Counterflow Combustion with Multiple Flames under High Strain Rates

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- Multi-branched flames are commonly found in unsteady combustors.
- They especially can appear with the extinction/ re-ignition behavior in vorticity-dominated flows with time-varying rates of strain *S*.
- Flamelet theory provides a useful model with reduced computational cost for multidimensional combustor analysis via CFD.
- Flamelet theory is based on counterflow similarity solutions in planar or axisymmetric configurations. *Peters* (2000), *Pierce & Moin* (2004)
- The theory has been developed only for single nonpremixed or premixed flames.
- Here, we extend the flamelet theory to three-dimensional configurations with multiple (one, two, or three) flames.

Governing Equations for 3D Reacting Counterflow

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0$$

$$\rho\frac{\partial Y_m}{\partial t} + \rho u_j\frac{\partial Y_m}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y_m}{\partial x_j}\right) + \rho\omega_m \;\; ; \;\; m = 1, 2, ..., N$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_j\frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\tau_{ij} = \mu\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right]$$

$$\rho\frac{\partial h}{\partial t} + \rho u_j\frac{\partial h}{\partial x_j} - \frac{\partial p}{\partial t} = \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial h}{\partial x_j}\right) - \rho\Sigma_{m=1}^{N} h_{f,m}\omega_m$$

$Le = 1$; $M << 1$

$\eta \equiv \int_0^y \rho(y')dy'$ for variable density flow.

Similarity form

$\rho = \rho(\eta)$; $h = h(\eta)$; $Y_m = Y_m(\eta)$

$\rho v = -S_1 f_1(\eta) - S_2 f_2(\eta)$; $u = S_1 x(df_1/d\eta)$; $w = S_2 z(df_2/d\eta)$.

ODEs in Similarity Analysis

Perfect gas , constant specific heats

$$
\begin{aligned}
f_1''' + (S_1 f_1 + S_2 f_2) f_1'' + S_1\left(\tilde{h} - (f_1')^2\right) &= 0 \\
f_2''' + (S_1 f_1 + S_2 f_2) f_2'' + S_2\left(\tilde{h} - (f_2')^2\right) &= 0 \\
f_1'(\infty) = \sqrt{\rho_{-\infty}} f_1'(-\infty) = f_2'(\infty) = \sqrt{\rho_{-\infty}} f_2'(-\infty) &= 1 \\
f_1(0) = f_2(0) &= 0
\end{aligned}
$$

$$
\begin{aligned}
Y_F'' + Pr(S_1 f_1 + S_2 f_2) Y_F' &= Pr\omega_F \\
Y_O'' + Pr(S_1 f_1 + S_2 f_2) Y_O' &= \nu Pr\omega_F \\
Y_F(\infty) = Y_{F,\infty} \ ; \ Y_F(-\infty) &= Y_{F,-\infty}
\end{aligned}
$$

$$
\begin{aligned}
\tilde{h}'' + Pr(S_1 f_1 + S_2 f_2)\tilde{h}' &= Pr\tilde{Q}\omega_F \\
\tilde{h}(\infty) = 1 \ ; \ \tilde{h}(-\infty) &= \frac{1}{\rho_{-\infty}}
\end{aligned}
$$

One-step Westbrook-Dryer kinetics for propane and oxygen

$$\frac{dY_F}{dt} = \omega_F = -\frac{A^* \rho_\infty^{*\,0.75}}{S_1^* + S_2^*} \tilde{h}^{-0.75} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}}$$

$$\omega_F = -\frac{Da}{\tilde{h}^{0.75}} Y_F^{0.1} Y_O^{1.65} e^{-50.237/\tilde{h}}$$

$A^* = 4.79 \ x10^8 \ (kg/m^3)^{-0.75}$

$T_{ambient} = 300 \ K.$

Reference Values: *Strain Rate* $S^* = S1^* + S2^* = 100/s$

Ambient Density $\rho^* = 10 \ kg/m^3$

$Da = K \, Da_{ref}$

$$Da_{ref} \equiv \frac{\tilde{A}(10kg/m^3)^{0.75}}{(100/s)} = 2.693 \ x \ 10^7 \ ; \ K \equiv \left[\frac{\rho_\infty^*}{10kg/m^3}\right]^{0.75} \frac{100/s}{S_1^* + S_2^*}$$

***K* increases with increasing pressure**
and decreases with increasing rate of strain

Conserved Scalars

$\alpha \equiv Y_F - \nu Y_O$ $\beta \equiv \tilde{h} + \nu Y_O \tilde{Q}$ $\nu = 0.275$

