Nonlinear Dynamics of Unsteady Premixed, Planar Flames.

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A. Liñán

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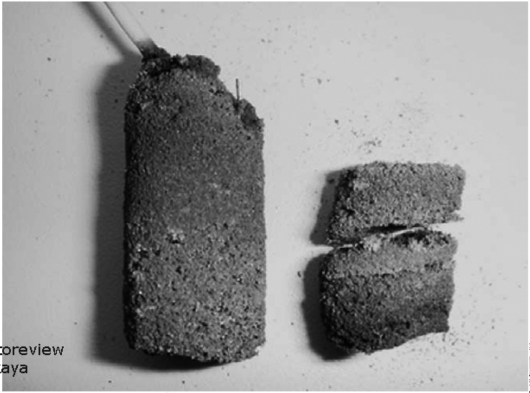
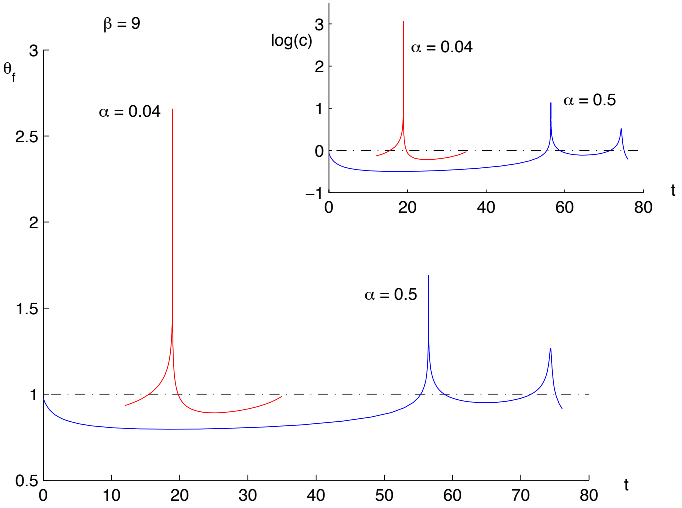
Physical problem. High-temperature Synthesis.



Historical retrospective of SHS: An autoreview
A. G. Merzhanov & I. P. Borovinskaya
Int. J. of SHS. 2008 vol. 17 pp242-265

Physical problem. Time evolution.



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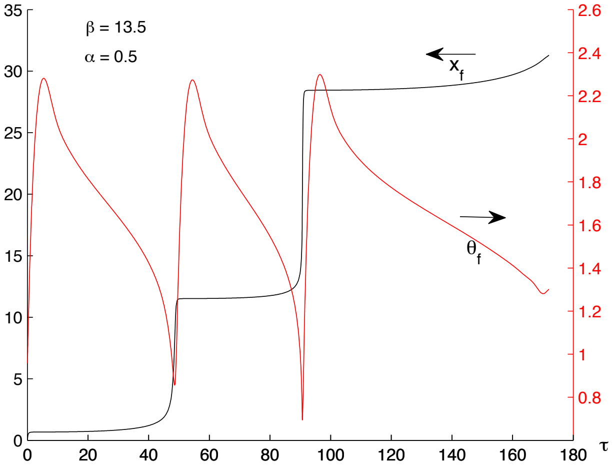
Flame displacement.



Planar, premixed flame in a solid.

Unsteady problem.

$$\frac{\partial \theta}{\partial t} + c\frac{\partial \theta}{\partial \xi} - \frac{\partial^2 \theta}{\partial \xi^2} = \beta\delta(\beta) Y \exp\left\{\frac{\beta(\theta-1)}{1+\alpha(\theta-1)}\right\}$$

$$\frac{\partial Y}{\partial t} + c\frac{\partial Y}{\partial \xi} - \underbrace{\frac{1}{Le}\frac{\partial^2 Y}{\partial \xi^2}}_{=0} = -\beta\delta(\beta) Y \exp\left\{\frac{\beta(\theta-1)}{1+\alpha(\theta-1)}\right\}$$

$$\theta = 0, \qquad Y = 1, \qquad \xi \to -\infty$$

$$\theta_\xi = 0, \qquad Y_\xi = 0, \qquad \xi \to \infty$$

- Zel'dovich number: $\beta = E(\tilde{T}_b - \tilde{T}_u)/R\tilde{T}_b^2 >> 1$
- Exothermicity: $\alpha = 1 - \tilde{T}_u/\tilde{T}_b \sim 1$

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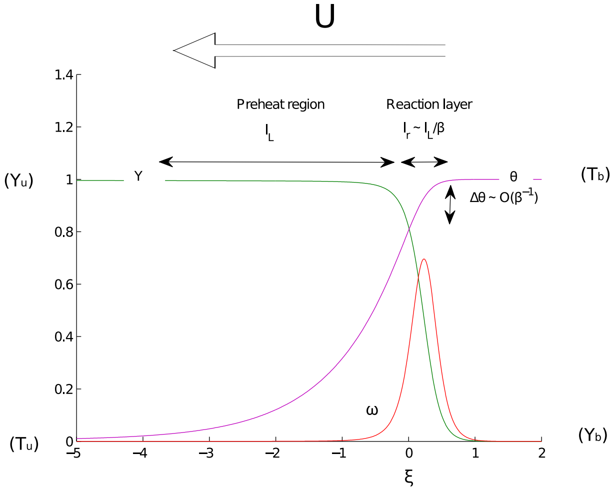
Steady flame structure.

Asymptotic structure for large β



Quasisteady reaction layer structure.

$$\frac{\partial \theta}{\partial t} + c\,\frac{\partial \theta}{\partial \xi} - \frac{\partial^2 \theta}{\partial \xi^2} = \beta \delta Y \exp\left\{ \frac{\beta\,(\theta - 1)}{1 + \alpha\,(\theta - 1)} \right\}$$

$$\frac{\partial Y}{\partial t} + c\,\frac{\partial Y}{\partial \xi} = -\beta \delta Y \exp\left\{ \frac{\beta\,(\theta - 1)}{1 + \alpha\,(\theta - 1)} \right\}$$

Boundary conditions?

