

# SIMPLIFIED FORMULATIONS FOR TURBULENT COMBUSTION OF HYDROGEN

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General Basic Equations  
Kolmogorov Turbulence Scaling  
Regimes of Turbulent Combustion  
Approaches to Turbulent Combustion  
Chemical-Kinetic Approximations  
Transport-Property Approximations  
Simplified Conservation Equations  
Turbulent Hydrogen Diffusion Flames

# REACTING NAVIER-STOKES CONSERVATION EQUATIONS

$$\partial\rho/\partial t + \nabla \cdot (\rho\mathbf{v}) = 0.$$

$$\partial\mathbf{v}/\partial t + \mathbf{v} \cdot \nabla\mathbf{v} = -(\nabla \cdot \mathbf{P})/\rho + \sum_{i=1}^N Y_i \mathbf{f}_i$$

$$\rho \frac{\partial}{\partial t} \left( h + \frac{1}{2} v^2 \right) + \rho \mathbf{v} \cdot \nabla \left( h + \frac{1}{2} v^2 \right) = \frac{\partial p}{\partial t} + \nabla \cdot [(p\mathbf{U} - \mathbf{P}) \cdot \mathbf{v}] + \rho \sum_{i=1}^N Y_i \mathbf{f}_i \cdot (\mathbf{v} + \mathbf{V}_i) - \nabla \cdot \mathbf{q}.$$

$$\partial Y_i / \partial t + \mathbf{v} \cdot \nabla Y_i = w_i / \rho - [\nabla \cdot (\rho Y_i \mathbf{V}_i)] / \rho$$

$$\mathbf{P} = \left[ \mathbf{p} + \left( \frac{2}{3} \mu - \kappa \right) (\nabla \cdot \mathbf{v}) \right] \mathbf{U} - \mu [(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T]$$

$$\mathbf{q} = -\lambda \nabla T + \rho \sum_{i=1}^N h_i Y_i \mathbf{V}_i + R^0 T \sum_{i=1}^N \sum_{j=1}^N \left( \frac{X_j D_{Ti}}{W_i D_{ij}} \right) (\mathbf{V}_i - \mathbf{V}_j) + \mathbf{q}_R$$

$$\begin{aligned} \nabla X_i = & \sum_{j=1}^N \left( \frac{X_i X_j}{D_{ij}} \right) (\mathbf{V}_j - \mathbf{V}_i) + (Y_i - X_i) \left( \frac{\nabla p}{p} \right) + \frac{\rho}{p} \sum_{j=1}^N Y_j Y_i (f_i - f_j) \\ & + \sum_{j=1}^N \left[ \left( \frac{X_i X_j}{\rho D_{ij}} \right) \left( \frac{D_{Tj}}{Y_j} - \frac{D_{Ti}}{Y_i} \right) \right] \frac{\nabla T}{T}, \quad i = 1, \dots, N. \end{aligned}$$

$$\mathbf{w}_i = W_i \sum_{k=1}^M (\mathbf{v}_{ik}'' - \mathbf{v}_{ik}') \mathbf{B}_k T^{\alpha_k} e^{-(E_k / R^0 T)} \sum_{j=1}^N \left( \frac{X_j p}{R^0 T} \right)^{v_{j,k}'}, \quad i = 1, \dots, N$$

