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

$$\partial\rho/\partial t + \nabla\cdot(\rho\nu) = 0.$$

$$\partial\nu/\partial t + \nu\cdot\nabla\nu = -(\nabla\cdot P)/\rho + \sum_{i=1}^{N} Y_i f_i$$

$$\rho\frac{\partial}{\partial t}\left(h + \frac{1}{2}\nu^2\right) + \rho\nu\cdot\nabla\left(h + \frac{1}{2}\nu^2\right) = \frac{\partial p}{\partial t} + \nabla\cdot[(pU - P)\cdot\nu] + \rho\sum_{i=1}^{N} Y_i f_i\cdot(\nu + V_i) - \nabla\cdot q.$$

$$\partial Y_i/\partial t + v\cdot\nabla Y_i = w_i/\rho - [\nabla\cdot(\rho Y_i V_i)]/\rho$$

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

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

$$\nabla X_i = \sum_{j=1}^{N} \left(\frac{X_i X_j}{D_{ij}} \right) (V_j - V_i) + (Y_i - X_i) \left(\frac{\nabla p}{p} \right) + \frac{\rho}{p} \sum_{j=1}^{N} Y_i Y_i (f_i - f_j)$$

$$+ \sum_{j=1}^{N} \left[\left(\frac{X_i X_j}{\rho D_{ij}} \right) \left(\frac{D_{Tj}}{Y_j} - \frac{D_{Ti}}{Y_i} \right) \right] \frac{\nabla T}{T}, \quad i = 1, \ldots, N.$$

$$w_i = W_i \sum_{k=1}^{M} \left(\nu''_{ik} - \nu'_{ik} \right) B_k T^{\alpha k} e^{-\left(E_k / R^0 T\right)} \sum_{j=1}^{N} \left(\frac{X_j p}{R^0 T} \right)^{\nu'_{j},k}, \quad i = 1, \ldots, N$$

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

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

$$h_i = h_i^o + \int_{T^0}^{T} c_{p,i} dT, \quad i = 1, \ldots, N$$

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

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^o	Standard heat of formation per unit mass for species i at temperature T^{o*}
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†
α_k	Exponent determining the temperature dependence of the frequency factor for the kth reaction*
κ	Bulk viscosity coefficient*
λ	Thermal conductivity*
μ	Coefficient for (shear) viscosity*
ν'_{ik}	Stoichiometric coefficient for species i appearing as a reactant in reaction k*
ν''_{ik}	Stoichiometric coefficient for species i appearing as a product in reaction k*
ρ	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

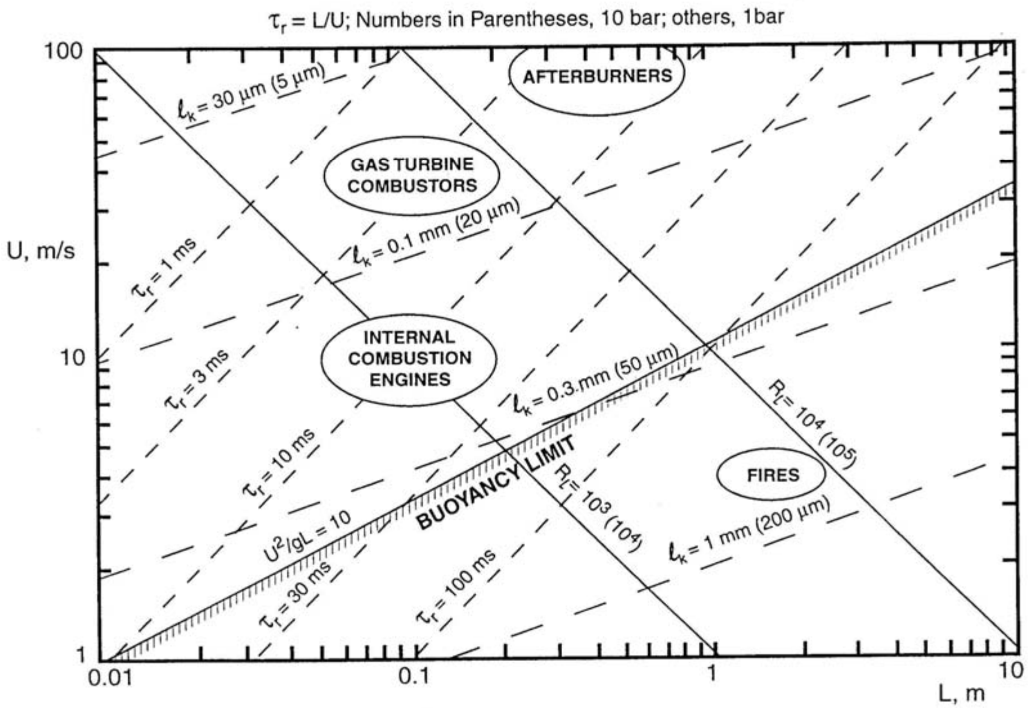
Turbulence Reynolds Number: $R_l = lu'/\nu$