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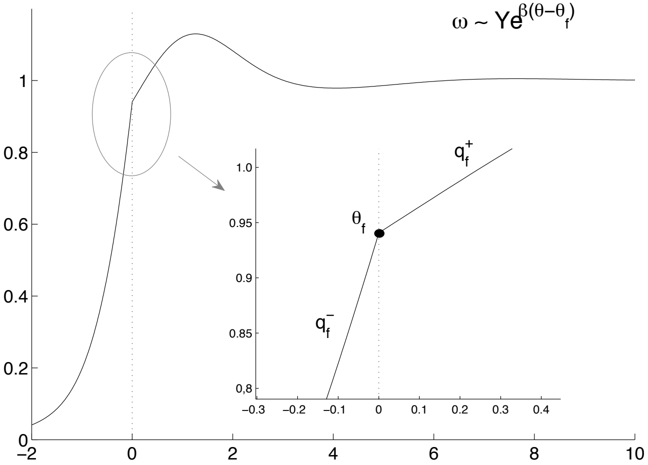
Quasisteady reaction layer structure.



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Quasisteady reaction layer structure.

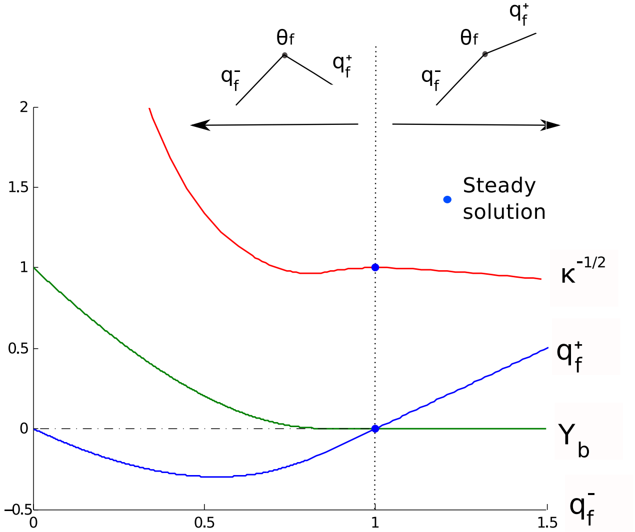
Solution.

Unburnt fuel: $$(1-q_f^-)\,\mathrm{Ln}\,Y_b + 1 - Y_b = 0$$

Heat fluxes jump: $$q_f^- = q_f^+ + 1 - Y_b$$

Flame velocity: $$c = \frac{1+\alpha(\theta_f - 1)}{\sqrt{\kappa(q_f^-)}}\, e^{\frac{(\beta/2)(\theta_f - 1)}{1+\alpha(\theta_f-1)}}$$

Quasisteady reaction layer structure.



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Reaction sheet formulation. Large β.

$$\frac{\partial \theta}{\partial t} + c\,\frac{\partial \theta}{\partial \xi} - \frac{\partial^2 \theta}{\partial \xi^2} = c \cdot (q_f^- - q_f^+) \cdot \delta(\xi)$$

$$\theta(\xi \to -\infty) = 0, \qquad \theta_\xi(\xi \to \infty) = 0$$

$$c = \frac{1 + \alpha(\theta_f - 1)}{\sqrt{\kappa(q_f^-)}}\, e^{\frac{(\beta/2)(\theta_f - 1)}{1 + \alpha(\theta_f - 1)}}$$

$$(1 - q_f^-) \ln Y_b + 1 - Y_b = 0$$

$$q_f^- = q_f^+ + 1 - Y_b$$

$$q_f^\pm = \theta_\xi(\xi = 0^\pm)/c, \qquad \theta_f(t) = \theta(0, t)$$

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$$q_f^- = q_f^+ + 1 - Y_b$$

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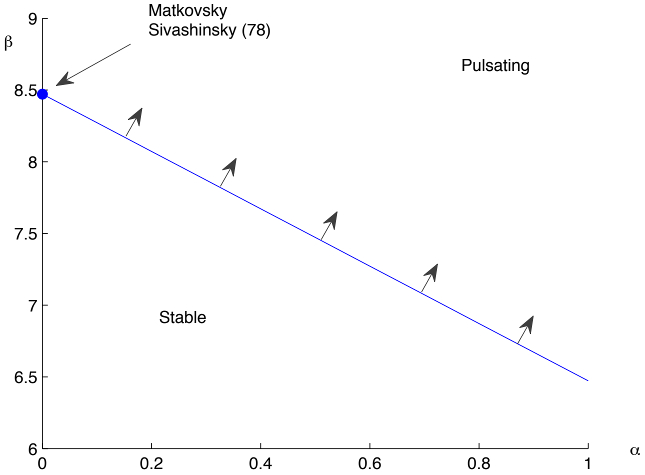
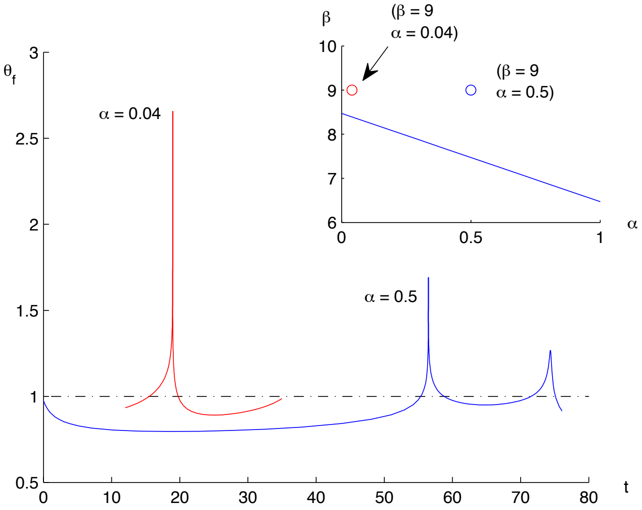
Stability of steady fronts.



Results.



θ_f
3
2.5
2
1.5
1
0.5
α = 0.04
α = 0.5
0
10
20
30
40
50
60
70
80
t
β
10
9
8
7
6
0
0.5
1
α
(β = 9
α = 0.04)
(β = 9
α = 0.5)

Unsteady propagation scales.

