Reduced-Order Models for the Prediction of Unsteady Heat Release in Acoustically Forced Combustion

PhD Defense

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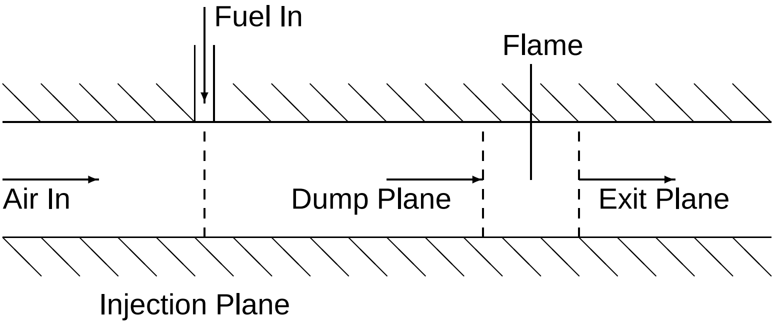
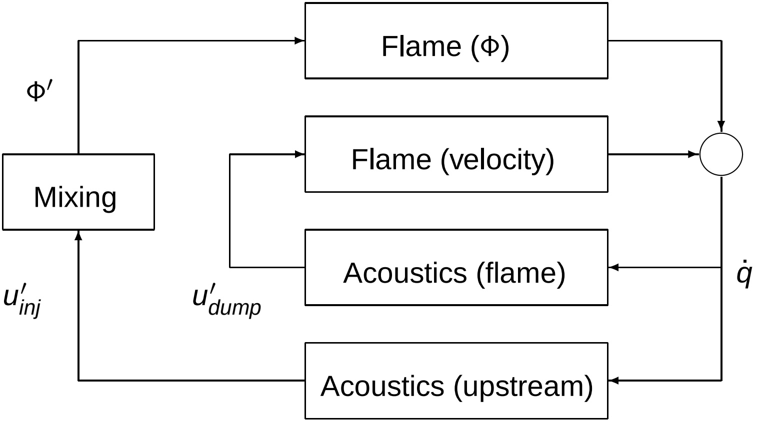
Motivation: Thermo-Acoustic Instabilities

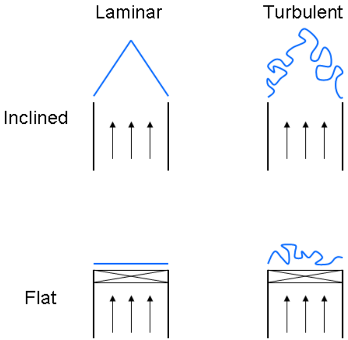


- Blowoff
- Flashback
- Reduced efficiency
- Premature degradation of hardware
- Elevated emissions

Anatomy of an instability



Anatomy of a Flame



Inclined flames

- Weak resonance with delay
- Scales with $Str = \frac{Lf}{U}$

Flat flames

- $2^n d$-order resonance
- Damping and stability vary

Approach

Part I: Highly Turbulent Combustion

- Derive various formulations for a dynamic WSR
- Look for scaling that agrees with reality

Part II: Laminar Combustion

- Experimentally investigate a laminar flat flame
- Use an FE model to study the flame numerically
- Derive an analytical model to search for scaling quantities
- Search for insights into the turbulent case

Part III: Moderately Turbulent Combustion

- Use Reynolds-averaging to simplify a 1-D model
- Look for scaling that agrees with reality

Part I: Highly Turbulent Combustion

Limiting Assumptions

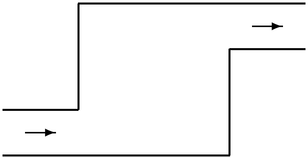
Highly turbulent implies very fast mixing.

- Spatial gradients are negligible in the reactor
- Incoming reactants are mixed instantly
- Leaving products are identical to the reactor contents
- The volume of the reactor is constant

Thus,

$$Da_t = \frac{t_t}{t_r} < 1$$

Governing Equations



$$\dot{Y}_i + {t_m}^{-1}\left(Y_i - Y_{i,in}\right) = \zeta_i$$

$$C_p\dot{T} + {t_m}^{-1}\sum_i Y_{i,in}\left(h_i - h_{i,in}\right) = -\sum_i h_i\zeta_i$$

Three WSR Models: Simple, Non-Simple Enthalpy, Multi-Step Kinetic

Simple WSR

Single-step reaction, Constant & equal C_p,

$$T = \Delta T c + T_0, \quad Y_i = \Delta Y_i c + Y_{i,0}$$

$$c' + (1 + \epsilon u)c = Da\, R(c)$$

$$R(c) = A \exp\left(-\frac{T_a}{T}\right)(1 - c)$$

$$c_0 = Da\, R(c_0) \qquad c_1' + (1 - Da\, R')c_1 = -u\, c_0$$

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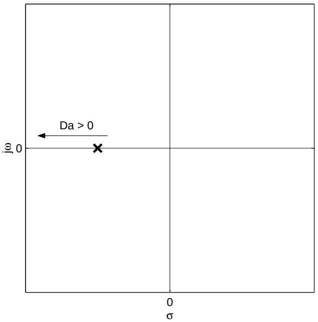
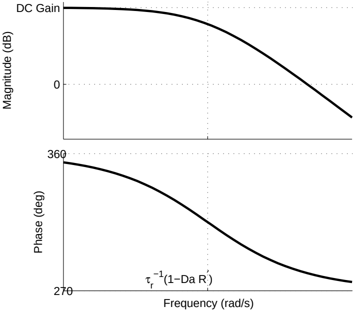
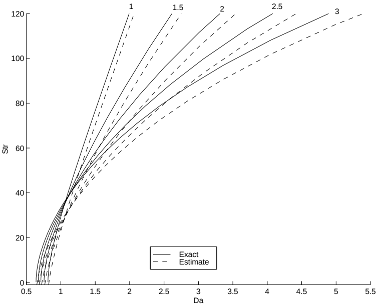
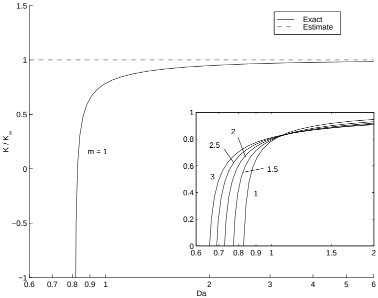
Simple WSR Solution









Non-Simple Enthalpy WSR

Single-step reaction

$$T = \Delta T \tau + T_0, \quad Y_i = \Delta Y_i c + Y_{i,0}$$

$$h(c,\tau) = (1-c) h_r(\tau) + c\, h_p(\tau)$$

$$\dot{m} = \dot{m}_0 (1 + \epsilon u(t)), \quad c_{in} = 0 + \epsilon v(t))$$

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$$(C_p \Delta T)\tau' + (h_r(\tau) - h_r(0)) = \Delta h(\tau) Da \cdot \hat{R}(\tau, c)$$
$$c' + c = Da \cdot \hat{R}(\tau, c).$$