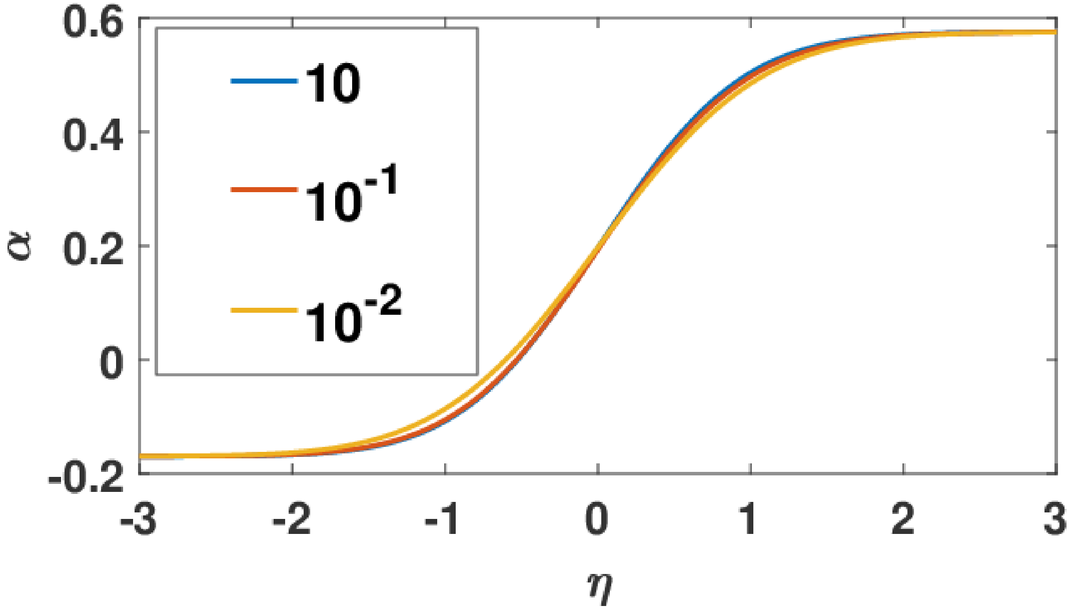
First case

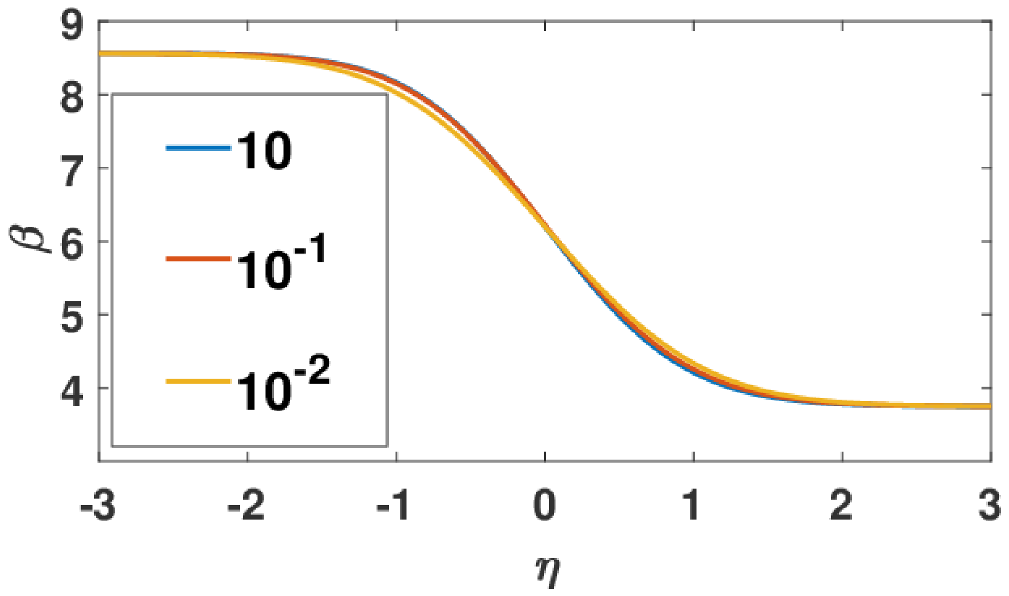
A fuel-lean mixture flows from left to right.

A fuel-rich mixture flows from right to left.

$S_1 = 0.25$; $S_2 = 0.75$; $Pr = Sc = 1.0$; K given in Legend

Monotonic behavior, little effect of strain distribution



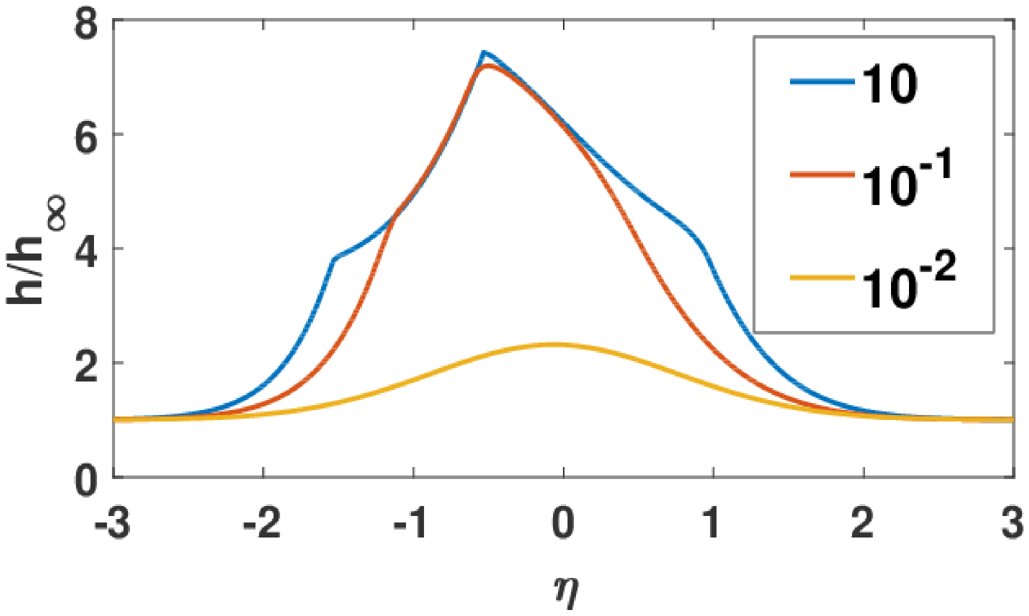


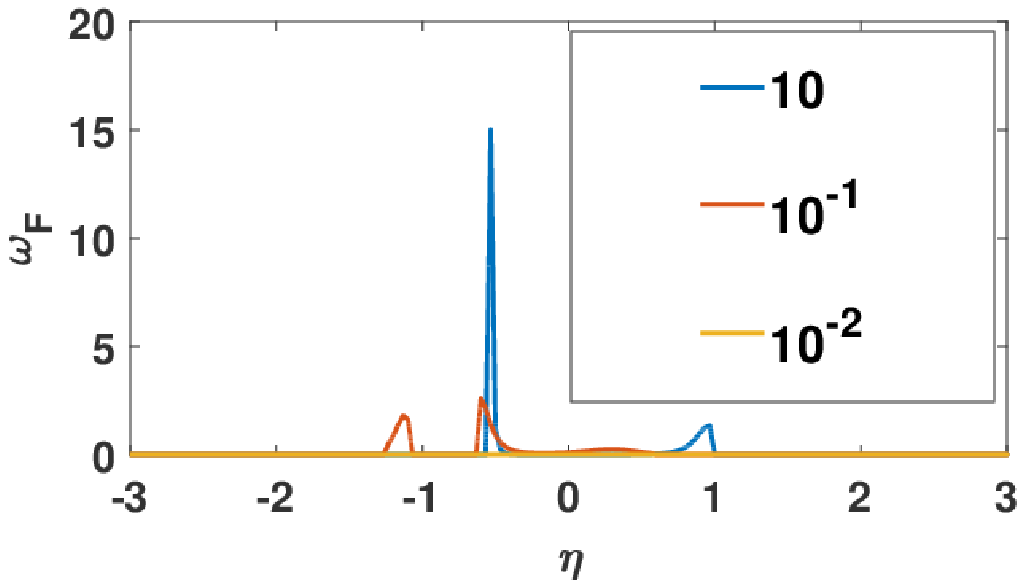
$S_1 = 0.25$; $S_2 = 0.75$; $Pr = Sc = 1.0$

-- **Three flames** can appear; fuel-lean premixed flame on left, diffusion flame in the middle, and fuel-rich premixed flame on right.

