

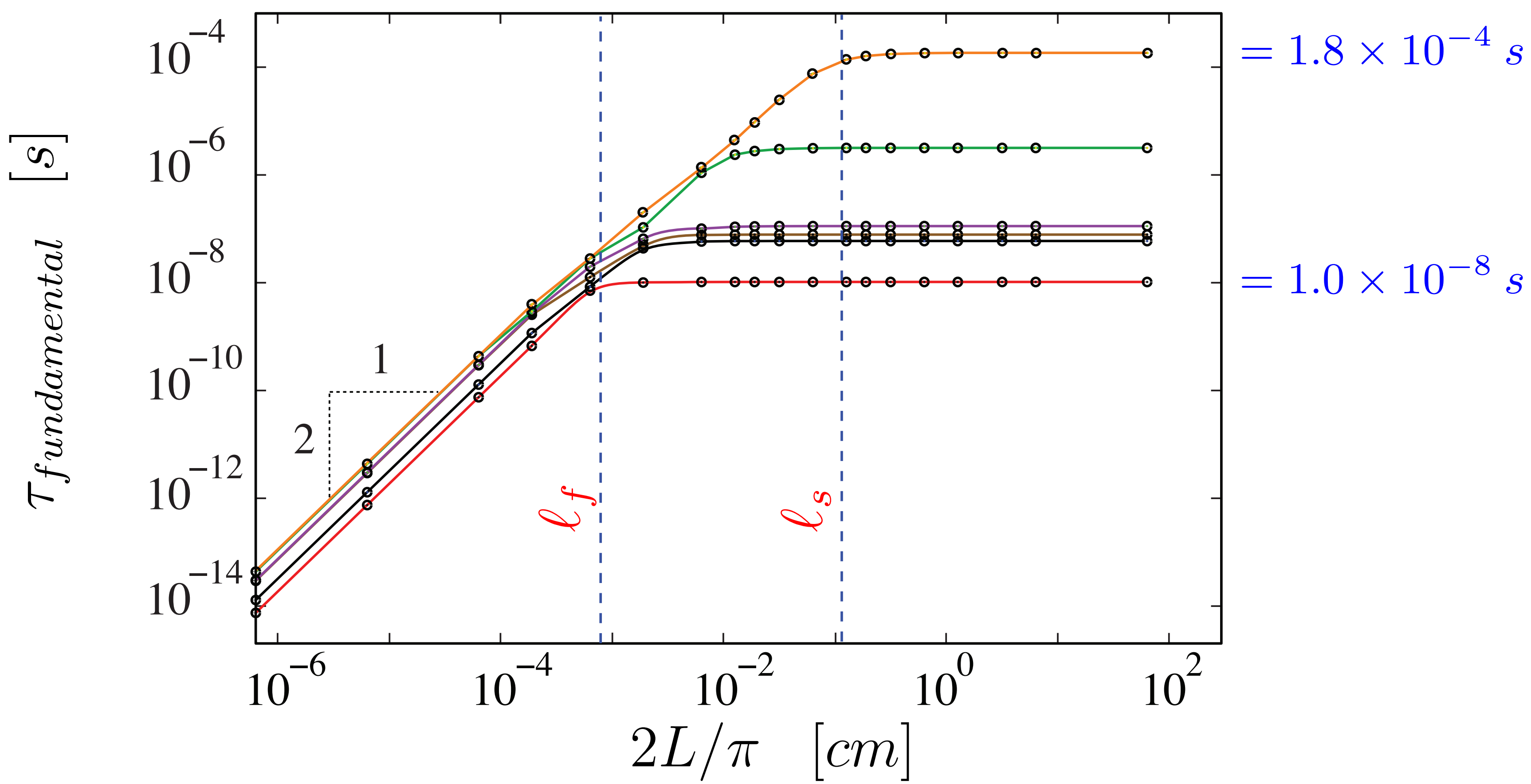
$$\boldsymbol{\mathcal{A}}^e \cdot \frac{d\boldsymbol{\mathcal{Z}}}{dt} = \left(\boldsymbol{\mathcal{J}}^e - \boldsymbol{\mathcal{B}}^e\right) \cdot \boldsymbol{\mathcal{Z}},$$

$\boldsymbol{\mathcal{A}}^e$ and $\left(\boldsymbol{\mathcal{J}}^e - \boldsymbol{\mathcal{B}}^e\right)$ are singular matrices.

- $L = 1\ cm$ and $D_{mix} = 64\ cm^2/s$,
- modified wavelength: $\widehat{\lambda} = 4L/(2\mathfrak{n} - 1)$,
- associated length scale: $\ell = \widehat{\lambda}/(2\pi) \;\Rightarrow\; \ell = \frac{2L}{(2\mathfrak{n}-1)\pi}$,



- $\ell_{finest} = 2.4 \times 10^{-4}\ cm,$
- $\ell_f = \sqrt{D_{mix}\tau_{fastest}} = 8.0 \times 10^{-4}\ cm,$
- $\ell_s = \sqrt{D_{mix}\tau_{slowest}} = 1.1 \times 10^{-1}\ cm,$



Summary

- Time and length scales are coupled.
- Short wavelength modes are dominated by diffusion, and coarse wavelength modes have time scales dominated by reaction.
- For a resolved diffusive structure, Fourier modes of sufficiently fine wavelength must be considered so that their associated time scale is of similar magnitude to the fastest chemical time scale.
- For a $p = 1\,atm, H_2{+}air$ laminar flame, the length scale where fast reaction balances diffusion is $\sim 2\ \mu m$; the associated fast time scale is $\sim 10\ ns$.