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$$\tau_1' + \left[1 - \beta Da \cdot \hat{R}_\tau\right] \tau_1 + \left[-\beta Da \cdot \hat{R}_c\right] c_1 = -u\beta c_0 + (\beta - \beta_0) v$$

$$c_1' + \left[-Da \cdot \hat{R}_\tau\right] \tau_1 + \left[1 - Da \cdot \hat{R}_c\right] c_1 = -u c_0 + v$$

Non-Simple Enthalpy WSR

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$$\hat{c} = \frac{C_{p,r}(\tau) - C_{p,p}(\tau)}{C_p(\tau, c)} \qquad \beta(\tau_0, c_0) = \frac{h_r(\tau_0) - h_p(\tau_0)}{C_p(\tau_0, c_0)\Delta T}$$

Non-Simple Enthalpy Solution

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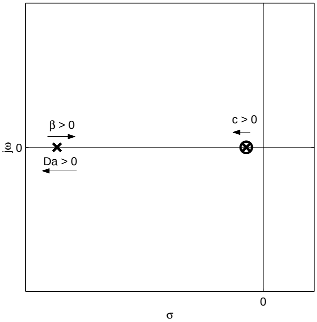

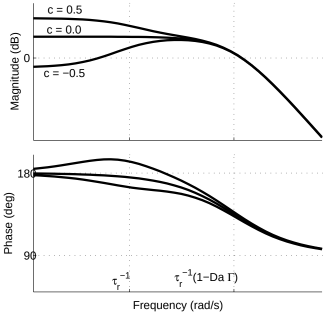

Multi-Step Chemical Kinetic WSR

Constant & equal C_p

$$\mathbf{X}_0 = \left\{ \begin{array}{c} T_0 \\ \mathbf{Y}_0 \end{array} \right\} \qquad \mathbf{X}_1 = \left\{ \begin{array}{c} T_1 \\ \mathbf{Y}_1 \end{array} \right\} \qquad \mathbf{q} = \left\{ \begin{array}{c} q_1 \\ \vdots \\ q_n \end{array} \right\}$$

$$\mathbf{X}_0 - \mathbf{X}_{0,inlet} = t_m \mathbf{A}_1 \cdot \mathbf{q}$$
$$\dot{\mathbf{X}}_1 + \left({t_m}^{-1} \mathbf{I} - \mathbf{A}_1 \cdot \mathbf{J} \right) \cdot \mathbf{X}_1 = \mathbf{B} \cdot \mathbf{U}.$$

$$\mathbf{q}_1 = \mathbf{J} \cdot \mathbf{X}_1$$

$$\dot{\mathbf{q}}_1 = \left(-t_m^{-1} \mathbf{I} + \mathbf{J} \cdot \mathbf{A}_1 \right) \cdot \mathbf{q}_1 + \mathbf{J} \cdot \mathbf{B} \cdot \mathbf{U}$$

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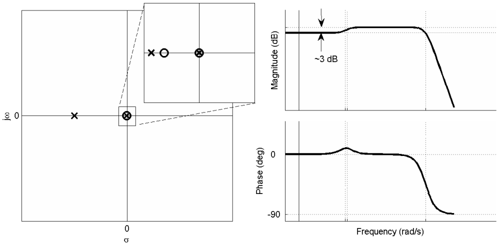
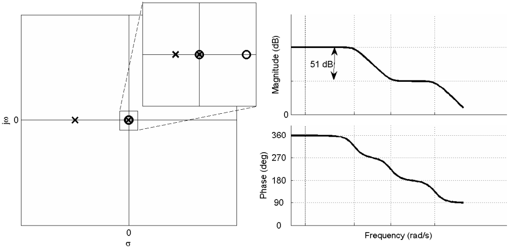
Multi-Step Results

Velocity Response



Equivalence Ratio Response



Summary

Summary of WSR Models

- Simple WSR

$$\omega_c = t_m{}^{-1}\left[1 - Da \cdot \hat{R}'(c_0)\right] \approx -t_r{}^{-1} R'(c_0)$$

- Non-Simple Enthalpy WSR

$$\omega_c = t_m{}^{-1}\left[1 - Da \cdot \hat{R}'(c_0)\right] \approx -t_r{}^{-1} R'(c_0)$$

- Multi-Step Chemical Kinetic WSR
  Multiple frequencies scaling with the various reaction times.

Part II: Laminar Combustion

Geometry & Limiting Assumptions

- 1-D symmetrical flow
- Single-step chemical kinetics
- *Non-unity Lewis number*

$$T = \Delta T\,\tau + T_0 \qquad Y_i = \Delta Y_i\,c + Y_{i,0}$$

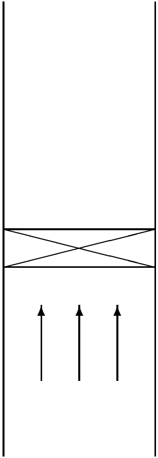
- Neglect density changes in space

$$\nabla \cdot \mathbf{u} \approx 0$$

- Typical non-dimensionalization

$$\hat{t} = \frac{t}{t_r} \qquad \hat{x} = \frac{x}{\delta} \qquad \hat{u} = \frac{u}{S_L}$$

$$\delta \equiv \sqrt{\alpha t_r} \qquad S_L \equiv \sqrt{\frac{\alpha}{t_r}}$$



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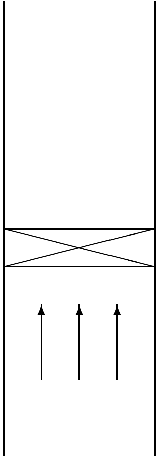

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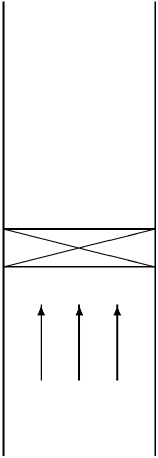

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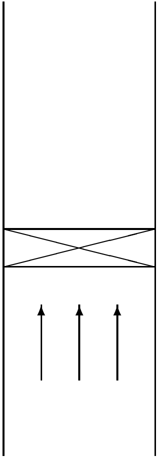

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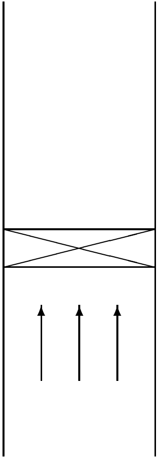

Governing Equations

$$\dot{c} + \hat{u}\, c' - \frac{1}{Le} c'' = R(c,\tau)$$
$$\dot{\tau} + \hat{u}\, \tau' - \tau'' = R(c,\tau)$$

$$\hat{u} = \hat{U} + \epsilon \exp(j\Omega\hat{t})$$

Static

$$\hat{U}\, c_0' - \frac{1}{Le} c_0'' = R(c_0,\tau_0)$$
$$\hat{U}\, \tau_0' - \tau_0'' = R(c_0,\tau_0)$$

Dynamic

$$(j\Omega - R_c)\, c_1 + \hat{U}\, c_1' - \frac{1}{Le} c_1'' = R_\tau \tau_1 - c_0'$$
$$(j\Omega - R_\tau)\, \tau_1 + \hat{U}\, \tau_1' - \tau_1'' = R_c c_1 - \tau_0'$$