-- Increase in strain rate and/or decrease in pressure causes fuel-rich premixed flame to merge into diffusion flame.

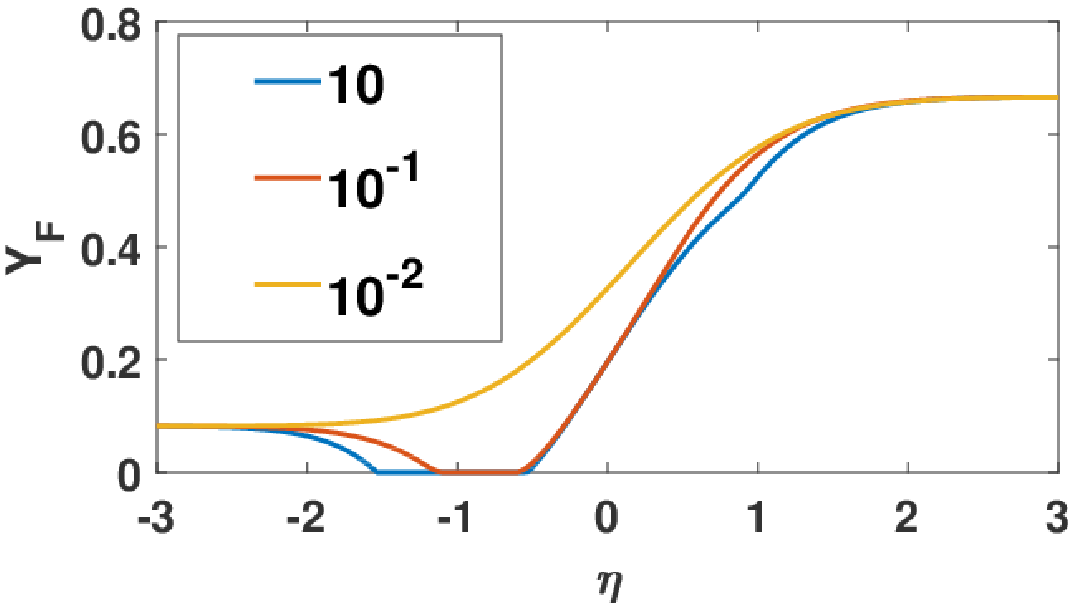
-- Further increase in strain rate or decrease in pressure causes fuel-lean flame to merge with diffusion flame and then extinction with further change.

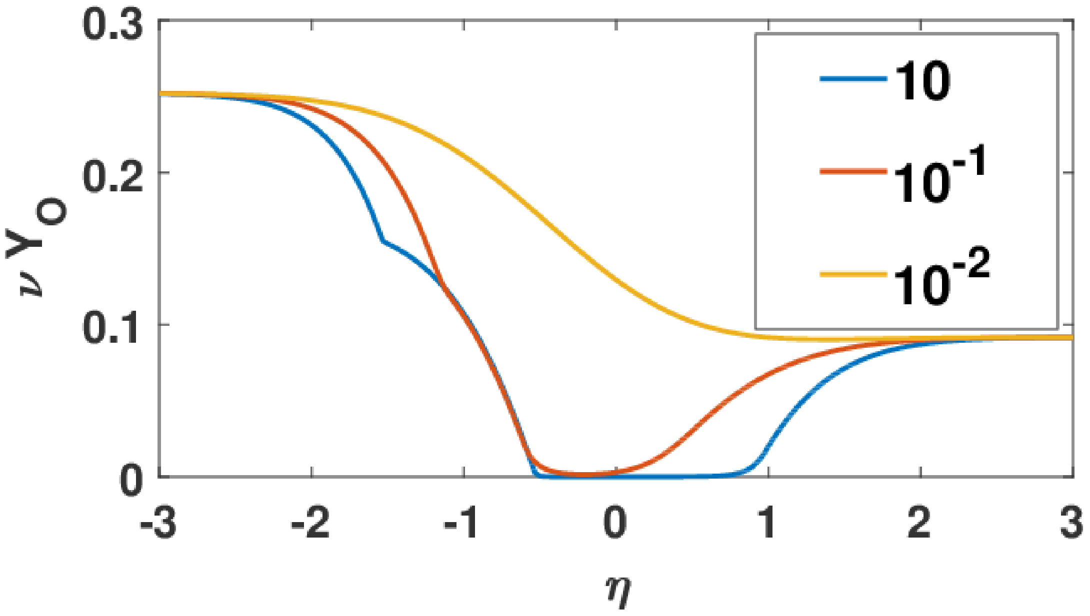




$S_1 = 0.25$; $S_2 = 0.75$; $Pr = Sc = 1.0$

-- A domain with no fuel but substantial oxygen exists between the fuel-lean premixed flame and the diffusion flame.
-- A domain with no oxygen but substantial fuel exists between the fuel-rich premixed flame and the diffusion flame.
-- The diffusion flame sits in the fuel-lean stream.
-- Merger and extinction are again shown with increasing strain rate and decreasing pressure.



