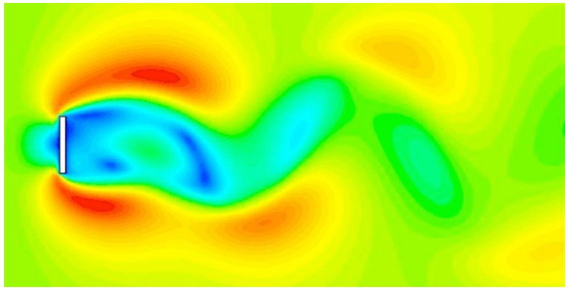
Chemical Reaction Modeling



Neal Davis

Species Transport Approach

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot \left(\rho \vec{v} Y_i\right) = -\nabla \cdot \vec{J}_i + R_i + S_i$$

Y_i = local mass fraction
R_i = rate of production, chemical reaction
S_i = rate of production, addition from dispersed phase
J_i = diffusion flux

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$$\vec{J}_i = -\rho D_{i,m} \nabla Y_i - D_{T,i} \frac{\nabla T}{T}$$

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$$\vec{J}_i = -\left(\rho D_{i,m} + \frac{\mu_t}{\mathrm{Sc}_t}\right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T}$$

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$$R_{\mathrm{kin},r} = \frac{A_r T^{\beta} \exp\left(\frac{E_r}{RT}\right)}{p_{r,d}^{N_{r,n}}} \prod_{n=1}^{n_{\max}} p_n^{N_{r,n}}$$

Mixture Fractions Approach (Non-Premixed Combustion)

$$\frac{\partial}{\partial t}\left(\rho \bar{f}\right) + \nabla \cdot \left(\rho \vec{v} \bar{f}\right) = -\nabla \cdot \left(\frac{\mu_{\mathrm{lam}} + \mu_{\mathrm{turb}}}{\sigma_t} \nabla \bar{f} \right) + S_m$$

$$f = \frac{Z_i - Z_{i,\mathrm{ox}}}{Z_{i,\mathrm{fuel}} - Z_{i,\mathrm{ox}}}$$

Reaction Progress Variable Approach (Premixed Combustion)

$$\frac{\partial}{\partial t}(\rho\bar{c}) + \nabla\cdot\left(\rho\vec{v}\bar{c}\right) = -\nabla\cdot\left(\frac{\mu_{\text{turb}}}{\text{Sc}_t}\nabla\bar{c}\right) + \rho S_c$$

$$c = \frac{\sum_k \alpha_k \left(Y_k - Y_k^u\right)}{\sum_k \alpha_k Y_k^{\text{eq}}} = \frac{Y_c}{Y_c^{\text{eq}}}$$

Composition PDF Transport Approach (Finite-Rate Chemistry)

$$\frac{\partial}{\partial t}(\rho P) + \frac{\partial}{\partial x_i}(\rho u_i P) + \frac{\partial}{\partial \psi_k}(\rho S_k P) = -\frac{\partial}{\partial x_i}\left[\rho \left\langle u_i'' | \psi \right\rangle P\right] + \frac{\partial}{\partial \psi_k}\left[\rho \left\langle \frac{1}{\rho}\frac{\partial J_{i,k}}{\partial x_i} | \psi \right\rangle P\right]$$