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Governing Equations

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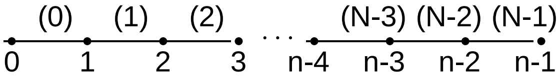
Dynamic

$$(j\Omega - R_c)\, c_1 + \hat{U}\, c_1' - \tfrac{1}{Le}\, c_1'' = R_\tau \tau_1 - c_0'$$
$$(j\Omega - R_\tau)\, \tau_1 + \hat{U}\, \tau_1' - \tau_1'' = R_c c_1 - \tau_0'$$

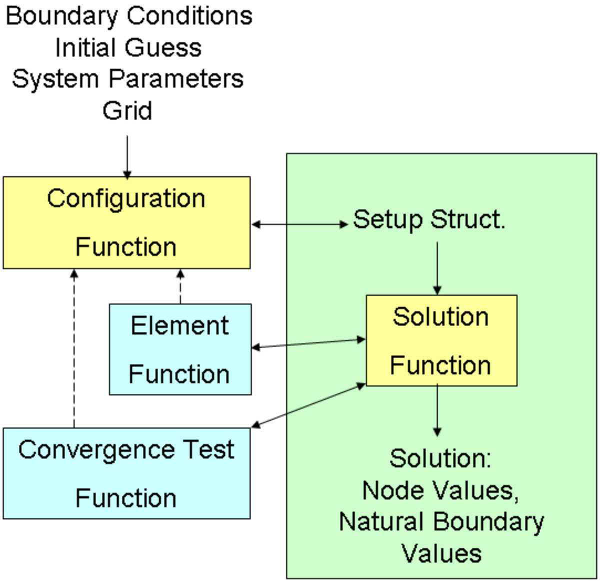
Finite Element Model

Defining the Element

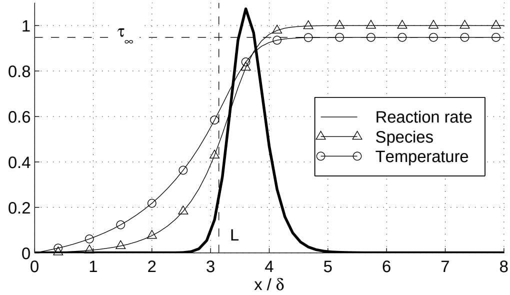


- Ahrrenius reaction rate
- Constant choice of t_r so that $R \approx O(1)$
- Linear interpolation functions
- Galerkin method of weighted residuals
- One-dimensional

A Brief Look at the Solver

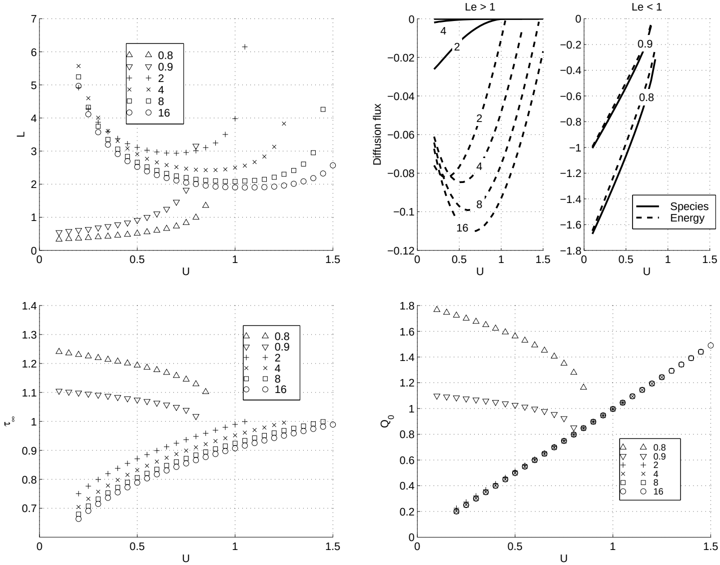


Static Solution



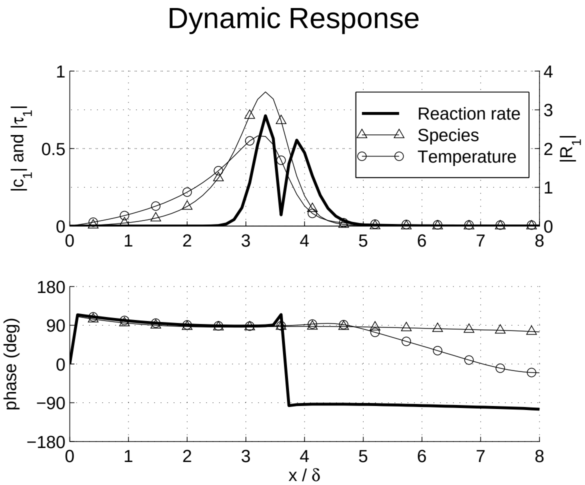
$U = 0.7$, $Le = 2.0$, 150-point grid

Static Results



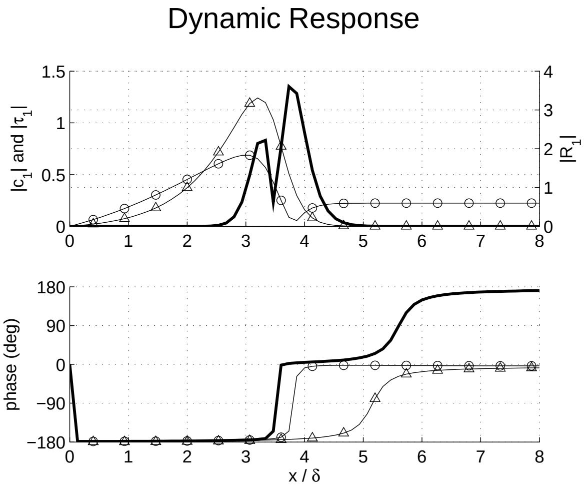
- Both estimates break down near $Le \approx 1$

Dynamic Solution



$U = 0.7$, $Le = 2.0$, $\Omega = 0.01$, 150-point grid

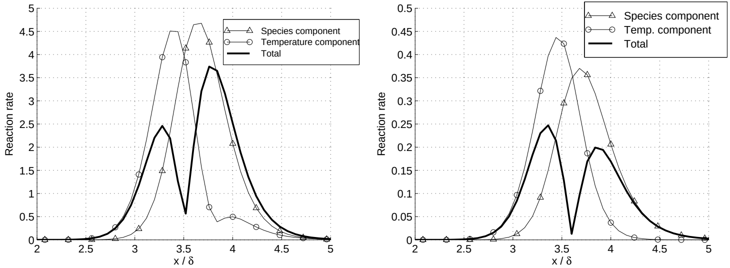
Dynamic Solution



$U = 0.7$, $Le = 2.0$, $\Omega = 1.0$, 150-point grid

Internal Structure

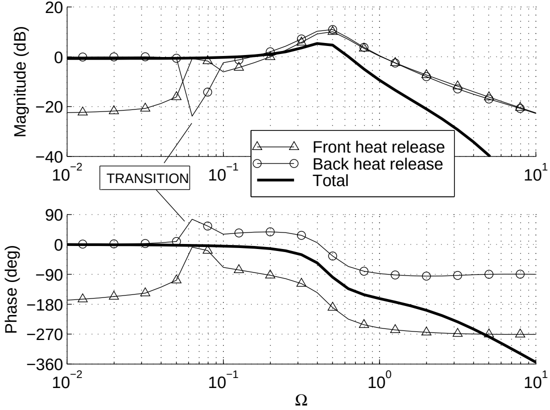
Heat release contribution from c and τ oscillations