$$p = \rho R^0 T \sum_{i=1}^N (Y_i / W_i)$$

$$h = \sum_{i=1}^N h_i Y_i$$

$$h_i = h_i^o + \int_{T_0}^T c_{p,i} dT, \quad i = 1, \dots, N$$

$$X_i = \frac{(Y_i / W_i)}{\sum_{j=1}^N (Y_j / W_j)}, \quad i = 1, \dots, N.$$

Symbols	Meaning
$B_k$	A constant in the frequency factor for the kth reaction*
$c_{pi}$	Specific heat at constant pressure for species i*
$D_{ij}$	Binary diffusion coefficient for species i and j*
$D_{Ti}$	Thermal diffusion coefficient for species i*
$E_k$	Activation energy for the kth reaction*
$f_i$	External force per unit mass on species i*
$h$	Enthalpy per unit mass for the gas mixture†
$h_i$	Specific enthalpy of species i†
$h_i^\circ$	Standard heat of formation per unit mass for species i at temperature $T^\circ$ *
$M$	Total number of chemical reactions occurring*
$N$	Total number of chemical species present*
$p$	Hydrostatic pressure†
$P$	Stress tensor†
$q$	Heat-flux vector†
$q_R$	Radiant heat-flux vector*
$R^0$	Universal gas constant*
$T$	Temperature†
$T^0$	A fixed, standard reference temperature*
$V_i$	Diffusion velocity of species i†
$v$	Mass-average velocity of the gas mixture†
$W_i$	Molecular weight of species i*
$w_i$	Rate of production of species i by chemical reactions (mass per unit volume per unit time)†
$X_i$	Mole fraction of species i†
$Y_i$	Mass fraction of species i†
$\alpha_k$	Exponent determining the temperature dependence of the frequency factor for the kth reaction*
$\kappa$	Bulk viscosity coefficient*
$\lambda$	Thermal conductivity*
$\mu$	Coefficient for (shear) viscosity*
$v'_{ik}$	Stoichiometric coefficient for species i appearing as a reactant in reaction k*
$v''_{ik}$	Stoichiometric coefficient for species i appearing as a product in reaction k*
$\rho$	Density†

\* Parameters that must be given in order to solve the conservation equations.

† Quantities determined by the equations given here.

# KOLMOGOROV SCALING

$l$  = Integral scale ,  $u'$  = RMS velocity fluctuation

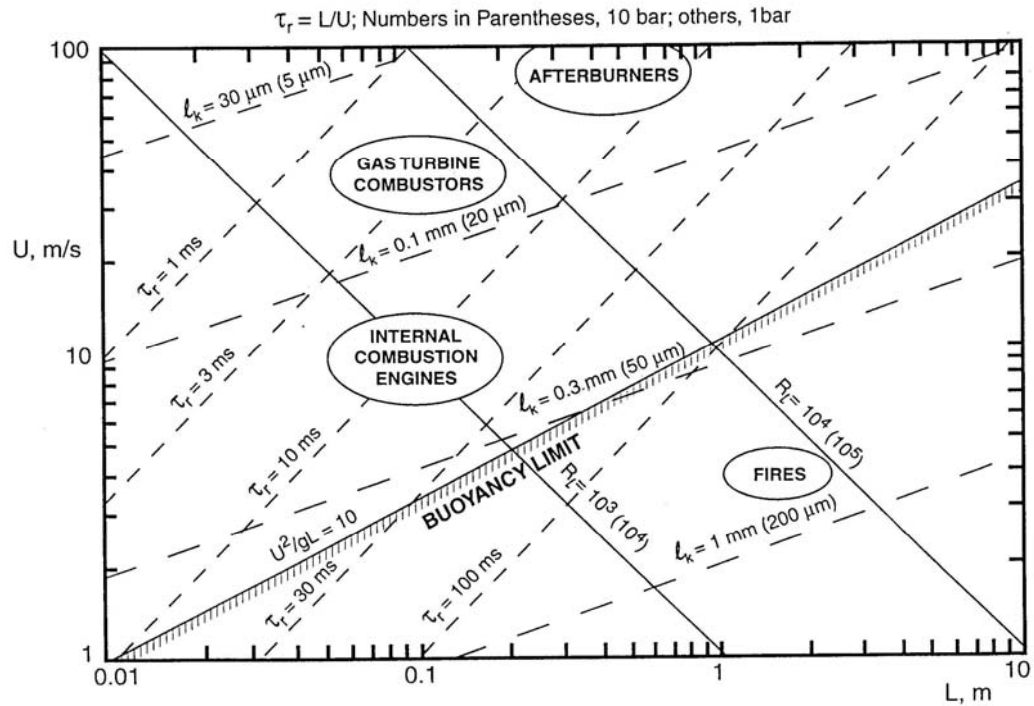
Turbulence Reynolds Number:  $R_l = lu' / \nu$