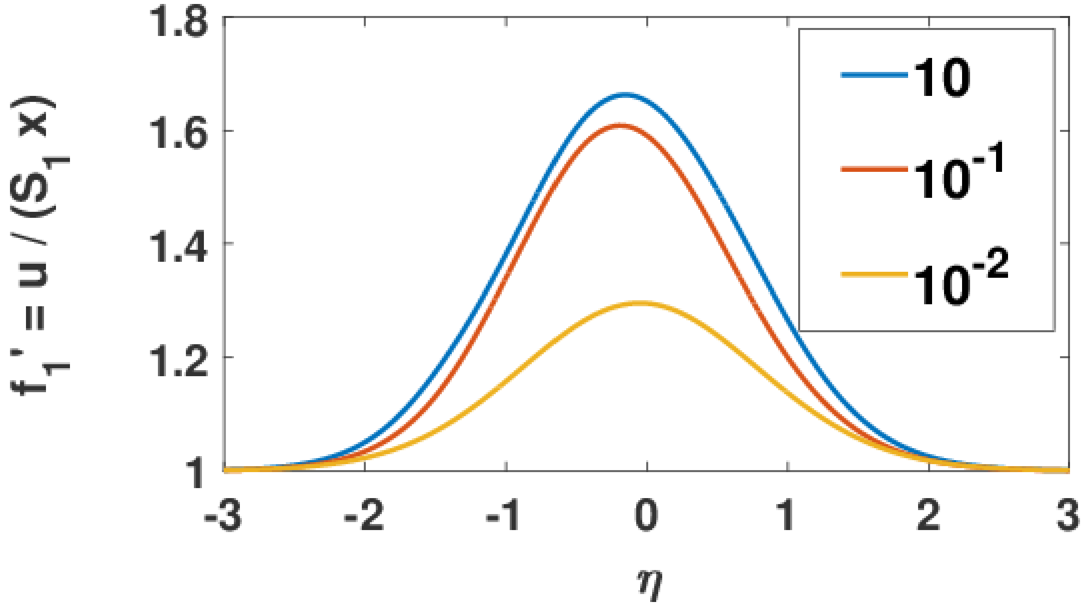


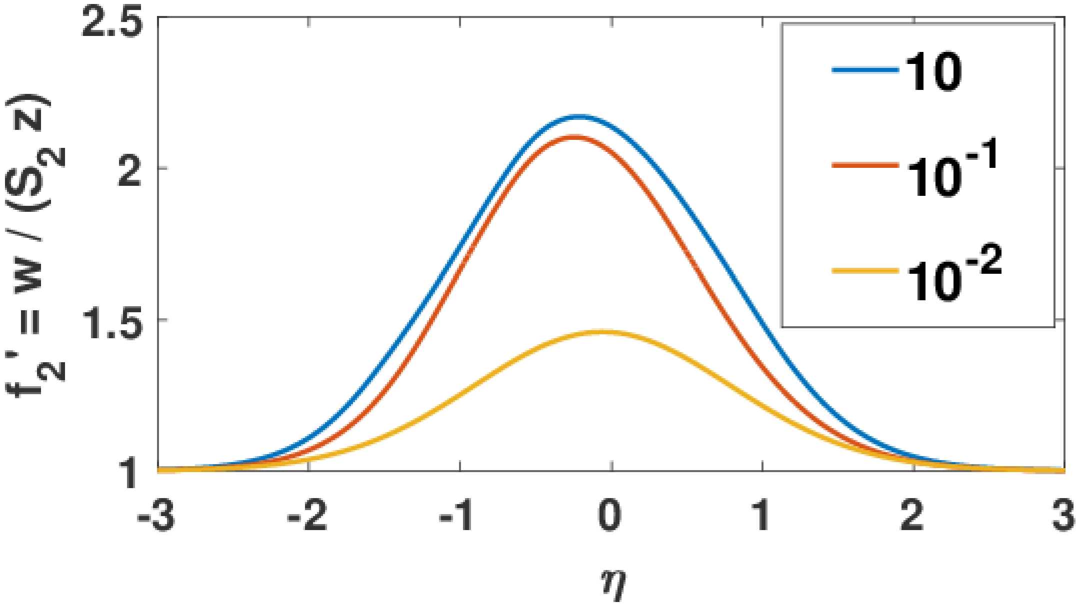
$S_1 = 0.25$; $S_2 = 0.75$; $Pr = Sc = 1.0$

-- In counterflows, the fluid in both streams is accelerates in the transverse directions away from the two symmetry planes. $\partial p/\partial x \sim -x$; $\partial p/\partial z \sim -z$; $u \sim x$; $w \sim z$.

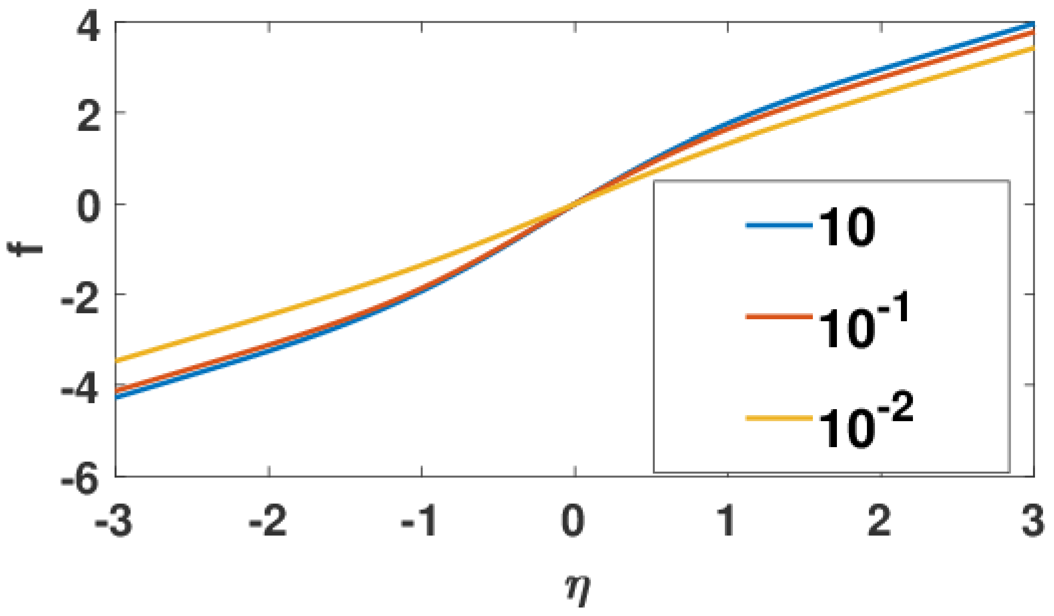
-- The flames result in domains of high temperature and low density which have greater acceleration due to the pressure gradient.

-- Overshoot of the transverse velocity occurs with greater velocities in the direction with greater normal strain rate.