Problem.

$$\frac{\partial \theta}{\partial t} + c\,\frac{\partial \theta}{\partial \xi} - \frac{\partial^2 \theta}{\partial \xi^2} = (q_f^- - q_f^+)\,c \cdot \delta(\xi)$$

$$\theta(\xi \to -\infty) = 0, \qquad \theta_\xi(\xi \to \infty) = 0$$

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Unsteady preheat (postheat) region.

$$c\,\frac{\Delta\theta}{\epsilon} \sim \frac{\Delta\theta}{\epsilon^2} \qquad \Rightarrow$$

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$$\theta(\xi \to -\infty) = 0, \qquad \theta_\xi(\xi \to \infty) = 0$$

Unsteady preheat (postheat) region.

$$c\,\frac{\Delta\theta}{\epsilon} \sim \frac{\Delta\theta}{\epsilon^2} \qquad \Rightarrow \qquad \epsilon \sim c^{-1}$$

Unsteady propagation scales.

Problem.

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Unsteady preheat (postheat) region.

$$c\,\frac{\Delta \theta}{\epsilon} \sim \frac{\Delta \theta}{\epsilon^2} \qquad \Rightarrow \qquad \begin{array}{l} \epsilon \sim c^{-1} \\ t_r \sim \dfrac{\epsilon}{c} \sim c^{-2} \end{array}$$

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Unsteady propagation scales.

Problem.

$$\frac{\partial \theta}{\partial t} + c\,\frac{\partial \theta}{\partial \xi} - \frac{\partial^2 \theta}{\partial \xi^2} = (q_f^- - q_f^+)\, c \cdot \delta(\xi)$$

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$$\varsigma = c \cdot x$$

$$d\tau = c^2 \cdot dt$$

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Unsteady propagation scales.

Problem.

$$\frac{\partial\theta}{\partial t} + c\,\frac{\partial\theta}{\partial\xi} - \frac{\partial^2\theta}{\partial\xi^2} = (q_f^- - q_f^+)\,c\cdot\delta(\xi)$$

$$\theta(\xi\to-\infty)=0, \qquad \theta_\xi(\xi\to\infty)=0$$

Unsteady preheat (postheat) region.

$$c\,\frac{\Delta\theta}{\epsilon} \sim \frac{\Delta\theta}{\epsilon^2} \quad\Rightarrow\quad \begin{array}{l} \epsilon \sim c^{-1} \\ t_r \sim \dfrac{\epsilon}{c} \sim c^{-2} \end{array}$$

$$\left.\begin{array}{l} \varsigma = c\cdot x \\ d\tau = c^2\cdot dt \end{array}\right\} \quad\Rightarrow\quad \theta_t \to \theta_t + \frac{c_t}{c}\varsigma\theta_\varsigma$$

Rescaled problem.

$$\theta_\tau + \left(1 + a(\tau)\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$

$$\theta(\varsigma \to -\infty) = 0, \qquad \theta_\varsigma(\varsigma \to \infty) = 0$$

$$a(\tau) = \frac{c_\tau}{c} \approx \frac{\beta}{2}\frac{\theta_{f\tau}}{(1 + \alpha\,(\theta_f - 1))^2}$$

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$$q_f^- - q_f^+ = 1 - Y_b$$

$$(1 - q_f^-)\ln Y_b + 1 - Y_b = 0$$

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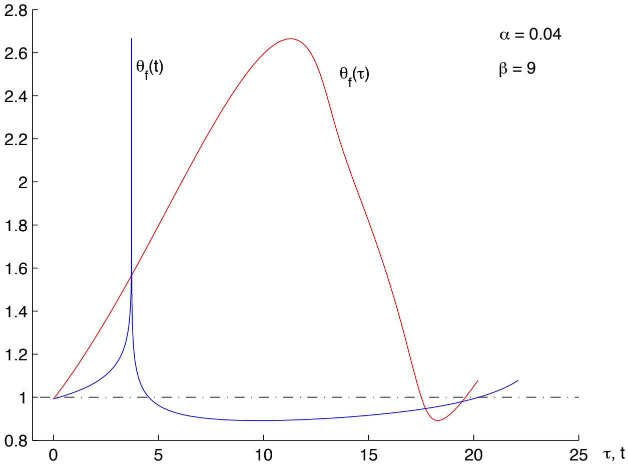
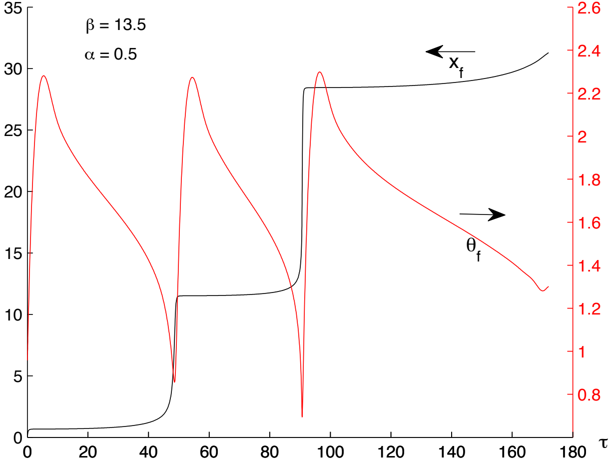
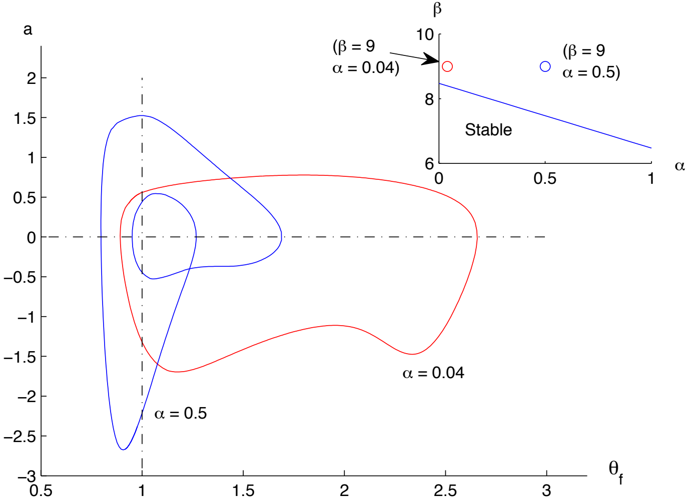
Time scales.