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

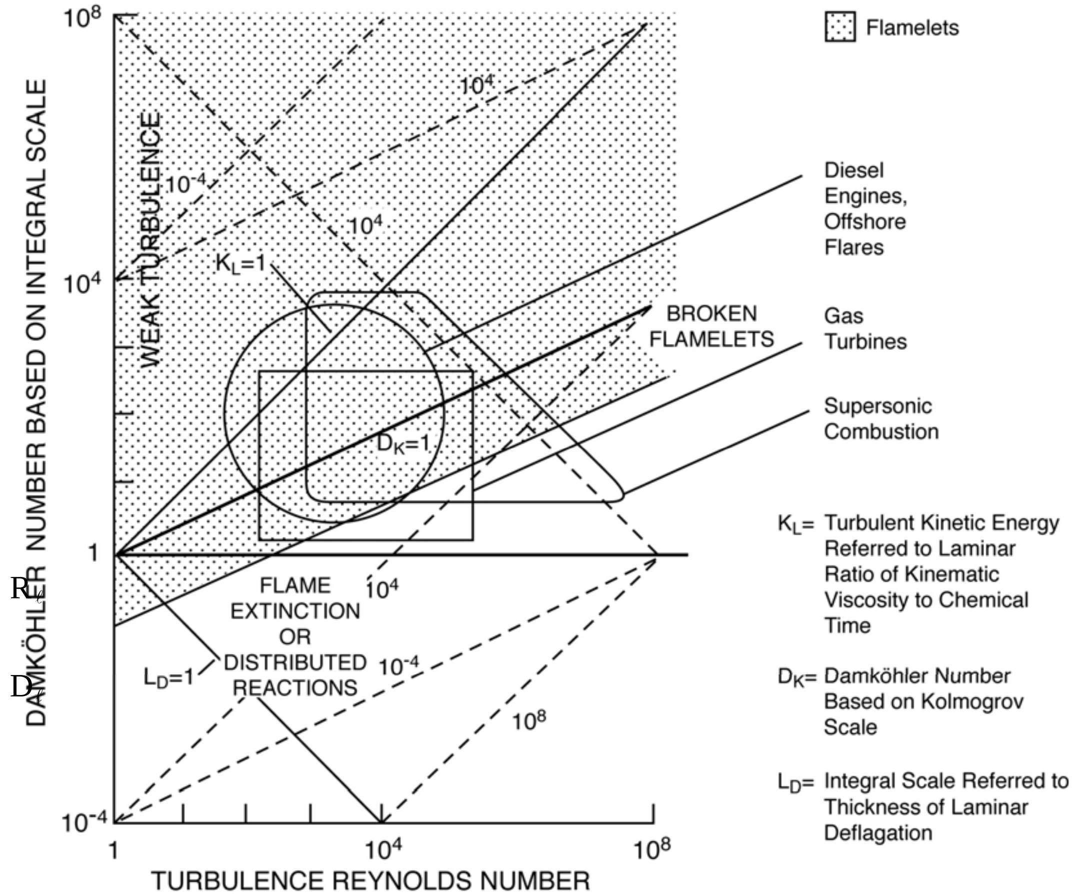
Kolmogorov scale: $\ell_k = \left(\nu^3 / \in\right)^{1/4} = \ell / R_\ell^{3/4}$