$\epsilon$  = Rate of dissipation of turbulent kinetic energy

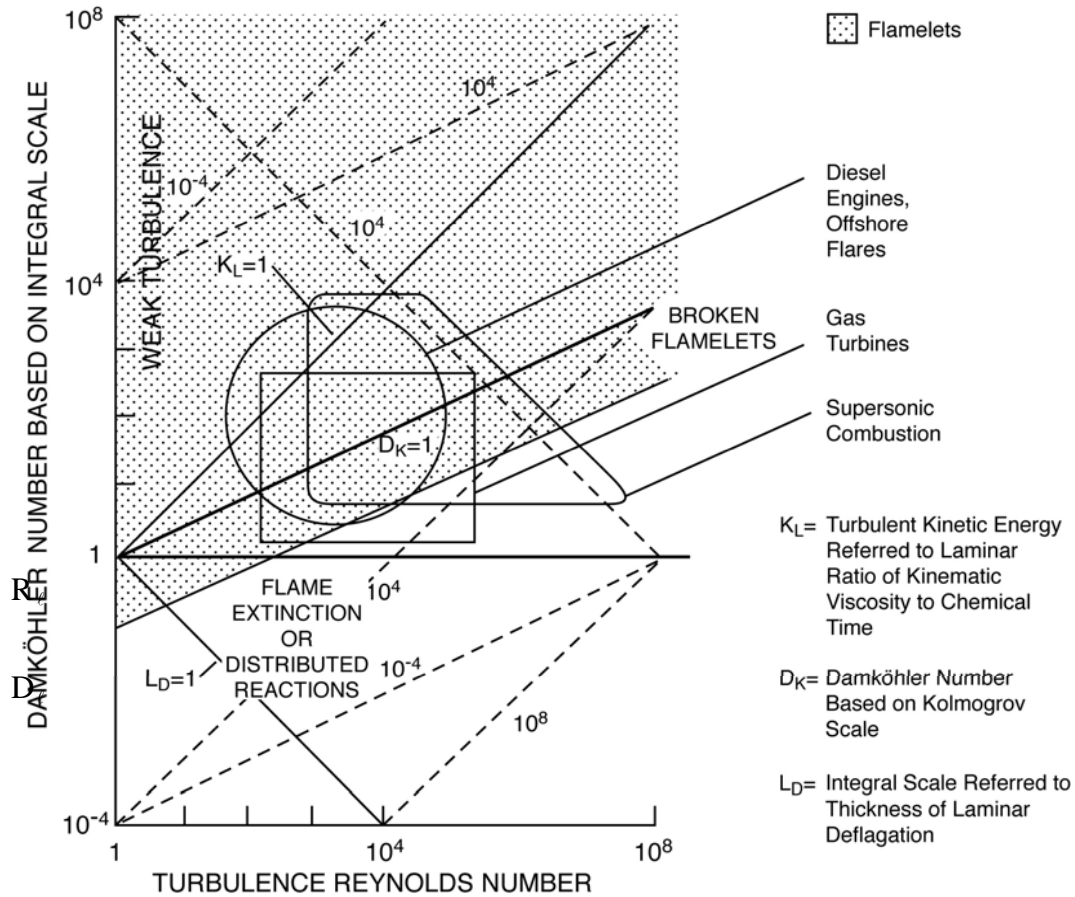
Kolmogorov scale:  $\ell_k = (\nu^3 / \epsilon)^{1/4} = \ell / R_l^{3/4}$

Kinetic energy in eddies of sizes between  $\frac{1}{k}$  and  $\frac{1}{k + dk}$  is  $E(k)dk$

Kolmogorov scaling:  $E(k) = \epsilon^{2/3} k^{-5/3}$  for the inertial range



Regimes of turbulent combustion in a diagram of a length scale of the system and a representative average velocity.



Regimes of turbulent combustion in a diagram of a turbulence Reynolds number and a Damköhler number, both based on the integral scale of the turbulence.