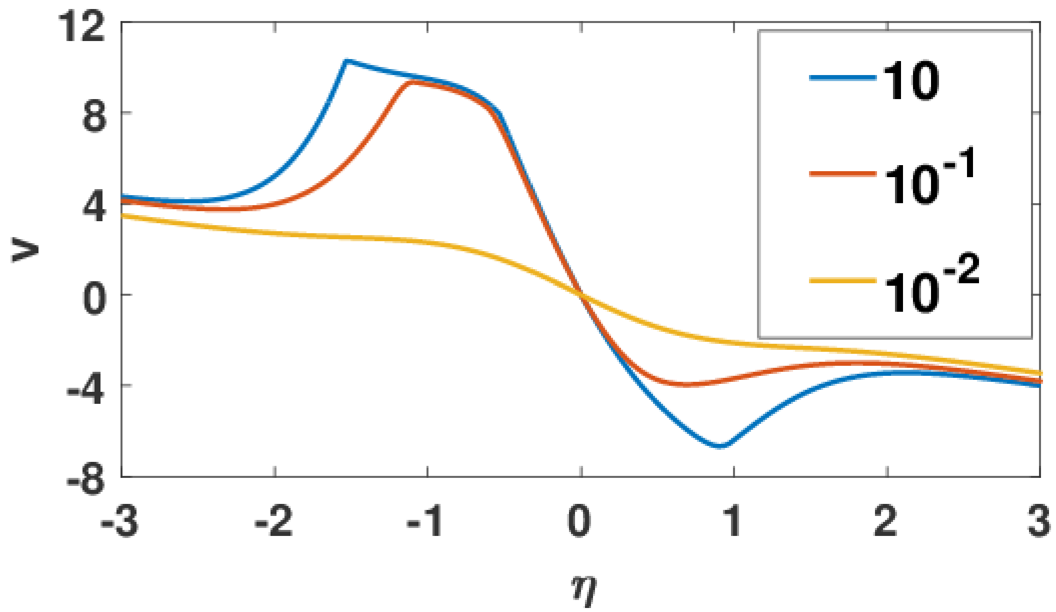


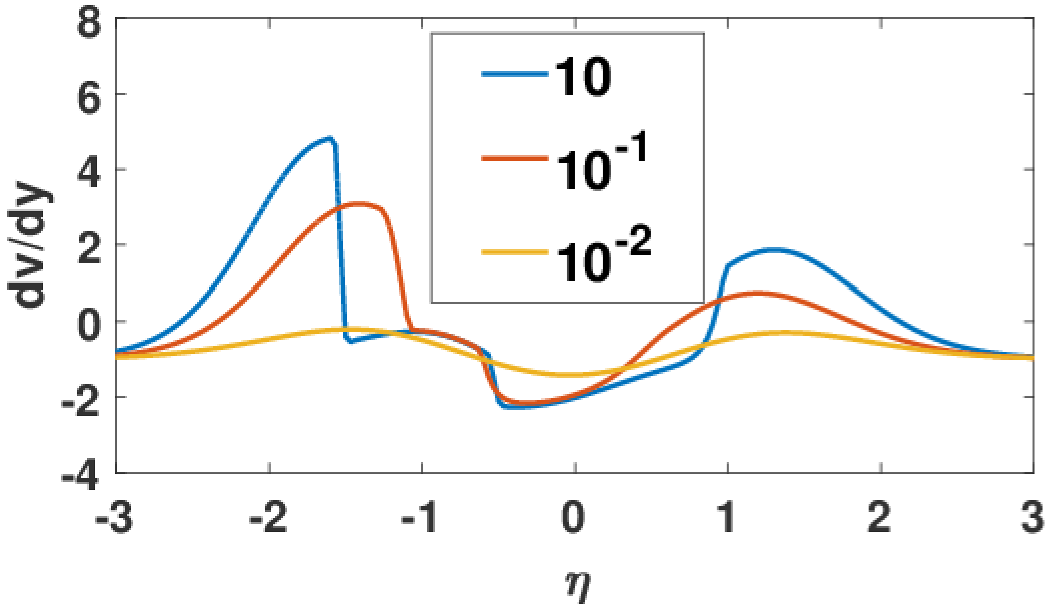
$S_1 = 0.25$; $S_2 = 0.75$; $Pr = Sc = 1.0$



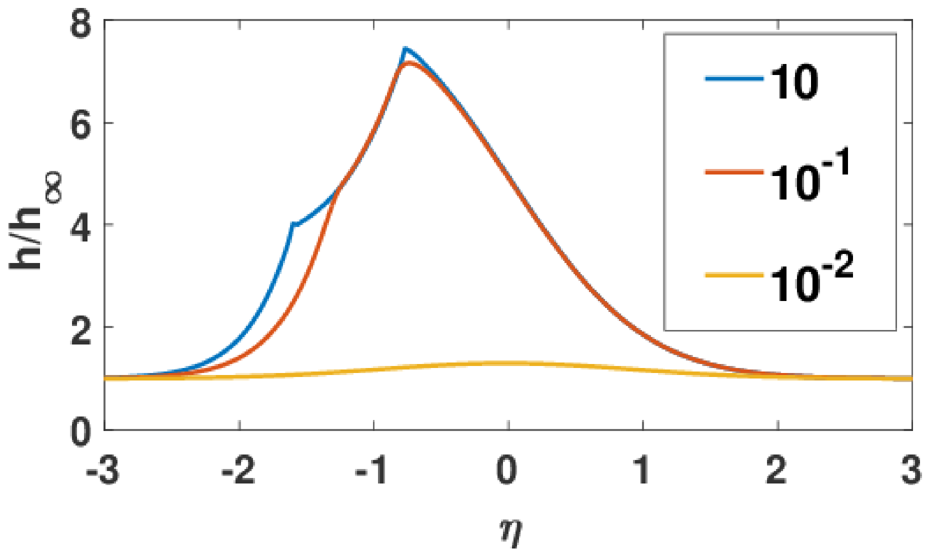
Contrary to impressions given in the literature, the velocity v in the counterflow direction is far from linear (or even monotonic) in y.

There can be local maxima and minima in both The velocity v and the normal strain rate $\partial v / \partial y$.





Fuel-lean Mixture Flowing Against Fuel



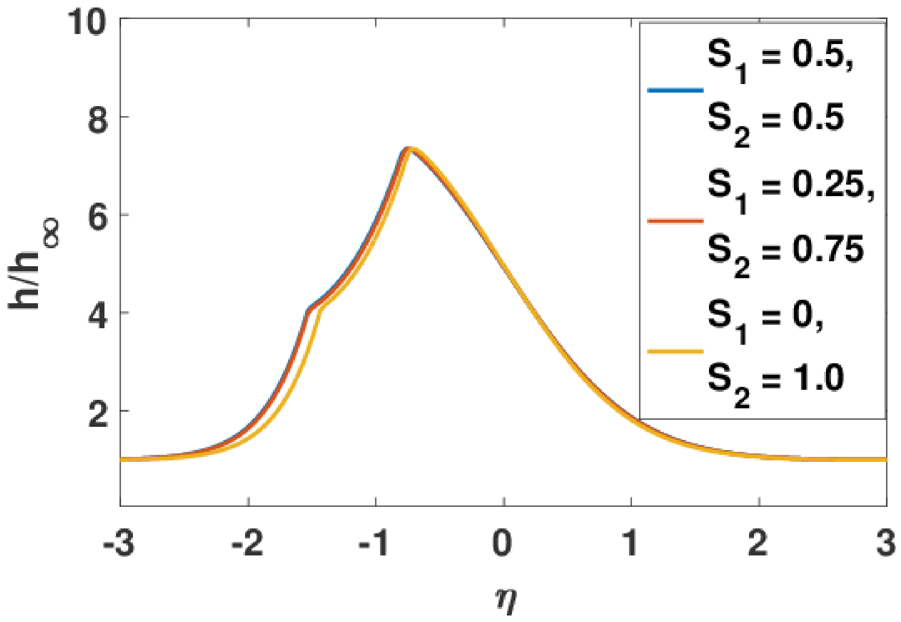
-- Here, results are presented for pure fuel flowing from the right counter to a fuel-lean combustible mixture from the left.