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

Kolmogorov scaling: $\mathrm{E}(\mathrm{k}) = \in^{2/3} \ \mathrm{k}^{-5/3}$ 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.

$$D_K = \tau_k / \tau_c = D_\ell / \sqrt{R_\ell},$$

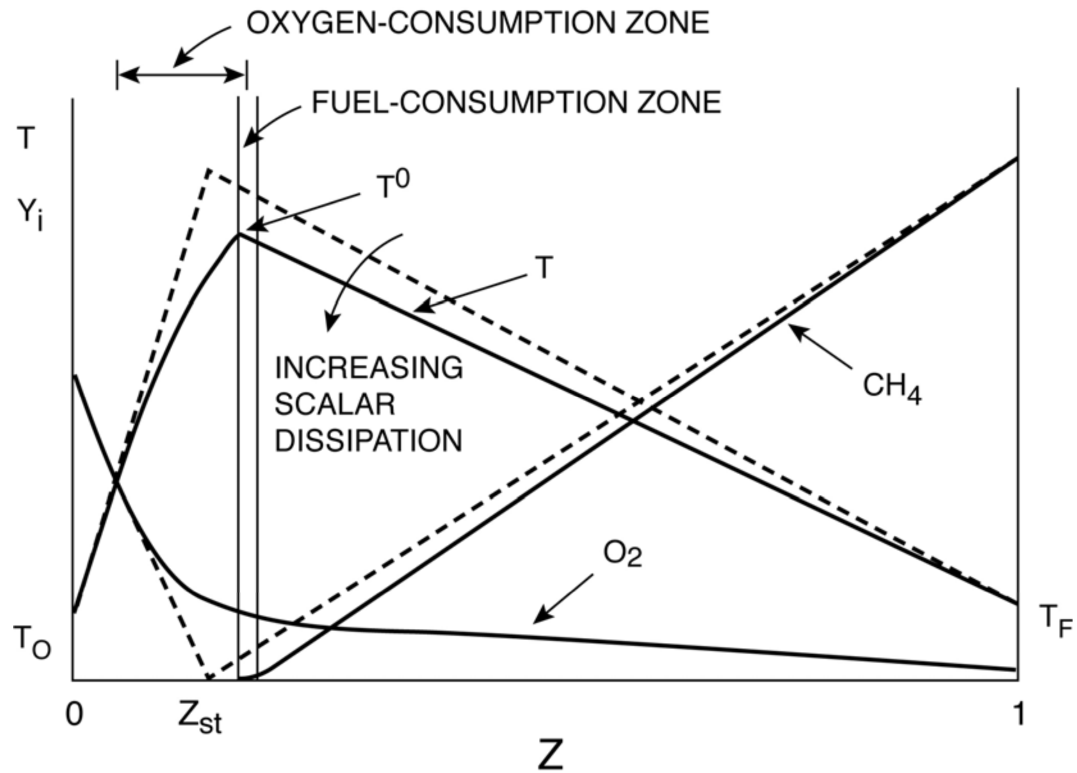
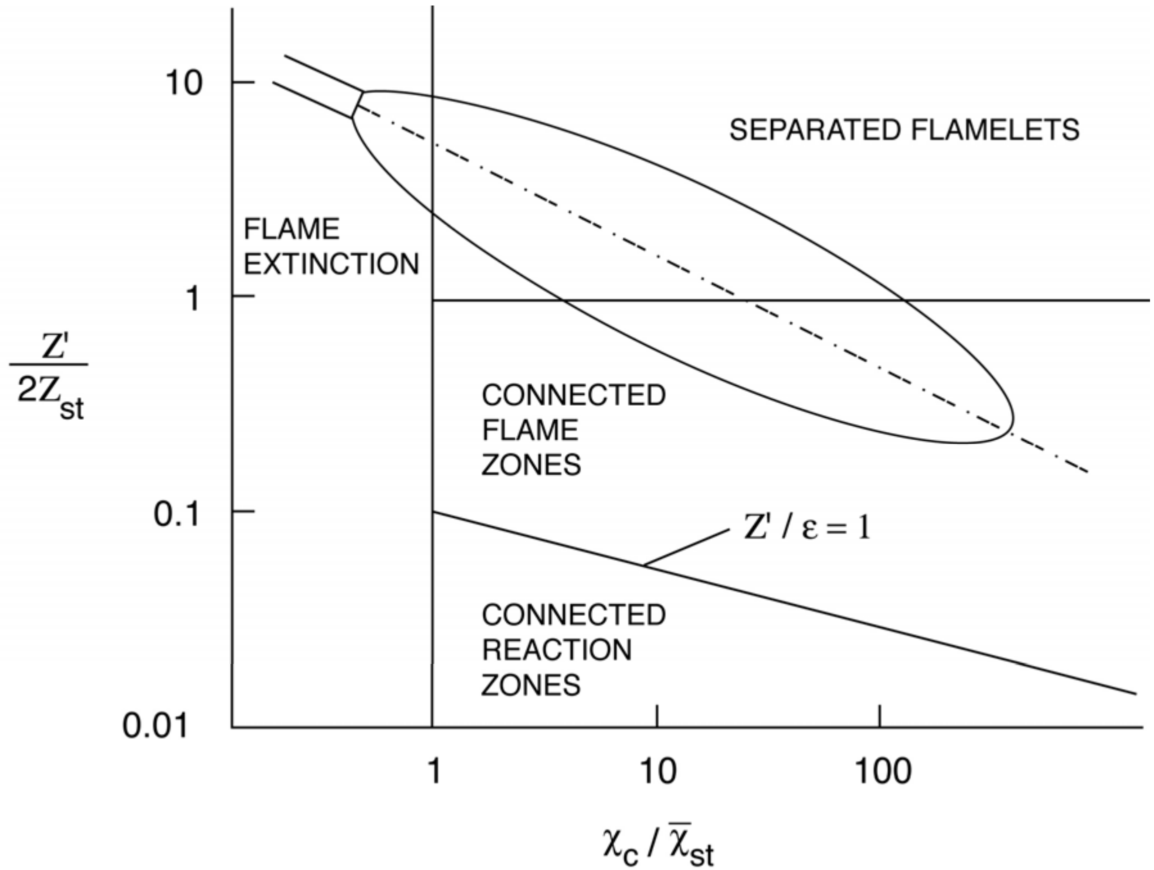