$$D_K = \tau_k / \tau_c = D_l / \sqrt{R_l},$$



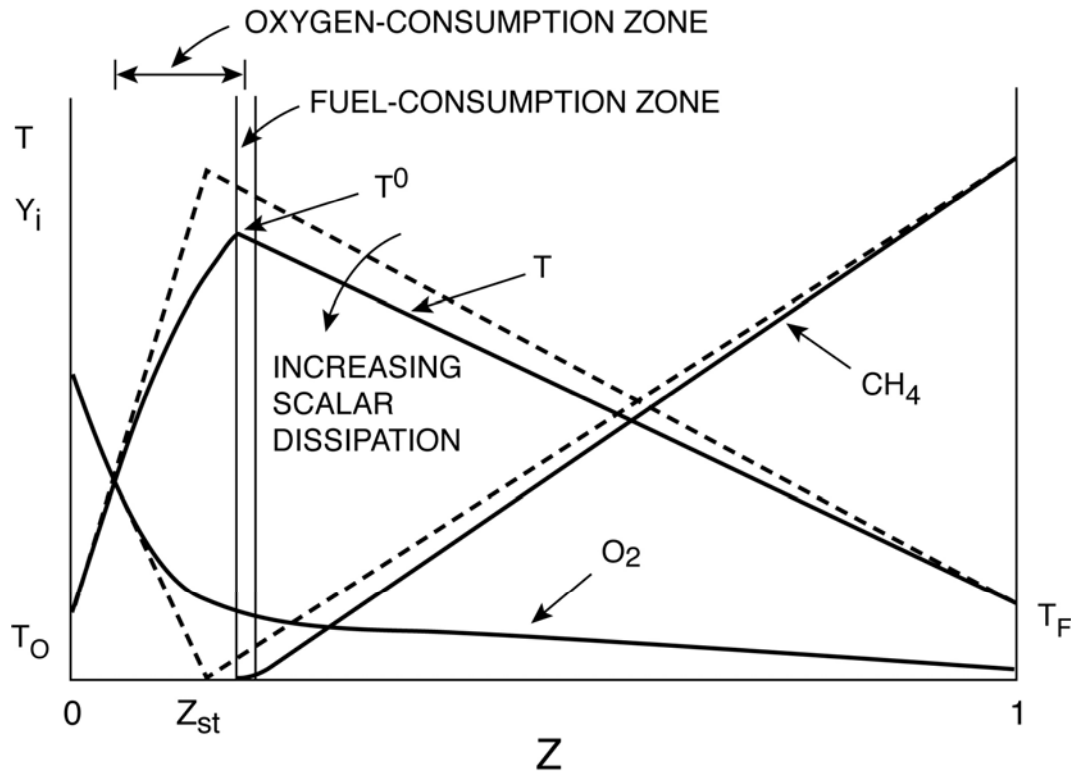
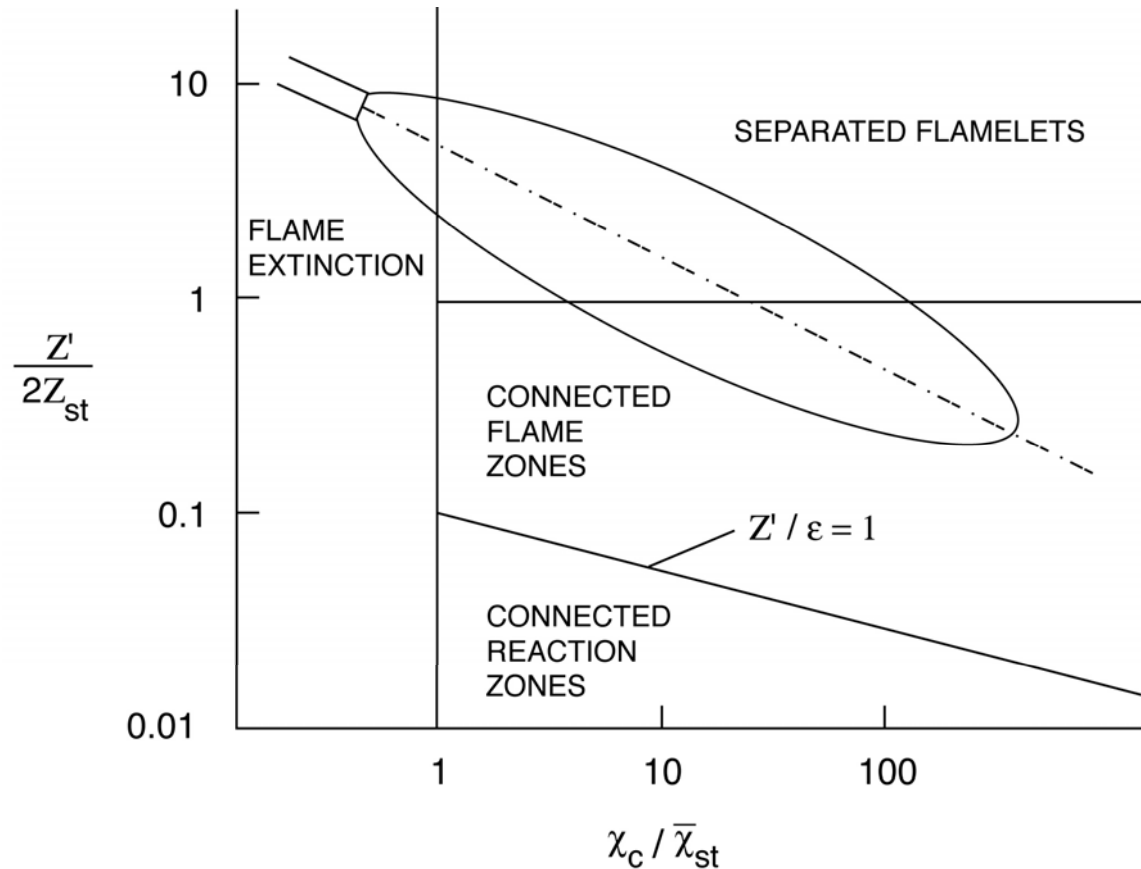