$U = 0.8$, $Le = 2.0$, (left) $\Omega = 0.02$, (right) $\Omega = 10.0$

Internal Structure

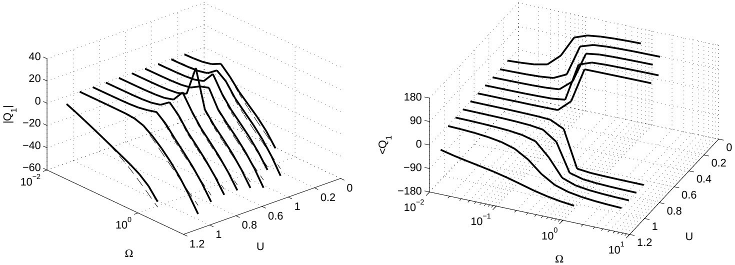
Front-half, back-half, and total heat release dynamics



$U = 0.8, Le = 2.0$

Dynamic Response

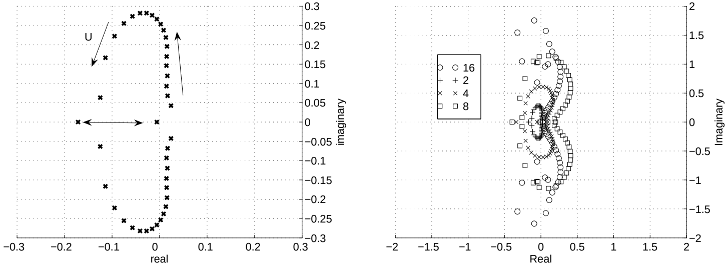
Heat release contribution from c and τ oscillations



$$Le = 2$$

Dynamic Response

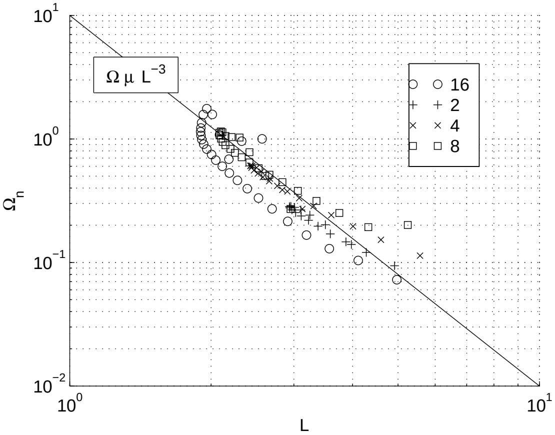
Complex root motion w.r.t. $\hat{U}$ for various Le



(left) $Le = 2$ only, (right) all Le

Scaling

Natural frequency as a function of standoff distance



Analytical Model

Ignition Reaction Model

$$\text{Ahrrenius:} \quad R = A\exp\left(-\frac{\tau_a}{\tau_0+\tau}\right)(1-c)$$

$$\text{Ignition:} \quad R = Ah\left(\tau - \tau_{ig}\right)(1-c)$$

Ignition Advantages

- A jump condition is simpler than an exponential
- The steady solution is still C^1 continuous
- Already proven to give good results for $Le = 1$

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- The steady solution is still C^1 continuous
- Already proven to give good results for $Le = 1$

Static Solution

Preheat

$$0 = Uc_0' - \frac{1}{Le}c_0'' \qquad \frac{c_0}{c_L} = \frac{\exp(U\,Le\,x) - 1}{\exp(U\,Le\,L) - 1}$$

$$0 = U\tau_0' - \tau_0'' \qquad \frac{\tau_0}{\tau_{ig}} = \frac{\exp(U\,x) - 1}{\exp(U\,L) - 1}$$

Flame

$$Uc_0' - \frac{1}{Le}c_0'' = A - Ac_0 \qquad c_0 = 1 - \Delta c \exp(\Lambda(x - L))$$

$$U\tau_0' - \tau_0'' = A - Ac_0 \qquad \tau_0 = \tau_{ig} + \Delta\tau\,[1 - \exp(\Lambda(x - L))]$$

Static Solution

Preheat

$$0 = Uc_0' - \frac{1}{Le}c_0''$$
$$0 = U\tau_0' - \tau_0''$$

$$\frac{c_0}{c_L} = \frac{\exp\left(U\,Le\,x\right) - 1}{\exp\left(U\,Le\,L\right) - 1}$$
$$\frac{\tau_0}{\tau_{ig}} = \frac{\exp\left(U\,x\right) - 1}{\exp\left(U\,L\right) - 1}$$

Flame

$$Uc_0' - \frac{1}{Le}c_0'' = A - Ac_0$$
$$U\tau_0' - \tau_0'' = A - Ac_0$$

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Static Solution

Preheat

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Flame

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Static Solution

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$$U\tau_0' - \tau_0'' = A - Ac_0 \qquad \tau_0 = \tau_{ig} + \Delta\tau\,[1 - \exp(\Lambda(x - L))]$$

$$\Lambda = \frac{U\,Le}{2}\left(1 - \sqrt{1 + \frac{4A}{U^2 Le}}\right)$$

Static Solution

Preheat

$$0 = Uc_0' - \frac{1}{Le}c_0''$$
$$0 = U\tau_0' - \tau_0''$$

$$\frac{c_0}{c_L} = \frac{\exp\left(U\,Le\,x\right) - 1}{\exp\left(U\,Le\,L\right) - 1}$$
$$\frac{\tau_0}{\tau_{ig}} = \frac{\exp\left(U\,x\right) - 1}{\exp\left(U\,L\right) - 1}$$

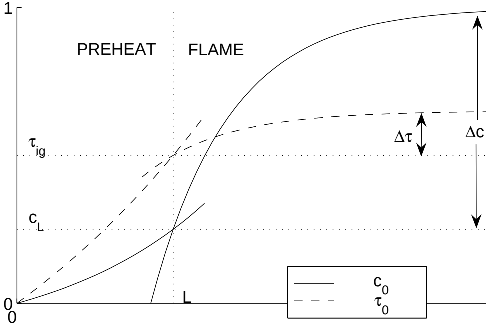
Flame

$$Uc_0' - \frac{1}{Le}c_0'' = A - Ac_0$$
$$U\tau_0' - \tau_0'' = A - Ac_0$$

$$c_0 = 1 - \Delta c\exp\left(\Lambda(x - L)\right)$$
$$\tau_0 = \tau_{ig} + \Delta\tau\left[1 - \exp\left(\Lambda(x - L)\right)\right]$$

Interfacial Matching

The offset distance, L, and Δc are still unknown.



$$(1-\Delta c) U\, Le\, n(U\, Le\, L) = -\Delta c\, \Lambda$$
$$\tau_{ig} U\, n(U\, L) = -\beta\, \Delta c\, \Lambda$$

Interfacial Matching

Alas! No exact solution.