Flame displacement.

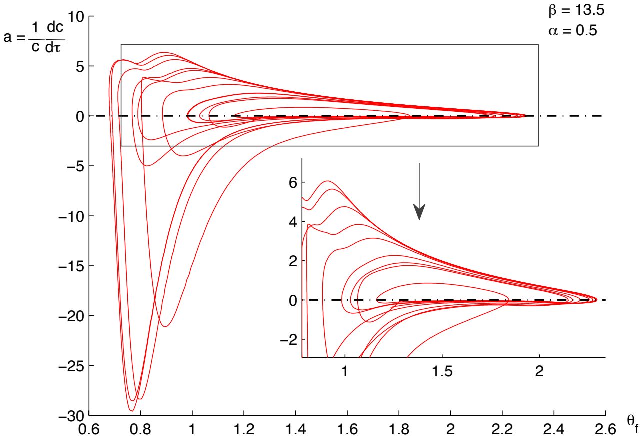


Phase plane.



a
2
1.5
1
0.5
0
−0.5
−1
−1.5
−2
−2.5
−3
0.5
1
1.5
2
2.5
3
θ_f
α = 0.5
α = 0.04
β
10
8
6
0
0.5
1
α
(β = 9
α = 0.04)
(β = 9
α = 0.5)
Stable

Chaotic dynamics.



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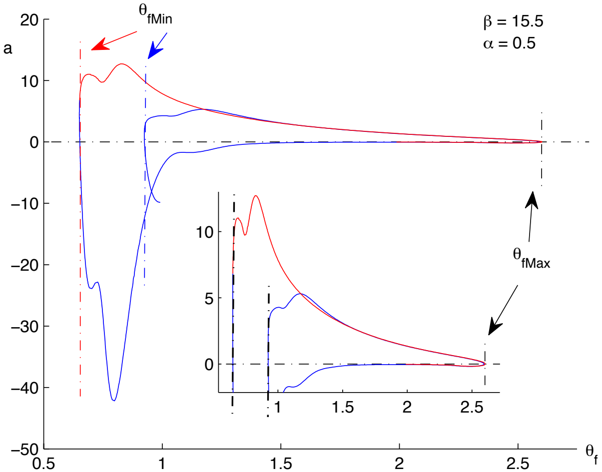
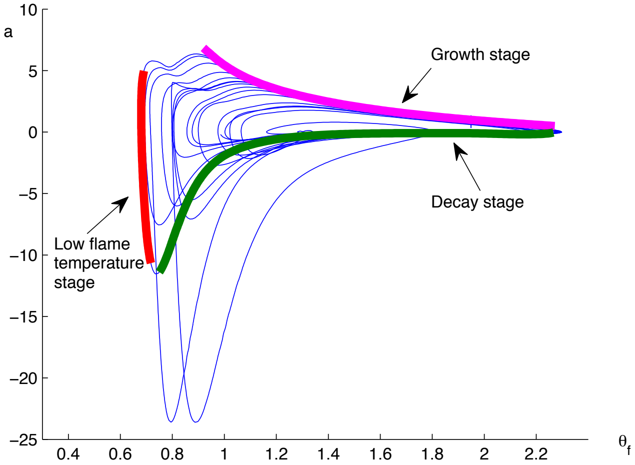
Cycle.



θfMin
β = 15.5
α = 0.5
a
20
10
0
−10
−20
−30
−40
−50
0.5
1
1.5
2
2.5
θf
θfMax
10
5
0
1
1.5
2
2.5

Stages.



a
10
5
0
−5
−10
−15
−20
−25
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
θf
Growth stage
Decay stage
Low flame temperature stage

Integral equation.

Problem.

$$\theta_\tau + \left(1 + a\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$

Integral equation.

$$\theta = \theta_f(\tau) + \int_0^\varsigma e^{s+as^2/2}\left\{q_f^\pm(\tau) + \int_0^s e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp\right\}ds$$

Integral equation.

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Integral equation.

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Integral equation.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$

Integral equation.

$$\theta = \theta_f(\tau) + \int_0^\varsigma e^{s+as^2/2}\left\{q_f^\pm(\tau) + \int_0^s e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp\right\}ds$$

$$a > 0 \quad \Rightarrow \quad q_f^\pm(\tau) = \int_{\pm\infty}^0 e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp$$

Integral equation.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$

Integral equation.

$$\theta = \theta_f(\tau) + \int_0^\varsigma e^{s+as^2/2}\left\{q_{\pm\infty}(\tau) + \int_0^s e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp\right\}ds$$

Large a. Uniform time derivative.

$$\theta_\tau(p\,;\tau) \approx \theta_{f_\tau}(\tau)$$

Integral equation.

Problem.

$$\theta_\tau + \left(1 + a\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = \left(q_f^- - q_f^+\right)\cdot\delta(\varsigma)$$

Integral equation.

$$\theta = \theta_f(\tau) + \int_0^\varsigma e^{s+as^2/2}\left\{q_{\pm\infty}(\tau) + \int_0^s e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp\right\}ds$$

Large a. Uniform time derivative.

$$\theta_\tau(p\,;\tau) \approx \theta_{f_\tau}(\tau)$$

$$q_{\pm\infty}(\tau) = \theta_{f_\tau}\sqrt{\frac{\pi e^{1/a}}{2a}}\left[\operatorname{erf}\left(\frac{1}{\sqrt{2a}}\right) \mp 1\right]$$

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Flame temperature dynamics.