Illustration of hydrocarbon-air flamelet structure as predicted by rate-ratio asymptotics.



Regimes of nonpremixed turbulent combustion in a diagram of a scalar-dissipation parameter related to a Damköhler number and the ratio of a representative mixture-fraction fluctuation to the mixture-fraction range that spans a diffusion flamelet.

$$\chi = 2\nu|\nabla Z|^2$$

# CATEGORIES OF APPROACHES TO ANALYSIS OF TURBULENT COMBUSTION

1. Phenomenological
  - a. Quasidimensional
  - b. Age Theories
  - c. Linear Eddy/One-Dimensional Turbulence
2. Fluids-Based
  - a. Direct Numerical Simulation (DNS)
  - b. Large-Eddy Simulation (LES)
  - c. Moment Methods (RANS)
    - i. Algebraic Closures
    - ii.  $k$ - $\varepsilon$  Modeling
    - iii. Reynolds-Stress Closure
3. Turbulent Burning Velocity ( $S_T$ )
  - a. Perturbations for Low Intensities and Large Scales
  - b. Moment-Method Modeling of the G Equation
  - c. Modeling Flame-Surface Evolution, such as Coherent-Flamelet Models (CFM)
  - d. Fractals
  - e. G-Equations Renormalization
  - f. Pseudosolitons
4. Probability-Density Function (PDF)
  - a. Flamelets
  - b. Presumed PDF
    - i.  $P(Z)$  for Diffusion Flames
    - ii.  $P(c)$  for Premixed Flames
    - iii.  $P(G)$  for Premixed Flames
  - c. Conditional Moment Closure (CMC)
  - d. PDF Transport
    - i. Linear Mean-Square Estimation (LMSE),  
also called Interaction by Exchange with the Mean (IEM)
    - ii. Coalescence-Dispersion (CD)
    - iii. Mapping Closure (MC)
    - iv. Euclidean Minimum Spanning Tree (EMST)

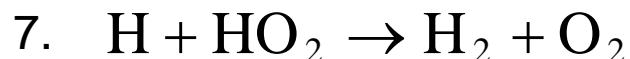
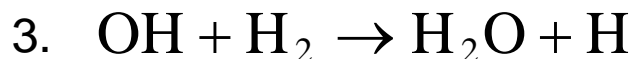
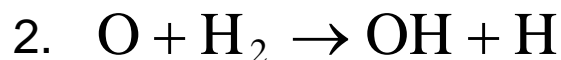
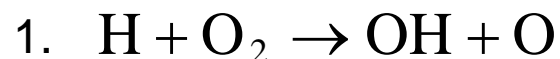
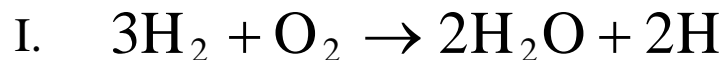
# FRONT-TRACKING EQUATION

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = S_L |\nabla G|$$

# MIXTURE-FRACTION EQUATION

$$\frac{\partial Z}{\partial t} + \mathbf{v} \cdot \nabla Z = \nabla \cdot (\rho D_{th} \nabla Z) / \rho$$