Illustration of hydrocarbon-air flamelet structure as predicted by rate-ratio asymptotics.



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.

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

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-ε 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

$$\partial G / \partial t + v \cdot \nabla G = S_L \left| \nabla G \right|$$

MIXTURE-FRACTION EQUATION

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

TWO-STEP CHEMICAL-KINETIC DESCRIPTION

I. $3H_2 + O_2 \rightarrow 2H_2O + 2H$

II. $2H \rightarrow H_2$

1. $H + O_2 \rightarrow OH + O$
2. $O + H_2 \rightarrow OH + H$
3. $OH + H_2 \rightarrow H_2O + H$
4. $2H + M \rightarrow H_2 + M$
5. $H + O_2 + M \rightarrow HO_2 + M$
6. $H + HO_2 \rightarrow 2OH$
7. $H + HO_2 \rightarrow H_2 + O_2$

Reactions 4–6: 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

$D_{Ti} = 0$,

$\kappa = 0$,

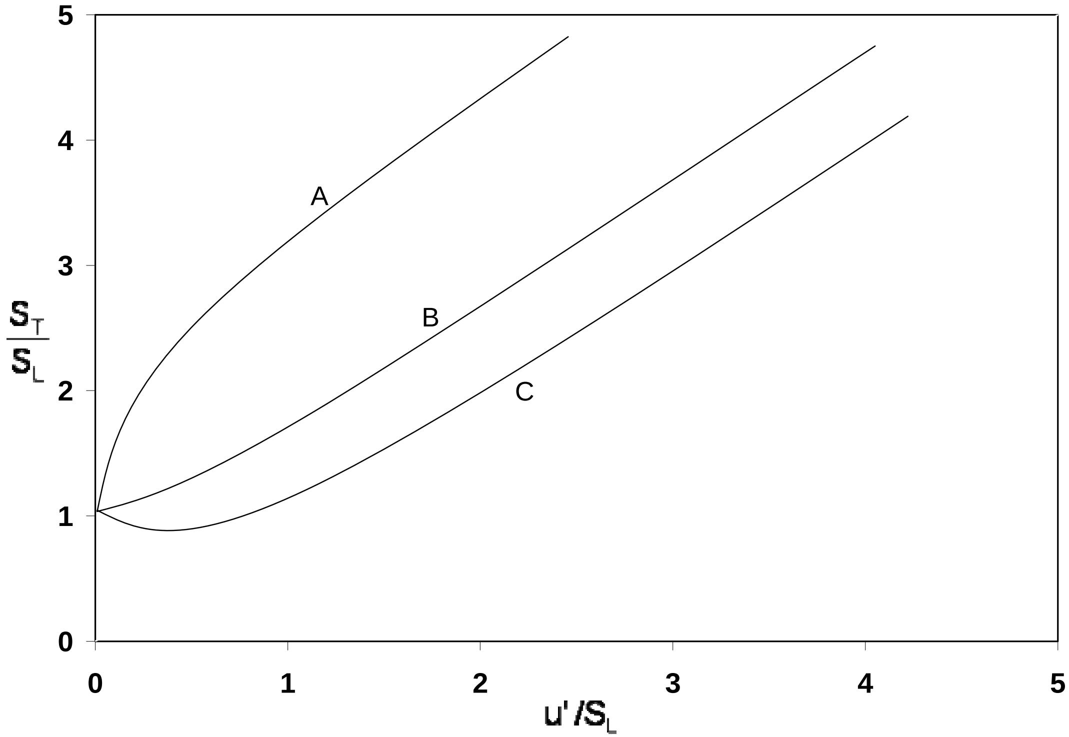
$Sc_{ij} = \mu / (\rho D_{ij}) = 1$,

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

$c_{pi} = c_p =$ constant

and

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



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

SIMPLIFIED CONSERVATION EQUATIONS

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

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

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

$$\rho Dh_T/Dt - \nabla\left[\left(\mu/Pr\right)\nabla h_T\right] = \partial p/\partial t - \sum_{i=1}^{N} h_i^o w_i - \nabla \cdot q_R$$

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

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

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

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

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

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

$$L_T(h_T) = Q_I\omega_I + Q_{II}\omega_{II}$$

$$Q_I = -2h^o_{H_2O}W_{H_2O} - 2h^o_H W_H$$

$$Q_{II} = 2h^o_H W_H$$

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

$$L_T(h_T) = (Q_I + Q_{II})\omega_{II},$$

NONPREMIXED TURBULENT BURKE-SCHUMANN HYDROGEN COMBUSTION

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

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

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

$L = L_O$ for Z < Z_L; L = L_F for Z > Z_L

Everywhere:

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

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

$N = (1 - L_O)/Z_L$ for $Z < Z_L$; $N = (L_F - 1)/(1 - Z_L)$ 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. $3H_2 + O_2 \rightarrow 2H_2O + 2H$ in a thin reaction zone at the highest temperature.