Growth stage attractor.

$$q_{\pm\infty}(\tau) = \theta_{f_\tau}\sqrt{\frac{\pi e^{1/a}}{2a}}\left[\mathrm{erf}\left(\frac{1}{\sqrt{2a}}\right) \mp 1\right]$$

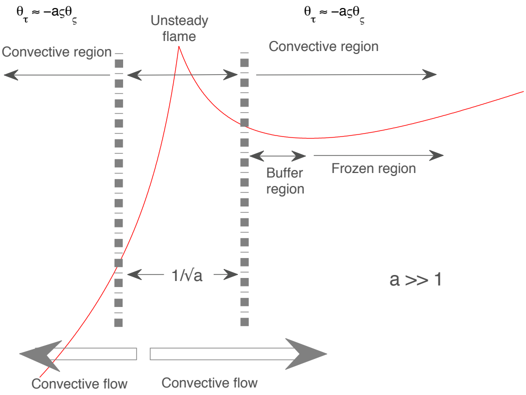
$$q_f^- - q_f^+ = 1 - Y_b(q_f^-)$$

$$(1 - q_f^-)\,\mathrm{Ln}\,Y_b + 1 - Y_b = 0$$

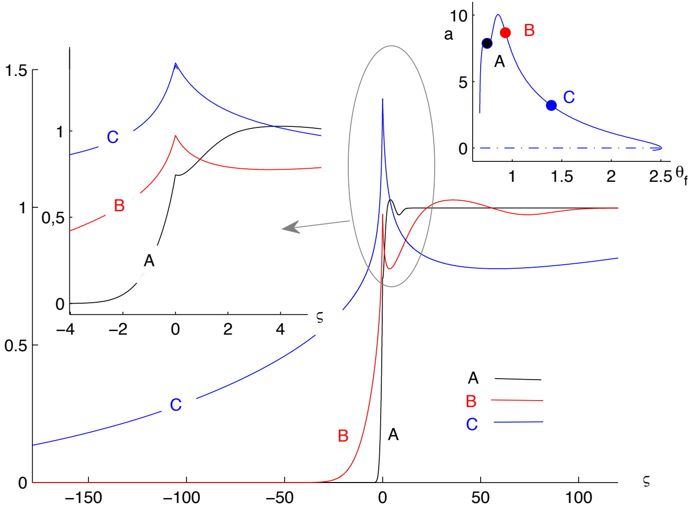
$$a = \frac{\beta}{2}\frac{\theta_{f_\tau}}{(1 + \alpha\,(\theta_f - 1))^2}$$

Spatial structure.

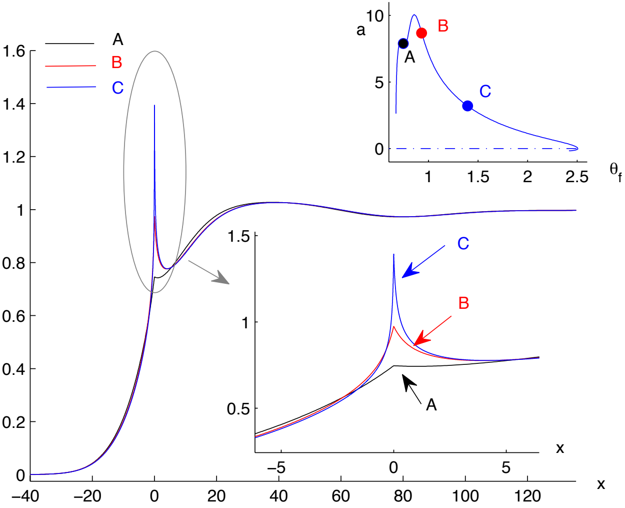
$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$



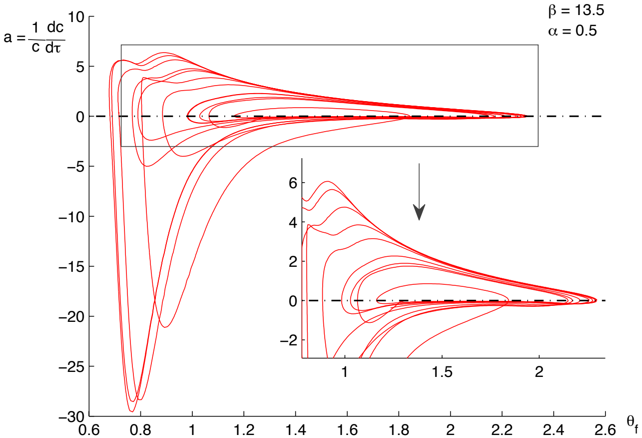
Scaled spatial variable.



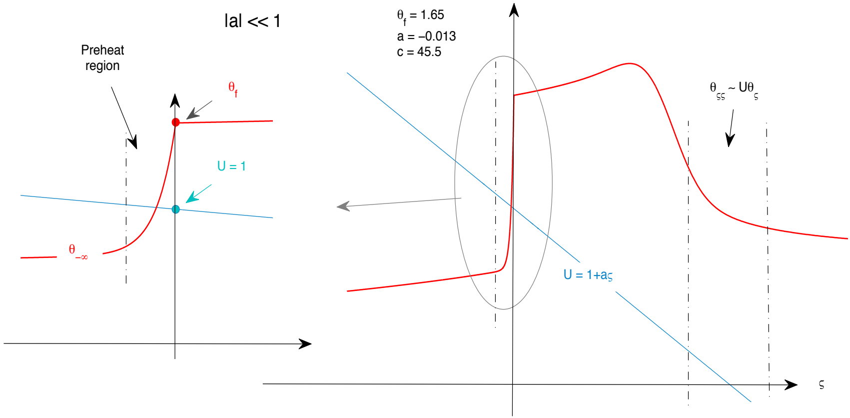
Physical spatial variable.



Chaotic dynamics.

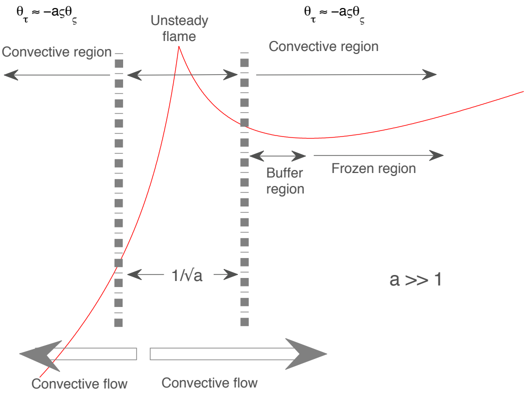


Scales. Small growth rates.