# TWO-STEP CHEMICAL-KINETIC DESCRIPTION



} Not Reversible

$$\alpha = \omega_{7f} / (\omega_6 + \omega_{7f}) = \omega_{7f} / \omega_5$$

$$\omega_I = \omega_{1f} - \omega_{1b} + (1 - \alpha)\omega_5 + \omega_{7b}$$

$$\omega_{II} = \omega_4 + \omega_5$$

## PARTIAL-EQUILIBRIUM APPROXIMATIONS

$$X_{OH} = X_H X_{H_2O} / (K_3 X_{H_2})$$

$$X_O = X_H^2 X_{H_2O} / (K_2 K_3 X_{H_2}^2)$$

$$X_H = K_1^{1/2} K_2^{1/2} K_3 X_{H_2}^{3/2} X_{O_2}^{1/2} / X_{H_2O}$$

$$X_{OH} = K_1^{1/2} K_2^{1/2} X_{H_2}^{1/2} X_{O_2}^{1/2}$$

$$X_O = K_1 K_3 X_{H_2} X_{O_2} / X_{H_2O}$$

# TRANSPORT-PROPERTY APPROXIMATIONS

$$D_{Ti} = 0,$$

$$\kappa = 0 ,$$

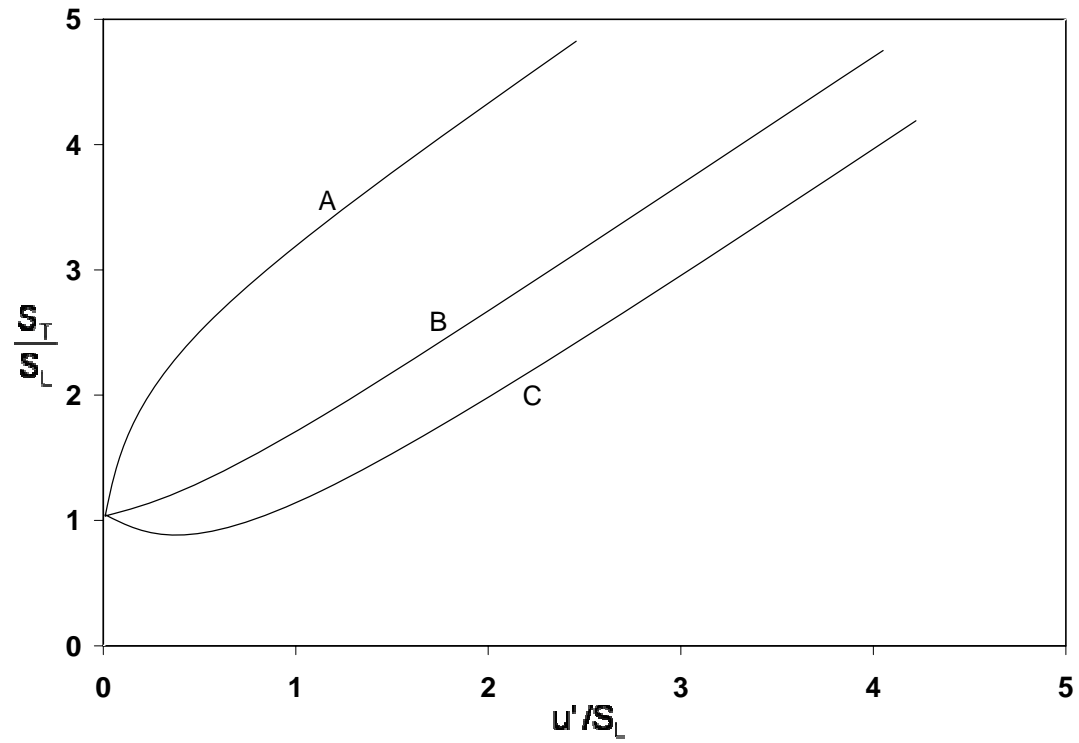
$$Sc_{ij} = \mu / (\rho D_{ij}) = 1 \quad ,$$

$$Pr = \mu c_p / \lambda = 1 \quad ,$$

$$c_{pi} = c_p = \text{constant}$$

and

$$D_{ij} = \text{constant}, \mu = \text{constant} \text{ or } C = \rho\mu = \text{constant}.$$



Schematic illustration of dependences of turbulent burning velocities on turbulence intensity.