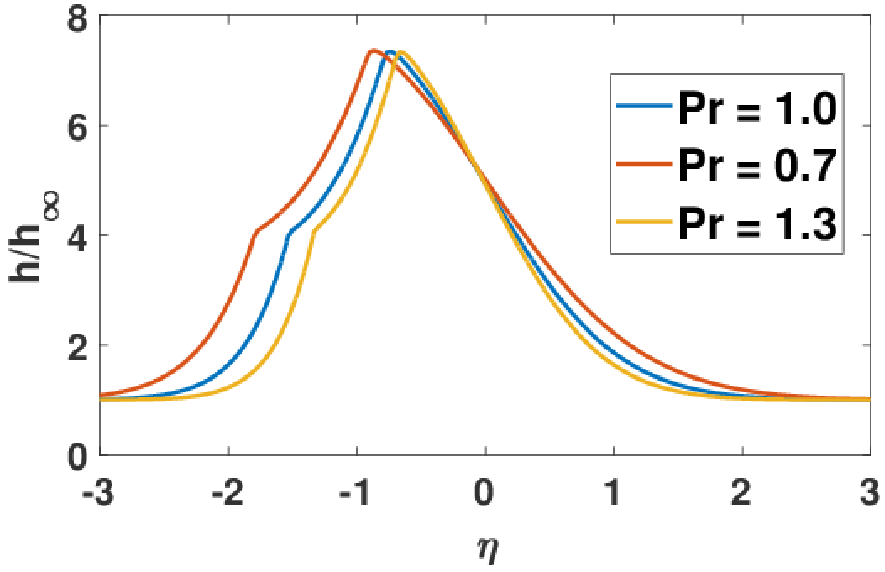
-- Only a fuel-lean premixed flame and a diffusion flame can occur.

-- Merging and extinction can follow as before with decreasing K value.

-- Strain rate distribution has little effect on scalar Properties; 3D, axisymmetric, and planar results are close.

-- Prandtl number has a more significant effect.





A new conserved scalar Σ must replace mixture fraction Z. It need not be physically meaningful but only monotonic in the y coordinate.

$$\Sigma'' + Pr(S_1 f_1 + S_2 f_2)\Sigma' = 0$$
$$\Sigma(\infty) = 1 \;;\; \Sigma(-\infty) = 0$$

$$\Sigma(\eta) = \frac{J(\eta)}{J(\infty)}$$
$$J(\eta) \equiv \int_{-\infty}^{\eta} e^{-I(\eta')} d\eta'$$
$$I(\eta) \equiv \int_{-\infty}^{\eta} Pr\Big[S_1 f_1(\zeta) + S_2 f_2(\zeta)\Big] d\zeta$$

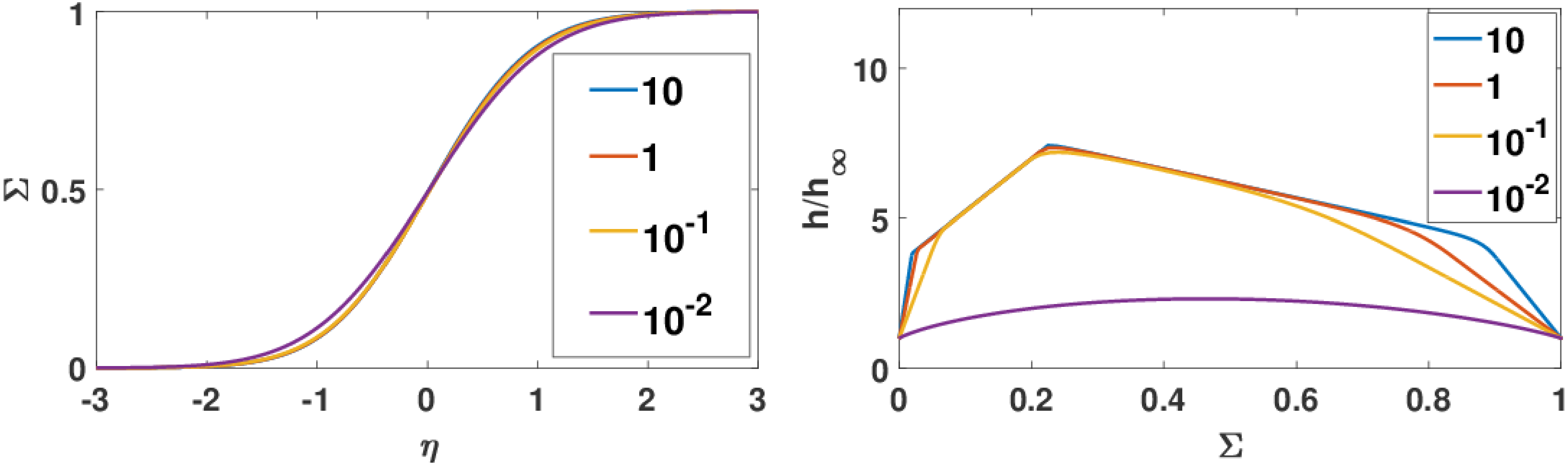
$$\Sigma = \frac{\alpha(\eta) - \alpha(-\infty)}{\alpha(\infty) - \alpha(-\infty)} = \frac{\beta(\eta) - \beta(-\infty)}{\beta(\infty) - \beta(-\infty)}$$

$$2\chi \frac{d^2 Y_m}{d\Sigma^2} + Pr\omega_m = 0 \;;\; m = 1, 2, ..., N$$
$$2\chi \frac{d^2 \tilde{h}}{d\Sigma^2} + Pr\tilde{Q}\omega_m = 0$$
$$\chi \equiv \frac{1}{2}\left(\frac{d\Sigma}{d\eta}\right)^2 = \frac{1}{2\rho^2}\left(\frac{d\Sigma}{dy}\right)^2 = \frac{1}{2}\frac{e^{-2I(\eta)}}{J^2(\infty)}$$

-- Σ is always a monotonic function of y or η while Z based on molecular species is not for multi-flame configuration. Z based on atomic species need not be monotonic in y for the unsteady state.