- High Le

$$\Delta c = \frac{-U\Lambda}{A}.$$

$$L = \frac{1}{U} \ln \left(\frac{1}{1 + \frac{U\tau_{ig}}{\Lambda\beta\Delta c}} \right)$$

- Low Le

$$\Delta c = 1 - \frac{\tau_{ig}}{\beta}$$

$$L = -\frac{1}{\Lambda} \left(\frac{\tau_{ig}/\beta}{1 - \tau_{ig}/\beta} \right)$$

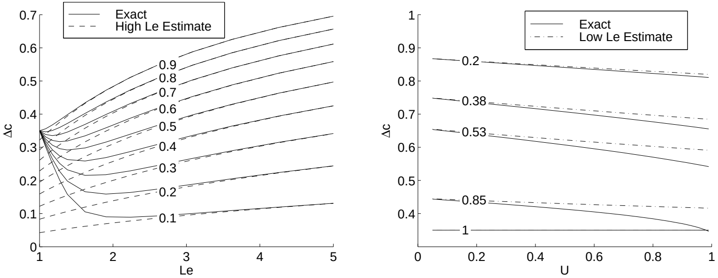
Interfacial Matching

When $U \to 1$, $L \to \infty$. The system of equations reduces precisely

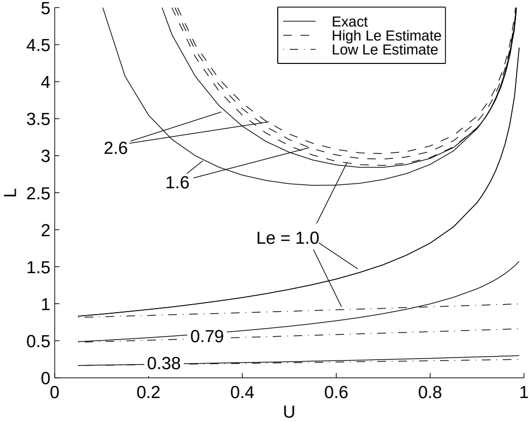
$$A = \frac{Le}{4}\left[\left(1 + \frac{2a}{Le}\right)^2 - 1\right]$$

$$a = \frac{\tau_{ig}}{1 - \tau_{ig}}$$

Static Results



Static Results



Dynamic Solution

$$(j\Omega - R_c)\, c_1 + \hat{U}\, c_1' - \frac{1}{Le}\, c_1'' = R_\tau \tau_1 - c_0'$$

$$(j\Omega - R_\tau)\, \tau_1 + \hat{U}\, \tau_1' - \tau_1'' = R_c c_1 - \tau_0'$$

Preheat

$$c_1 = p^+ \exp\left(k^+ (x - L)\right) + p^- \exp\left(k^- (x - L)\right) - \frac{c_0'}{j\Omega}$$

$$\tau_1 = b^+ \exp\left(d^+ (x - L)\right) + b^- \exp\left(d^- (x - L)\right) - \frac{\tau_0'}{j\Omega}$$

Flame

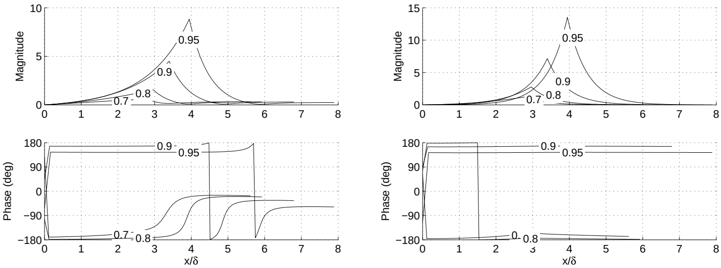
$$c_1 = P \exp\left(K\,(x - L)\right) - \frac{c_0'}{j\Omega}$$

$$\tau_1 = B \exp\left(D\,(x - L)\right) + PG \exp\left(K\,(x - L)\right) - \frac{\tau_0'}{j\Omega}$$

Dynamic Solution

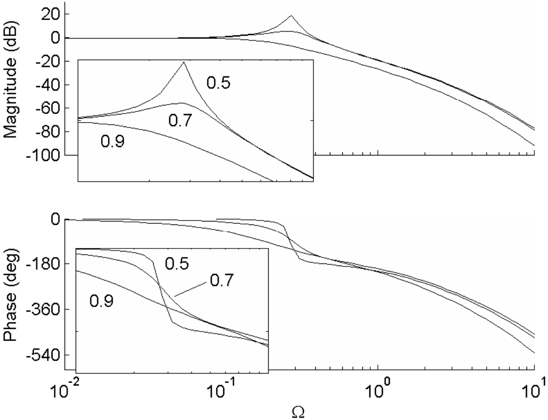
$$\mathbf{M}(\Omega) \cdot \left\{ \begin{array}{c} p^{+} \\ p^{-} \\ P \\ b^{+} \\ b^{-} \\ B \end{array} \right\} = \left\{ \begin{array}{c} c_0'(0)\,/\,j\Omega \\ \tau_0'(0)\,/\,j\Omega \\ 0 \\ 0 \\ 0 \\ 0 \end{array} \right\}$$

Dynamic Results



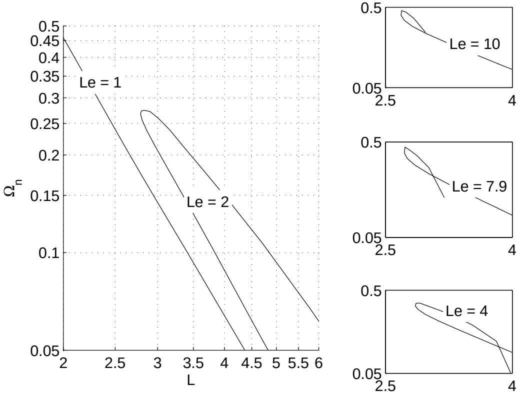
$Le = 2$, $\Omega = 0.1$, (left) species (right) temperature

Dynamic Results



$Le = 2$

Scaling



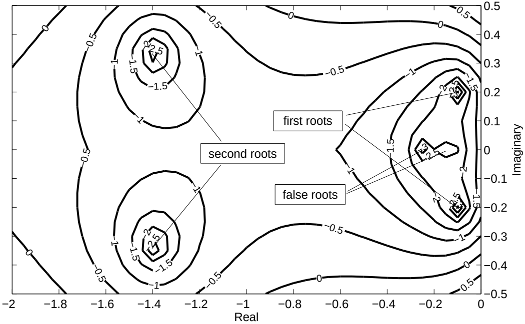
Eigen Values

Consider the homogeneous case:

$$\mathbf{M}(\lambda) \cdot \begin{Bmatrix} p^+ \\ p^- \\ P \\ b^+ \\ b^- \\ B \end{Bmatrix} = 0$$

$$\det(\, \mathbf{M}(\lambda)\,) = 0$$

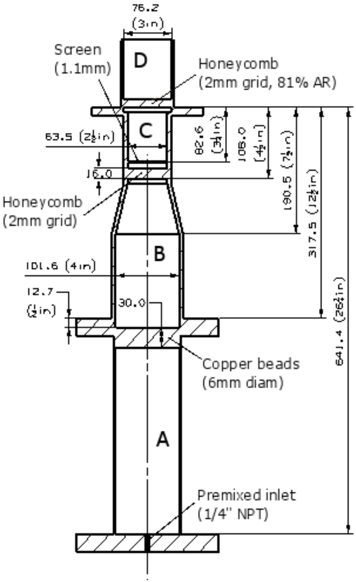
Eigen Values



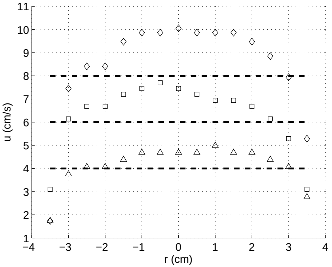
$\log_{10}\left(\det\left(\mathbf{M}\right)\det\left(\mathbf{M}\right)^{*}\right)$ as a function of λ in complex space