# SIMPLIFIED CONSERVATION EQUATIONS

$$D/Dt = \partial/\partial t + \mathbf{v} \cdot \nabla,$$

$$\rho D Y_i / Dt - \nabla [(\mu / S_i) \nabla Y_i] = w_i$$

$$h_T = h - \sum_{i=1}^N h_i^c Y_i$$

$$\rho D h_T / Dt - \nabla [(\mu / Pr) \nabla h_T] = \partial p / \partial t - \sum_{i=1}^N h_i^o w_i - \nabla \cdot \mathbf{q}_R$$

$$w_i = W_i [(\mathbf{v}_{iI}'' - \mathbf{v}_{iI}') \omega_I + (\mathbf{v}_{iII}'' - \mathbf{v}_{iII}') \omega_{II}]$$

$$L_i(Y_i) = \rho D Y_i / Dt - \nabla \cdot [(\mu / S_i) \nabla Y_i]$$

$$L_T(h_T) = \rho D h_T / Dt - \nabla \cdot [(\mu / Pr) \nabla h_T]$$

$$L_{H_2O}(Y_{H_2O} / W_{H_2O}) = -2L_{O_2}(Y_{O_2} / W_{O_2}) = 2\omega_I$$

$$L_{H_2}(Y_{H_2} / W_{H_2}) = \omega_{II} - 3\omega_I$$

$$L_H(Y_H / W_H) = 2\omega_I - 3\omega_{II}$$

$$L_T(\mathbf{h}_T) = Q_I \omega_I + Q_{II} \omega_{II}$$

$$Q_I = -2h_{H_2O}^o W_{H_2O} - 2h_H^o W_H$$

$$Q_{II} = 2h_H^o W_H$$

$$L_{H_2O}(Y_{H_2O}/W_{H_2O}) = -L_{H_2}(Y_{H_2}/W_{H_2}) = -2L_{O_2}(Y_{O_2}/W_{O_2}) = 2\omega_{II}$$

$$L_T(\mathbf{h}_T) = (Q_I + Q_{II})\omega_{II},$$

# NONPREMIXED TURBULENT BURKE-SCHUMANN HYDROGEN COMBUSTION

$$Z_L = Z_{st} / [Z_{st} + (L_O/L_F)(1 - Z_{st})]$$

$$L_O = S_{O_2} / Pr$$

$$L_F = S_{H_2} / Pr$$

$$L = L_O \quad \text{for } Z < Z_L; \quad L = L_F \quad \text{for } Z > Z_L$$

Everywhere:

$$\rho L DZ / Dt = \nabla \cdot (\rho D_{th} \nabla Z)$$

$$(\rho D_{th} = \mu / Pr)$$

$$N = (1 - L_O)/Z_L \text{ for } Z < Z_L; \quad N = (L_F - 1)/(1 - Z_L) \text{ for } Z > Z_L$$

For  $Z < Z_L$ :

$$Y_{O_2} = Y_{O_2\infty} (1 - Z/Z_L)$$

$$2L_F W_{H_2} h_T = (Q_I + Q_{II}) Y_{H_2\infty} Z_L (H + Z/Z_L)$$

For  $Z > Z_L$ :

$$Y_{H_2} = Y_{H_2\infty} (Z - Z_L)/(1 - Z_L)$$

$$2L_F W_{H_2} h_T = (Q_I + Q_{II}) Y_{H_2\infty} Z_L [H + (1 - Z)/(1 - Z_L)]$$

Everywhere:

$$\rho DH/Dt + \rho NDZ/Dt = \nabla \cdot (\rho D_{th} \nabla H)$$

# FINITE-RATE CHEMISTRY NONPREMIXED TURBULENT HYDROGEN COMBUSTION (1)

- I.  $3\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} + 2\text{H}$  in a thin reaction zone at the highest temperature.
- II.  $2\text{H} \rightarrow \text{H}_2$  and/or  $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$  in thicker recombination zones on each side.

Partial equilibrium of  $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$  occurs at the reaction zone of I.