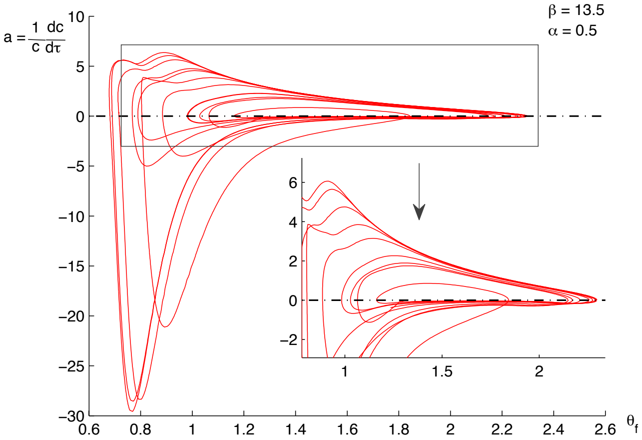


Spatial structure.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = (q_f^- - q_f^+)\cdot\delta(\varsigma)$$



Chaotic dynamics.



Integral equation.

Problem.

$$\theta_\tau + \left(1 + a\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = \left(q_f^- - q_f^+\right)\cdot\delta(\varsigma)$$

Integral equation.

$$\theta = \theta_f(\tau) + \int_0^\varsigma e^{s+as^2/2}\left\{q_f^\pm(\tau) + \int_0^s e^{-(p+ap^2/2)}\theta_\tau(p\,;\tau)dp\right\}ds$$

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Scales. Heat conduction layers.

Problem.

$$\theta_\tau + \left(1 + a\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2}$$

Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2}$$

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Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2} \qquad \Rightarrow \qquad U_c \ell_c \sim 1$$

Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2} \qquad \Rightarrow \qquad U_c \ell_c \sim 1$$

$$U_c \sim 1 + a\ell_c$$

Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2} \qquad \Rightarrow \qquad U_c \ell_c \sim 1$$

$$U_c \sim 1 + a\ell_c$$

Large growth rates. $|a| \gg 1$

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Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Heat conduction layers

$$U_c \frac{\Delta\theta}{\ell_c} \sim \frac{\Delta\theta}{\ell_c^2} \qquad \Rightarrow \qquad U_c \ell_c \sim 1$$

$$U_c \sim 1 + a\ell_c \approx a\ell_c$$

Large growth rates. $|a| \gg 1$

Scales. Heat conduction layers.

Problem.

$$\theta_\tau + (1 + a\,\varsigma)\,\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

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Large growth rates. $|a| \gg 1$

$$|a|\ell_c^2 \sim 1 \qquad \Rightarrow$$

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Large growth rates. $|a| \gg 1$

$$|a|\ell_c^2 \sim 1 \qquad \Rightarrow \qquad \ell_c \sim \frac{1}{\sqrt{a}} \ll 1, \qquad U_c \sim \sqrt{a} \gg 1$$

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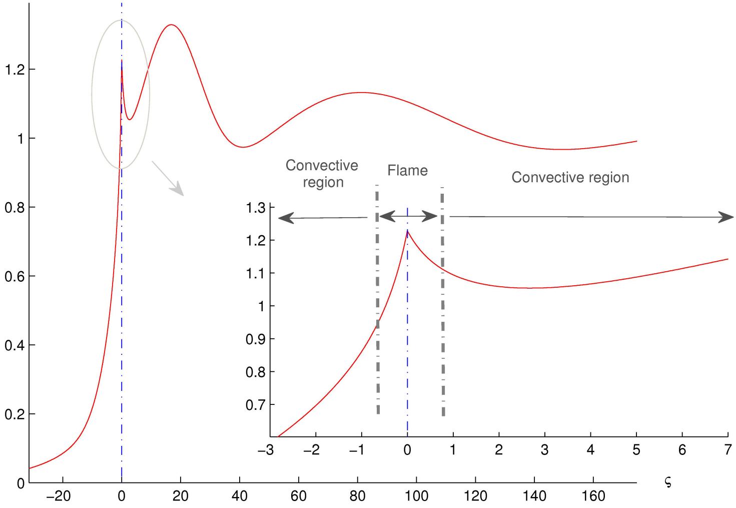
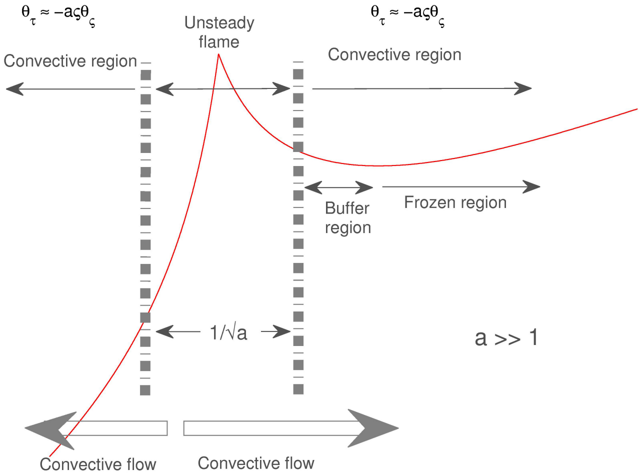
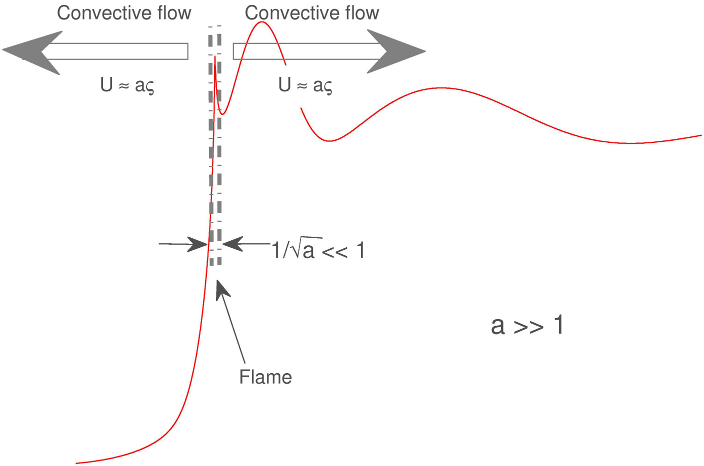
Large growth rates. Spatial structure.