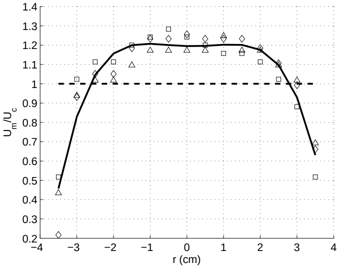
Experimental Investigation

Experimental Setup



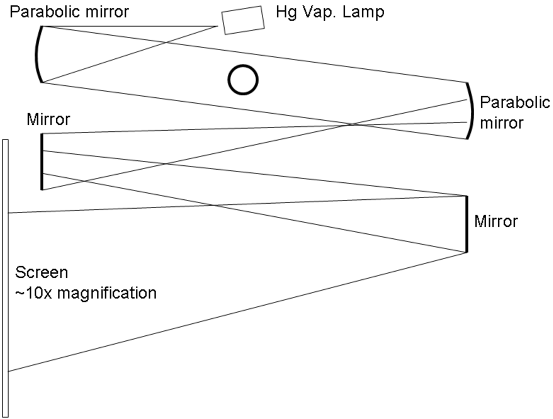
Velocity Profile Measurements



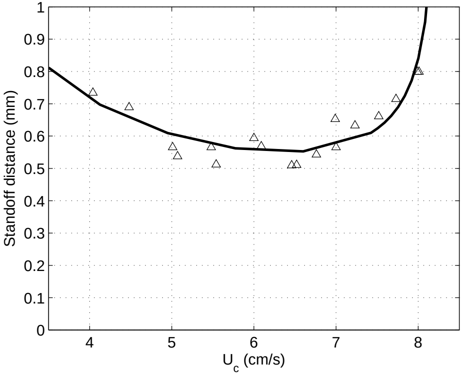


- Approximately 5*mm* above the honeycomb
- The honeycomb is 7*cm* in diameter
- Mean velocities are $4cm/s$, $6cm/s$, and $8cm/s$

Heat Release Rate

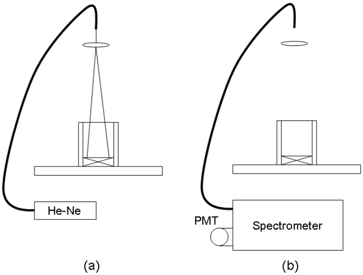


Heat Release Rate



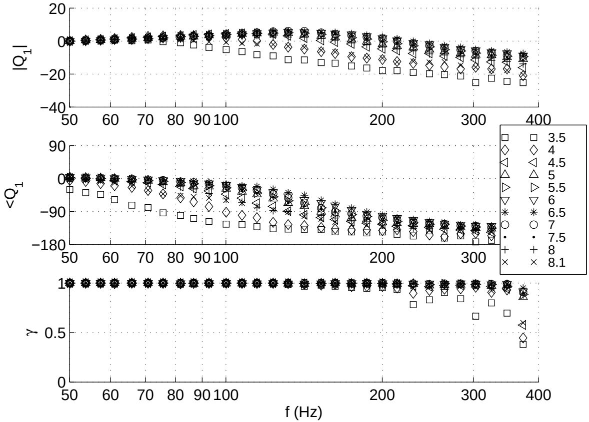
$$L \approx C \left(\frac{U_c}{U_L}\right)^{-1.15} \left(1 - \frac{U_c}{U_L}\right)^{-0.34}$$

Heat Release Rate

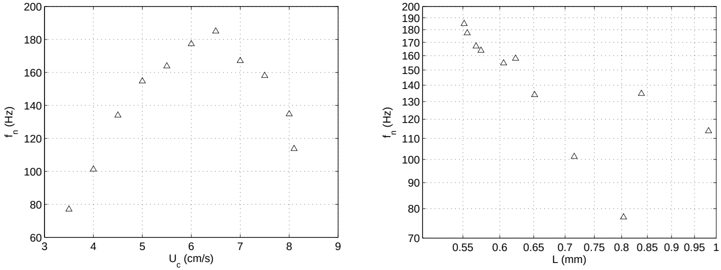


- The optics are focused to roughly a $4cm$ diameter via the He-Ne laser
- The fiber is connected to a spectrometer at $308nm$ (OH^*)

Transfer Function Measurements

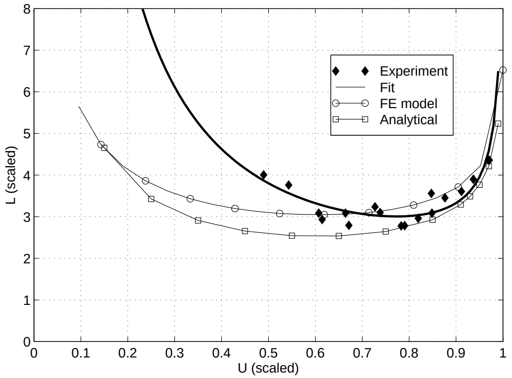


Scaling

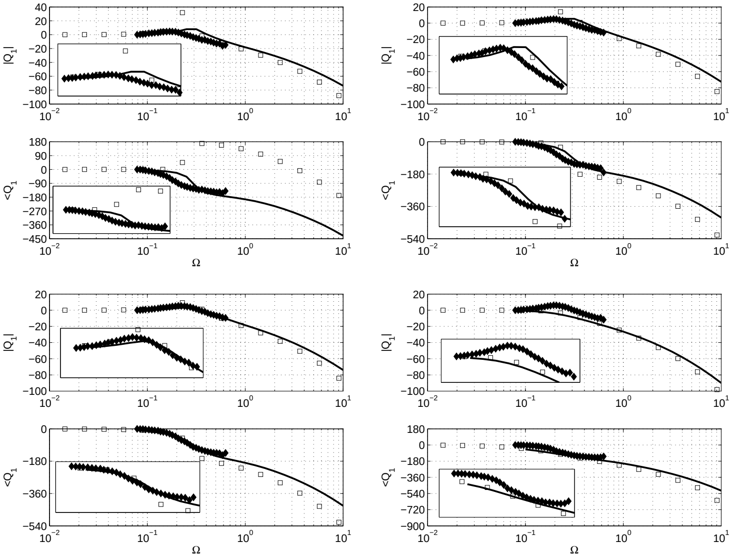

200
180
160
140
120
100
80
60
3
4
5
6
7
8
9
f_n (Hz)
U_c (cm/s)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
0.55
0.6
0.65
0.7
0.75
0.8
0.85
0.9
0.95
1
f_n (Hz)
L (mm)