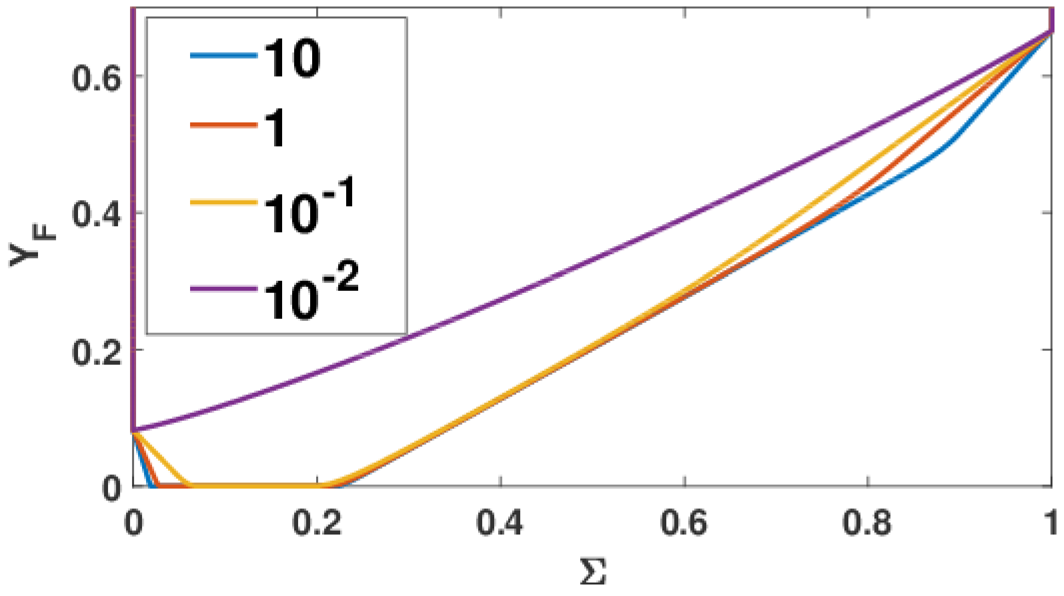
-- For the simple steady-state diffusion-flame-only case, $\Sigma = Z$.

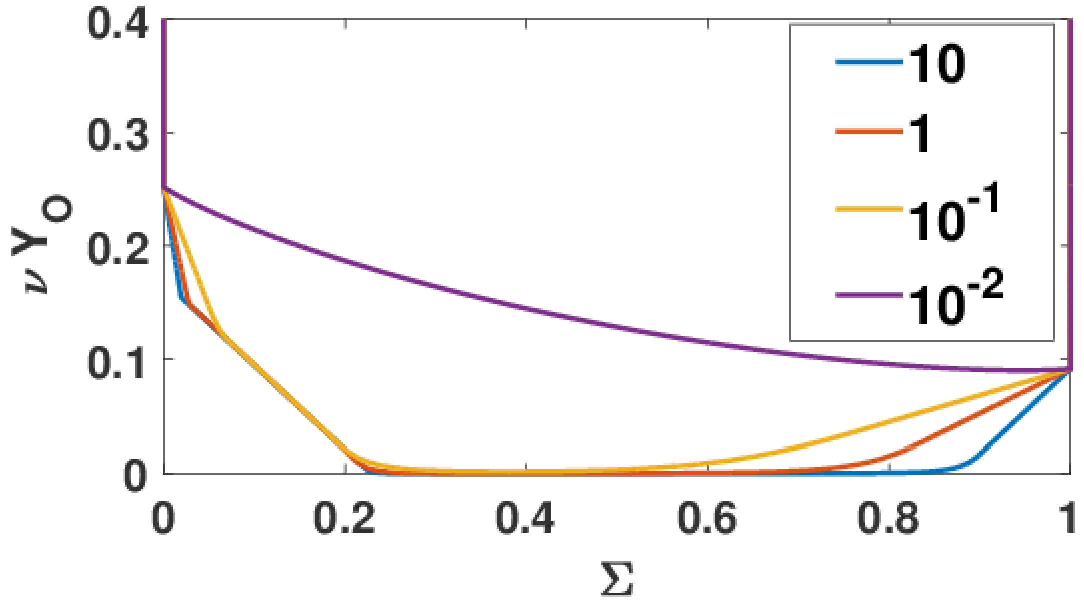
-- At high Da or K values, $n+1$ linear segments appear for scalar variables versus Σ where n is the number of flames.



-- Consistent results with *h* behavior are found for fuel and oxygen mass fractions.

-- The scalar dissipation χ is non-zero only in non-linear regions and especially large in the "corner" regions.





Conclusions

-- Flamelet theory has been extended to three dimensions and to multi-flame configurations.

-- A formalism has been established unifying various reacting counterflows: a single diffusion flame, a single premixed flame, a two-flame situation with a combustible mixture flowing in one direction, and a three-flame situation with combustible mixtures flowing in both directions.

-- Density variations due to combustion result in previously unidentified but substantial velocity overshoots, nonlinear variation in counterflow velocity, and variation in normal strain rate.

-- The dependence of multiple-flame existence, flame merging, and extinction on pressure, imposed strain rate, distribution of strain rate, and Prandtl number has been established.

Conclusions continued

-- A generalized variable Σ to replace mixture fraction and a new generalized scalar dissipation rate have been identified.