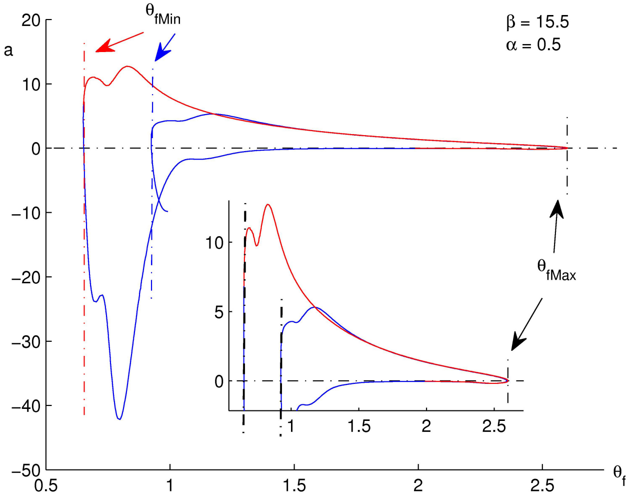
Scales. Large growth rates.



Scales. Large growth rates.



Cycle.



θ_{fMin}
$\beta = 15.5$
$\alpha = 0.5$
a
20
10
0
−10
−20
−30
−40
−50
0.5
1
1.5
2
2.5
θ_f
θ_{fMax}
10
5
0
1
1.5
2
2.5

Flame temperature dynamics.

Problem.

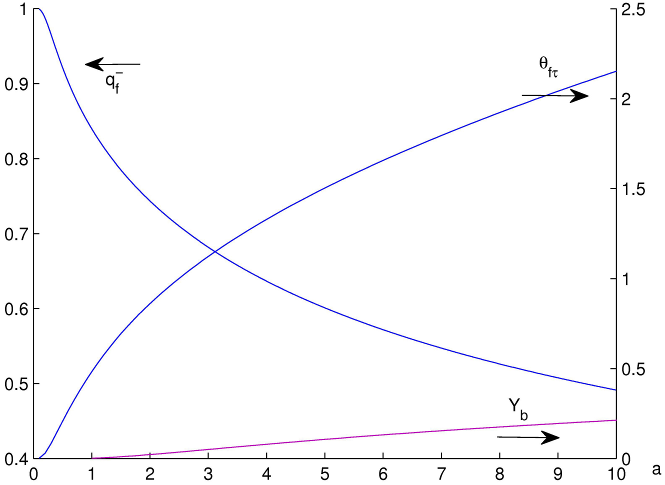
$$\frac{q_f^-}{1 - Y_b(q_f^-)} = \frac{1}{2}\left(\text{erf}\left(\frac{1}{\sqrt{2a}}\right) + 1\right)$$

$$2\theta_{f\tau}\sqrt{\frac{\pi e^{1/a}}{2a}} = 1 - Y_b(q_f^-)$$

$$(1 - q_f^-)\ln Y_b + 1 - Y_b = 0$$

$$a = \frac{\beta}{2}\frac{\theta_{f\tau}}{(1 + \alpha(\theta_f - 1))^2}$$

Universal growth stage. Large *a*.



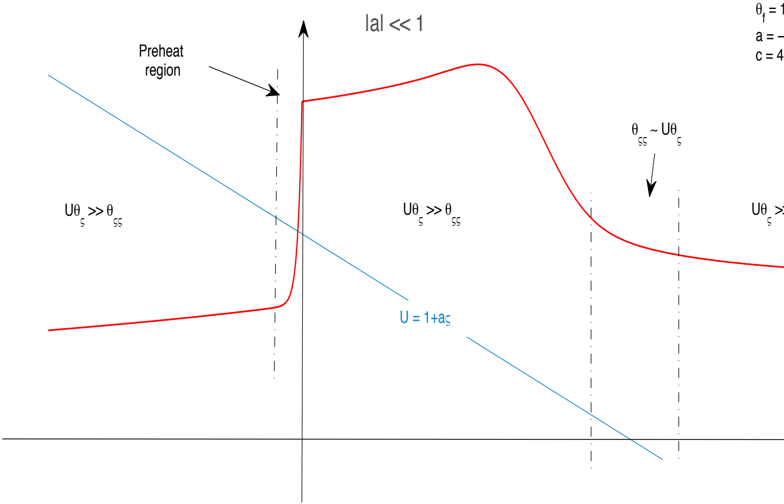
Quasisteady reaction layer.

Problem.

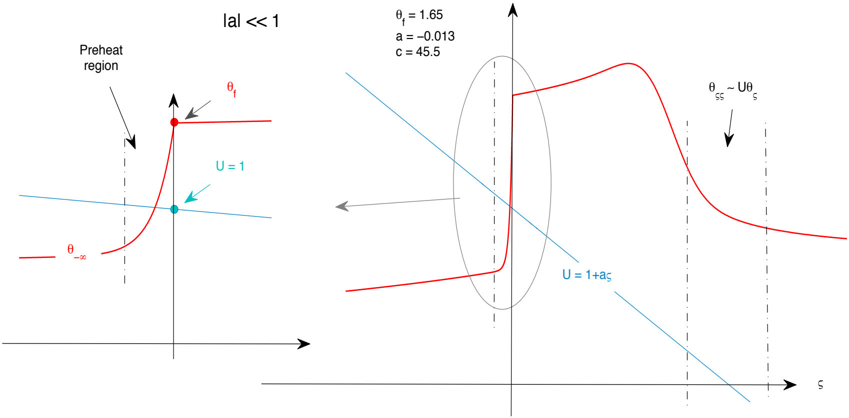
$$\mathcal{O}\left(\beta^{-1}\left(\frac{d\theta_f}{d\tau},\frac{\partial\theta}{\partial\xi},\ldots\right)\right)-\frac{\partial^2\varphi}{\partial\mu^2}=\kappa\, Y\exp\left\{\frac{\varphi}{1+\beta^{-1}\Lambda\varphi}\right\}$$

$$\mathcal{O}\left(\beta^{-1}\frac{\partial Y}{\partial\tau},\ldots\right)+\frac{\partial Y}{\partial\mu}=-\kappa\, Y\exp\left\{\frac{\varphi}{1+\beta^{-1}\Lambda\varphi}\right\}$$