Comparison of Laminar Models and Data

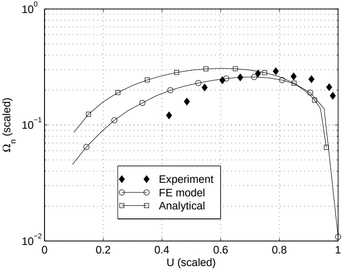
Static Comparison

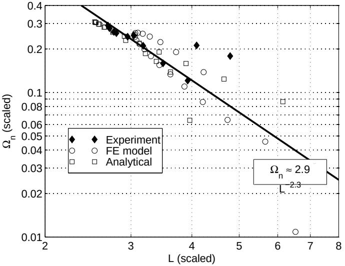


Transfer Function Comparison



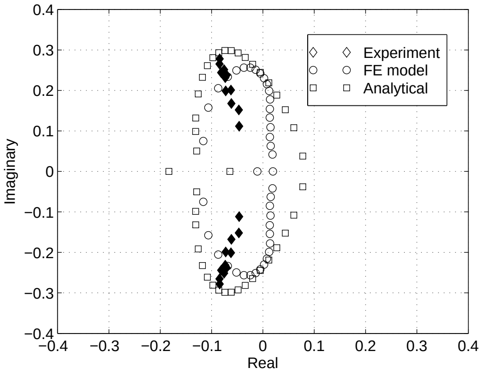
Frequency Comparison





- FE velocity is scaled by the blowoff velocity
- Experimental is scaled by methane flame diffusivity and reaction time
- Velocity disagreement is due to preheating from the ceramic

Root Loci



Preheating from the ceramic also explains the model's instability.

Part III: Moderately Turbulent Combustion

Governing Equations

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T - \nabla \cdot (\alpha \nabla T) = -\frac{\Delta T}{Y_{f,0}} \zeta_f$$

$$\frac{\partial Y_i}{\partial t} + \mathbf{u} \cdot \nabla Y_i - \nabla \cdot (D_i \nabla Y_i) = \zeta_i$$

- Reynolds averaging eliminates uncorrelated oscillations
- Assume turbulence dominates molecular and thermal diffusion

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$$\frac{\partial \langle T \rangle}{\partial t} + (u + v) \frac{\partial \langle T \rangle}{\partial x} - D_T \frac{\partial^2 \langle T \rangle}{\partial x^2} = -\frac{\Delta T}{Y_{f,0}} \langle \zeta_f \rangle$$

$$\frac{\partial \langle Y_i \rangle}{\partial t} + (U + v) \frac{\partial \langle Y_i \rangle}{\partial x} - D_T \frac{\partial^2 \langle Y_i \rangle}{\partial x^2} = \langle \zeta_i \rangle$$

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- Reynolds averaging eliminates uncorrelated oscillations
- Assume turbulence dominates molecular and thermal diffusion

$$\dot{c} + (\hat{U} + \hat{v})c' - c'' = R(c)$$

Turbulent Ignition Model

$$R(c) = A\,h(c - c_{ig})\,h(1 - c)$$

- "Switches on" at c_{ig} and "switches off" when the fuel is exhausted
- Obeys Ranalli's observation that heat release is proportional to volume
- Analytically simple

Analytical Solution

Static Solution

Preheat

$$\hat{U}c_0' - c_0'' = 0$$

Flame

$$\hat{U}c_0' - c_0'' = A$$

Equilibrium

$$\hat{U}c_0' - c_0'' = 0$$

Static Solution

Preheat

$$c_0^{(p)} = c_{ig} \frac{\exp(\hat{U}x) - 1}{\exp(\hat{U}L_f) - 1}$$

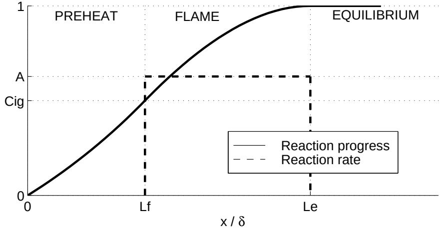
Flame

$$c_0^{(f)} = 1 - \frac{A}{U^2}\left[\exp\left(U(\hat{x} - L_e)\right) - 1\right] + \frac{A}{U}(\hat{x} - L_e)$$

Equilibrium

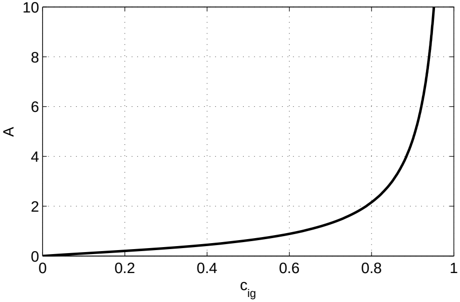
$$c_0^{(e)} = 1$$

Static Solution



- Interface matching applied just like with the PFR
- Yields leading and trailing edge positions
- The reaction coefficient is solved similarly (iteratively)

Static Solution



- Interface matching applied just like with the PFR
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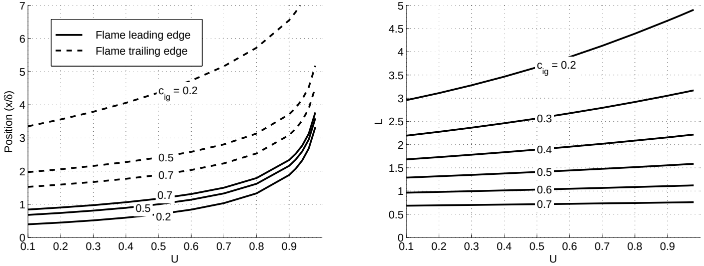
Static Results



(left) Flame leading and trailing edges (right) flame thickness

Dynamic Solution

$$j\Omega c_1 + \hat{U} c_1' - c_1'' = -c_0'$$

- All three regions have the same governing equation
- The jump conditions and the particular solution shape the response

$$c_1^{(p)} = B^{(p)+} \exp\left(k^+ \hat{x}\right) + B^{(p)-} \exp\left(k^- \hat{x}\right) - \frac{c_0'}{j\Omega}$$

$$c_1^{(f)} = B^{(f)+} \exp\left(k^+ \left(\hat{x} - L_e\right)\right) + B^{(f)-} \exp\left(k^- \left(\hat{x} - L_e\right)\right) - \frac{c_0'}{j\Omega}$$

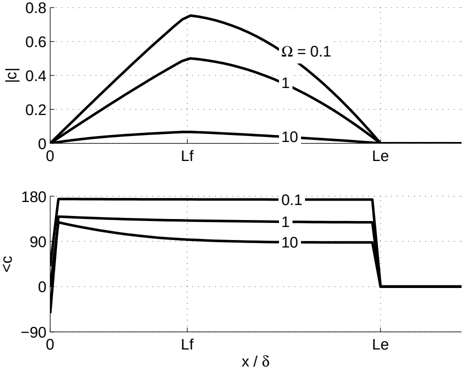
$$c_1^{(e)} = 0$$

Interfacial Matching

$$\mathbf{P}(\Omega) \cdot \mathbf{M}(\Omega)^{-1} = \begin{Bmatrix} B^{(p)+} \\ B^{(p)-} \\ B^{(f)+} \\ B^{(f)-} \end{Bmatrix}$$