II. $2H \rightarrow H_2$ and/or $2H_2 + O_2 \rightarrow 2H_2O$ in thicker recombination zones on each side.

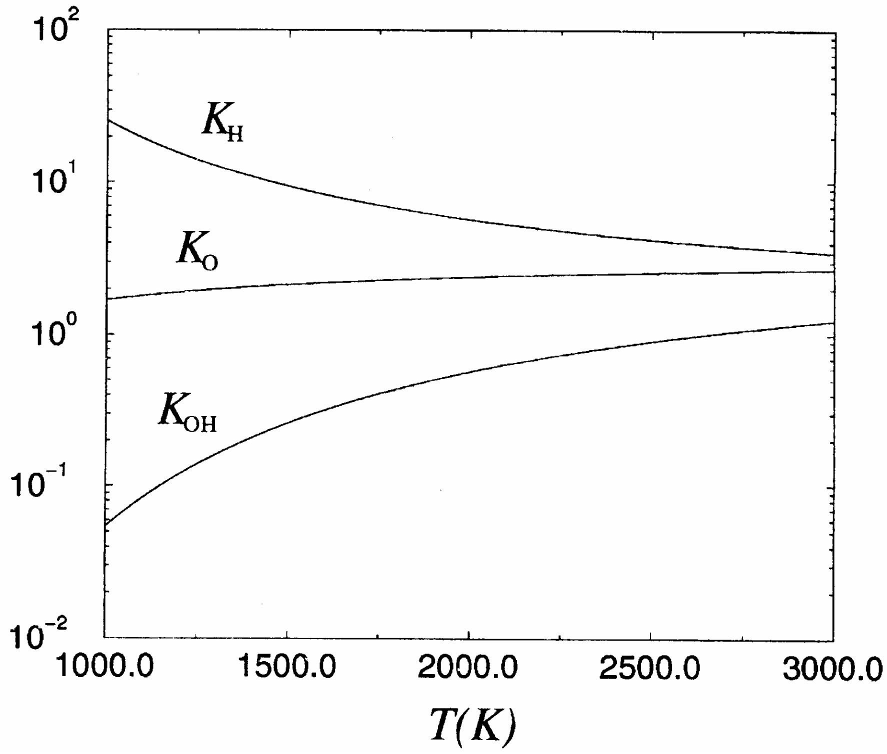
Partial equilibrium of $H + O_2 \rightarrow OH + O$ occurs at the reaction zone of I.

$$X_H = K_H X_{O_2}^{1/2} / X_{H_2O} \qquad K_H = K_1^{1/2} K_2^{1/2} K_3$$

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

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

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



FINITE-RATE CHEMISTRY NONPREMIXED TURBULENT HYDROGEN COMBUSTION (2)

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

$$L_{H}\left(Y_{H}/W_{H}\right) = 4L_{O_2}\left(Y_{O_2}/W_{O_2}\right) - 2L_{H_2}\left(Y_{H_2}/W_{H_2}\right)$$

$$L_{T}\left(h_{T}\right) = Q_{II}\left[L_{H_2}\left(Y_{H_2}/W_{H_2}\right) - 3L_{O_2}\left(Y_{O_2}/W_{O_2}\right)\right] - Q_{I}L_{O_2}\left(Y_{O_2}/W_{O_2}\right)$$

$$L_{H_2}\left(Y_{H_2}/W_{H_2}\right) - 3L_{O_2}\left(Y_{O_2}/W_{O_2}\right) = \omega_4 + \omega_5$$

At the stoichiometric surface of $3H_2 + O_2 \rightarrow 2H_2O + 2H$

(Z_{st}=0.036, not 0.024) $Y_{O_2} = 0, \quad Y_{H_2} = 0$

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.