$$X_{\text{H}} = K_{\text{H}} X_{\text{O}_2}^{1/2} / X_{\text{H}_2\text{O}}$$

$$K_{\text{H}} = K_1^{1/2} K_2^{1/2} K_3$$

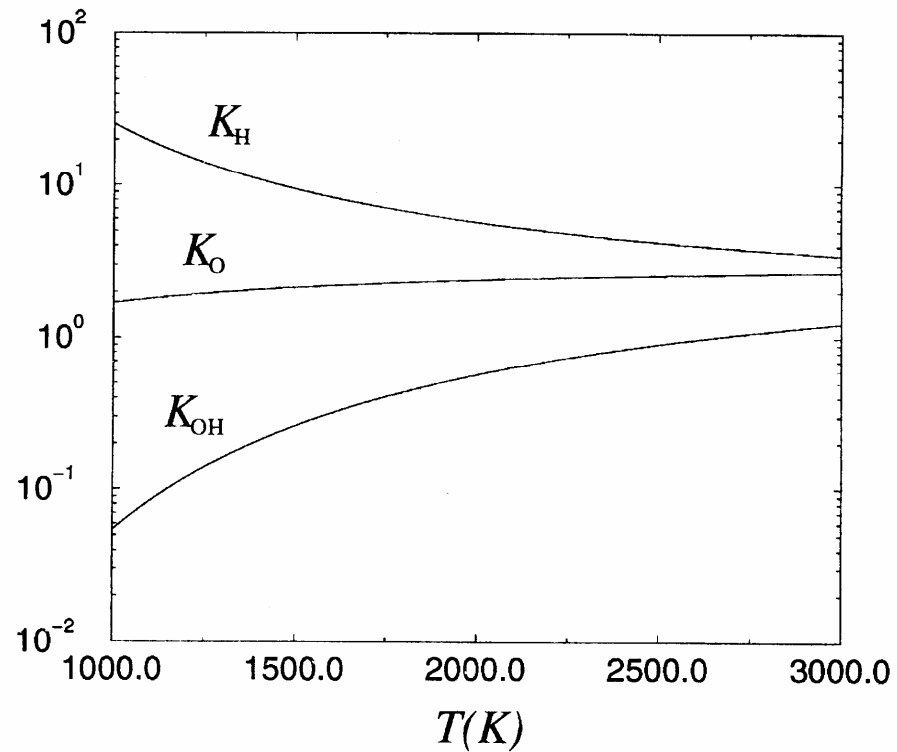
$$X_{\text{OH}} = K_{\text{OH}} X_{\text{H}_2}^{1/2} X_{\text{O}_2}^{1/2}$$

$$K_{\text{OH}} = K_1^{1/2} K_2^{1/2}$$

$$X_{\text{O}} = K_{\text{O}} X_{\text{H}_2} X_{\text{O}_2} / X_{\text{H}_2\text{O}}$$

$$K_{\text{O}} = K_1 K_3$$

# THE PARTIAL-EQUILIBRIUM QUANTITIES $K_H$ , $K_{OH}$ and $K_O$ AS FUNCTIONS OF TEMPERATURE



# FINITE-RATE CHEMISTRY NONPREMIXED TURBULENT HYDROGEN COMBUSTION (2)

$$L_{\text{H}_2\text{O}}(Y_{\text{H}_2\text{O}}/W_{\text{H}_2\text{O}}) = -2L_{\text{O}_2}(Y_{\text{O}_2}/W_{\text{O}_2})$$

$$L_{\text{H}}(Y_{\text{H}}/W_{\text{H}}) = 4L_{\text{O}_2}(Y_{\text{O}_2}/W_{\text{O}_2}) - 2L_{\text{H}_2}(Y_{\text{H}_2}/W_{\text{H}_2})$$

$$L_{\text{T}}(h_{\text{T}}) = Q_{\text{II}}[L_{\text{H}_2}(Y_{\text{H}_2}/W_{\text{H}_2}) - 3L_{\text{O}_2}(Y_{\text{O}_2}/W_{\text{O}_2})] - Q_{\text{I}}L_{\text{O}_2}(Y_{\text{O}_2}/W_{\text{O}_2})$$

$$L_{\text{H}_2}(Y_{\text{H}_2}/W_{\text{H}_2}) - 3L_{\text{O}_2}(Y_{\text{O}_2}/W_{\text{O}_2}) = \omega_4 + \omega_5$$

At the stoichiometric surface of  $3\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} + 2\text{H}$

$$(Z_{\text{st}}=0.036, \text{ not } 0.024) \quad Y_{\text{O}_2} = 0, \quad Y_{\text{H}_2} = 0$$



# CONCLUSIONS

- Turbulent hydrogen combustion obeys the reacting Navier-Stokes equations with fluid-mechanical turbulence.
- There are four broad categories of approaches to the description of turbulent combustion, with optimal approaches differing in different regimes of regime diagrams.
- Of the flamelet and distributed-reaction limiting regimes, most applications lie closer to the flamelet regime.
- A formulation specific to hydrogen can be based on two-step reduced chemistry and account for finite-rate recombination in nonpremixed turbulent combustion.
- It is important to account for Schmidt and Prandtl numbers different from unity in treating turbulent hydrogen combustion.