- Jump conditions are accounted for in **M**
- Particular solution is accounted for in **P**

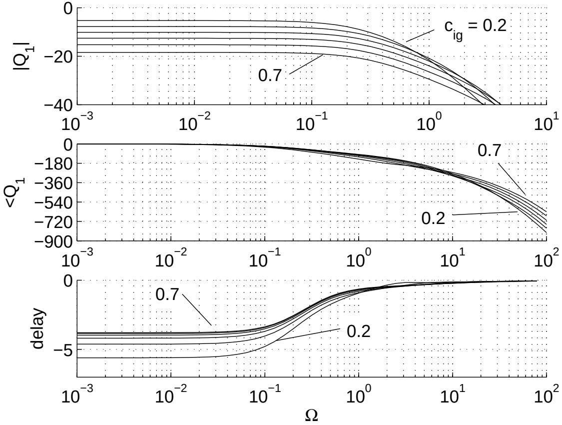
Dyamic Solution



- Discontinuities at L_f and L_e
- Phase is almost constant
- Unsteady heat release is determined entirely at L_f and L_e

Results and Analysis

Frequency Response



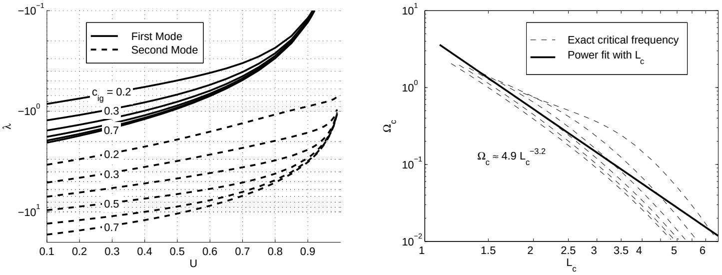
Eigen Values

$$\det(\mathbf{M}(\lambda)) = 0$$

$$J \sinh(\beta \mathcal{L}) \sinh(\beta L_f) + \beta \sinh(\beta L_e) = 0$$

$$\beta = \sqrt{\frac{\hat{U}^2}{4} + \lambda} \qquad J = \frac{-\hat{U}}{1 - \exp\left(-\hat{U}\mathcal{L}\right)}$$

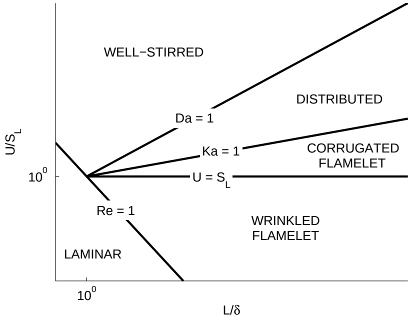
Eigen Values



- Eigen values scale crudely as a power of L_c
  $\lambda_1 \propto {L_c}^{-3.2}$
- Delay is determined entirely by pole locations
  $t_\infty = \sum_{n=1}^{\infty} \frac{1}{\lambda_n}$

Unifying the Model Results

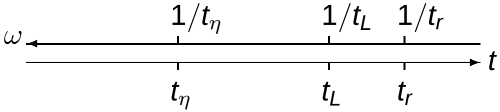
The Bhorgi Diagram



$$Da = \frac{t_L}{t_r}$$
$$= \left(\frac{L}{\delta}\right)\left(\frac{u_L}{S_L}\right)^{-1}$$

$$Ka = \frac{t_r}{t_\eta} = \frac{\delta/S_L}{L/u_L} Re_L^{1/2}$$
$$= \left(\frac{u_L}{S_L}\right)^{3/2}\left(\frac{L}{\delta}\right)^{-1/2}$$

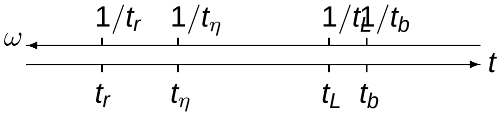
Highly Turbulent Combustion



Scales with the reaction time

$$\Omega_c = \omega_c \, t_r \approx 1$$

Moderately Turbulent Combustion



- Flat flames scale as a power law with distance

$$\Omega_c \propto \left(\frac{L_c}{\delta_t}\right)^{-m} = Da^{-m/2}$$

- Inclined flames scale with the Strouhal number

$$\Omega_c \propto \left(\frac{U}{S_L}\right)\left(\frac{L}{\delta}\right)^{-1} = Da^{-1}$$

Laminar Combustion

- Flat laminar flames scale as a power law with displacement

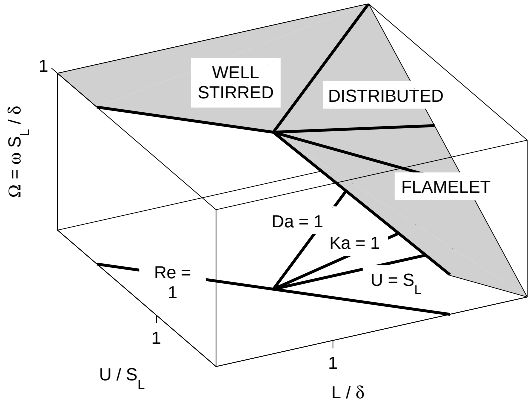
$$\Omega_c \propto L^{-m}$$

- Inclined laminar flames scale with the Strouhal number

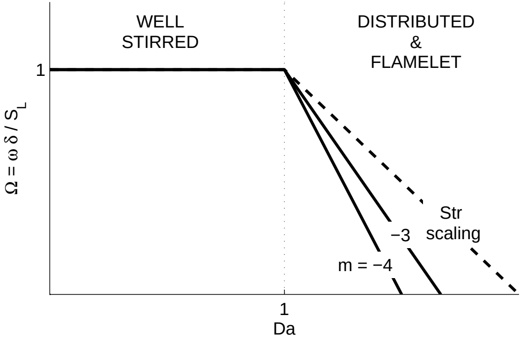
$$\Omega_c \propto \frac{U}{L}$$

- Turbulent structures die off and do not play a major role in the laminar regime

The Extended Bhorgi Diagram



The Extended Bhorgi Diagram



Future Work

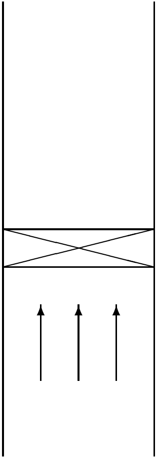
Additional Laminar Work

1. Experimental laminar transition study:

   Study the transition from flat, burner-stabilized flames to inclined flames.

2. Unify flamelet and laminar models:

   Write a 2-D model valid during the transition from flat to inclined flame.



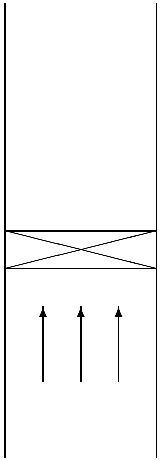
Additional Turbulent Work

3. Experimental turbulent transition study

   Study the transition from flat, burner-stabilized flames to inclined flames.

4. Unify flamelet and Reynold-averaged models

   Write a 2-D model valid during the transition from flat to inclined flame. What is the effect of turbulent flame thickness on the flamelet analysis?



Questions