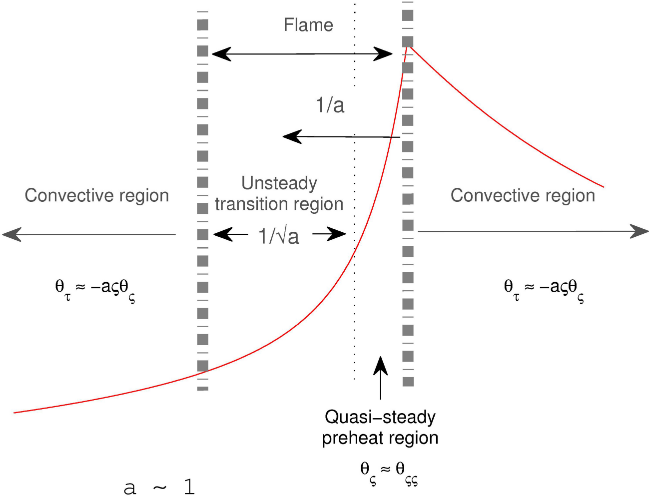
Scales. Small growth rates.



Scales. Small growth rates.



Order unity growth rates.



$a \sim 1$

Flame temperature dynamics.

Problem.

$$\theta_{f\tau} = \left(1 - q_f^- - Y_b(q_f^-)\right) G(a)$$

$$q_{f\tau}^- = \theta_{f\tau} - q_f^- \, H(a)$$

$$(1 - q_f^-) \, \mathrm{Ln}\, Y_b + 1 - Y_b = 0$$

$$a = \frac{\beta}{2} \frac{\theta_{f\tau}}{(1 + \alpha\,(\theta_f - 1))^2}$$

Scales. Heat conduction layers.

Problem.

$$\theta_\tau + \left(1 + a\,\varsigma\right)\theta_\varsigma - \theta_{\varsigma\varsigma} = 0$$

Diffusive layers

$$\frac{U_c}{\ell_c} \sim \frac{1}{\ell_c^2} \qquad \Rightarrow \qquad U_c \ell_c \sim 1$$

$$U = 1 + a\varsigma = a(\varsigma - \varsigma_0) \qquad \Rightarrow \qquad U_c \sim |a|\ell_c$$

Small growth rates. $|a| \ll 1$

$$|a|\ell_c^2 \sim 1 \qquad \Rightarrow$$

Scales. Heat conduction layers.

Problem.

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Small growth rates. $|a| \ll 1$

$$|a| \ell_c^2 \sim 1 \qquad \Rightarrow \qquad \ell_c \sim \frac{1}{\sqrt{|a|}} \gg 1$$

$$U_c \sim \sqrt{|a|} \ll 1$$

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Scales. Heat conduction layers.

Problem.

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Small growth rates. $|a| \ll 1$

$$|a| \ell_c^2 \sim 1 \qquad \Rightarrow \qquad \frac{1}{|a|} \gg \ell_c \sim \frac{1}{\sqrt{|a|}} \gg 1$$

$$U_c \sim \sqrt{|a|} \ll 1$$

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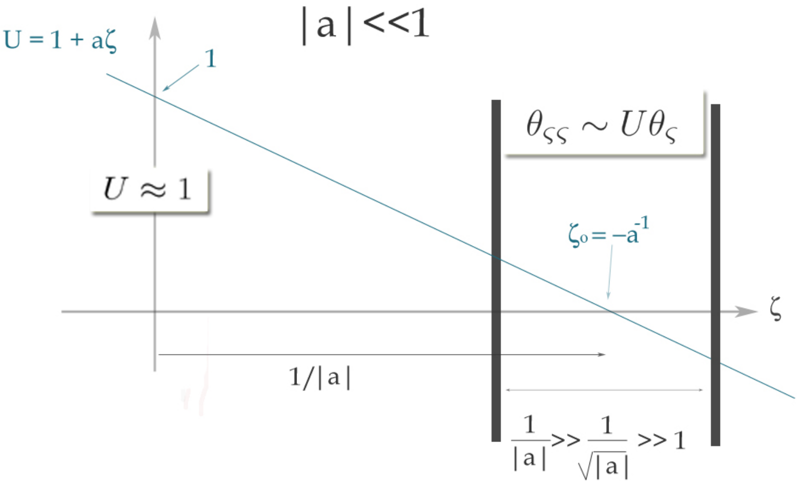
Scales. Small growth rates.



Convective regions.

Negligible diffusion.

$$|\varsigma| \gg \ell_{diff} \qquad \Rightarrow \qquad \theta_\tau \approx (1 + a\,\varsigma)\,\theta_\varsigma \qquad \gg \theta_{\varsigma\varsigma}$$

Characteristic lines.

Constant temperature along:

$$\frac{\varsigma}{c} = \frac{\varsigma_0}{c_0} + \int_{\tau_0}^{\tau} \frac{d\tau}{c}$$

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Characteristic length.

$$\varsigma = \varsigma_0 \frac{c}{c_0}$$

Convective regions.

Negligible diffusion.

$$|\varsigma| \gg \ell_{diff} \qquad \Rightarrow \qquad \theta_\tau \approx (1 + a\,\varsigma)\,\theta_\varsigma \qquad \gg \theta_{\varsigma\varsigma}$$

Characteristic lines.

Constant temperature along:

$$\frac{\varsigma}{c} = \frac{\varsigma_0}{c_0} + \int_{\tau_0}^{\tau} \frac{d\tau}{c}$$

Characteristic length.

$$\varsigma = \varsigma_0 \frac{c}{c_0} \qquad \Rightarrow \qquad \lambda \sim \lambda_0 \frac{c}{c_0}$$

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Future work.

- Decay and low flame temperature stages.
- Gaseous flames lean flames with $L_{O_2} \approx 1$.
- Oscillations close to the flammability limits.
- Realistic kinetic simplified models.