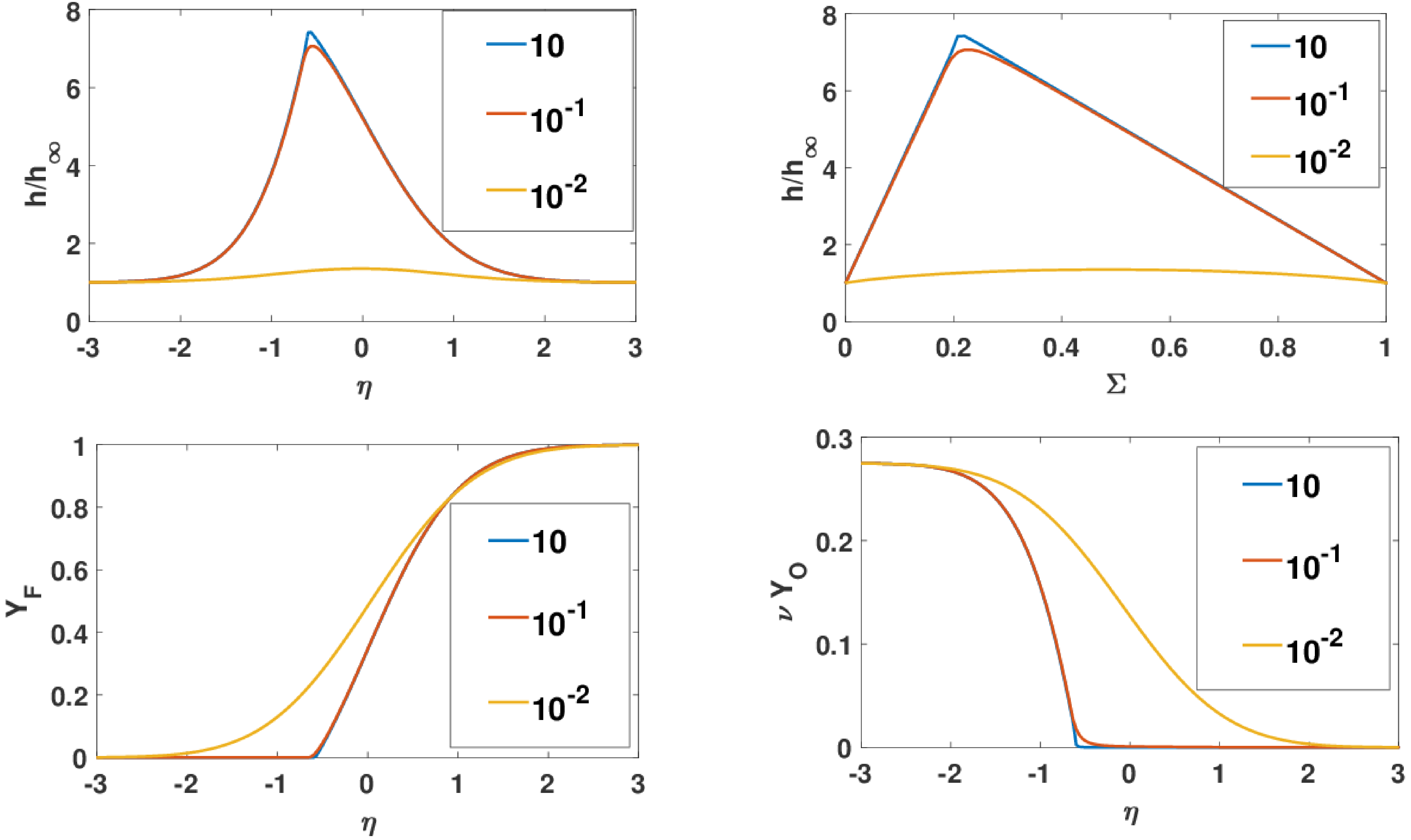
-- Extensions of this flamelet theory for detailed kinetics, detailed transport, and real-fluid equations of state are needed.

-- A basis has been provided for development of sub-grid models for LES using the multi-flamelet approach.

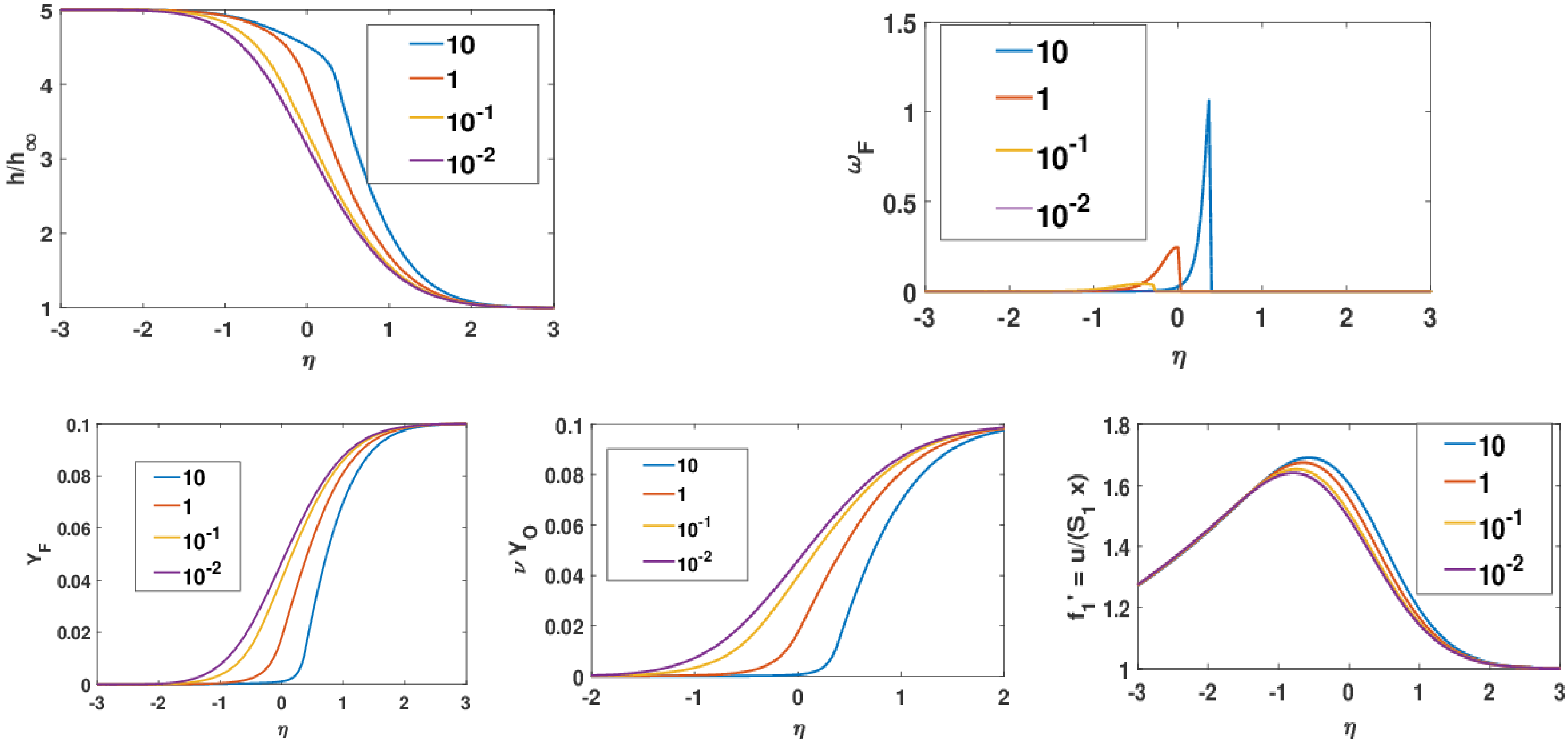
-- A basis has been provided for further exploration of multi-branched flames in highly strained, three-dimensional flows.

Thank you.

Single Diffusion Flame



Single Premixed Flame



Fuel-rich Mixture flowing against Oxygen