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The Nondimensionalization of the Chemically Reacting Navier-Stokes Equations

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In this memorandum, we present the nondimensionalization of the chemically reacting Navier-Stokes equations. The scales of the conserved variables often seen in chemically reacting flows are disparate. For instance, energy can be on the order of ten thousand joules per cubic meter and concentrations can be on the order of ten one-thousandths of kilo-moles per cubic meter. This disparity can lead to ill-conditioned linear systems associated with implicit temporal integration, which become more difficult to converge. We demonstrate and derive here a nondimensional state that is utilized within our formulation. Free parameters are established for the nondimensionalization and the choice of their reference values explained. We then demonstrate the change in disparity of values by comparing a nondimensional and dimensional result of a splitter plate simulation.

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1.3.2 Results for a chemically reacting hydrogen-air shear layer solution demonstrating the variety of scales found in the conservation variables for chemically reacting flow simulations. The ratio in scales found here for maximum values of the conservation variables changed from $\max\left(\rho e_t / C_{H_2O_2}\right) \approx 1e12$ to $\max\left(\hat{\rho e_t / C_{H_2O_2}}\right) \approx 1e5$. 14

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EXECUTIVE SUMMARY

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THE NONDIMENSIONALIZATION OF THE CHEMICALLY REACTING NAVIER-STOKES EQUATIONS

1. NONDIMENSIONALIZATION

1.1 Chemically Reacting Navier-Stokes Equations

We quickly review the governing equations of the chemically reacting Navier-Stokes equations as described by Johnson and Kercher [1]. Let $\Omega \subset \mathbb{R}^d$ be a given d-dimensional domain with boundary $\partial\Omega$, over which an outward oriented normal $n : \partial\Omega \to \mathbb{R}^d$ is defined, and $T \subset \mathbb{R}^+$ is a given temporal interval. We consider the nonlinear conservation law governing the unsteady chemically reacting Navier-Stokes equations, in strong form, defined for piecewise smooth, $\mathbb{R}^m$-valued functions y, and gradient ∇y, given as

$$\frac{\partial y}{\partial t} + \nabla \cdot \mathcal{F}\left(y, \nabla y\right) - \mathcal{S}\left(y\right) = 0 \text{ in } \Omega \times T, \tag{1.1.1}$$

$$y\left(\cdot, t_0\right) - y_0 = 0 \text{ in } \Omega, \tag{1.1.2}$$

$$n \cdot \mathcal{F}\left(y, \nabla y\right) - n \cdot \mathcal{F}_{\partial}\left(y, \nabla y\right) = 0 \text{ on } \partial\Omega \times T, \tag{1.1.3}$$

$$G_{\partial}\left(y_{\partial}\right) : \left(y^{+} - y_{\partial}\right) \otimes n = 0 \text{ on } \partial\Omega \times T, \tag{1.1.4}$$

where t denotes time, $\mathcal{F} : \mathbb{R}^m \to \mathbb{R}^{m \times d}$ is a given flux function, $\mathcal{S} : \mathbb{R}^m \to \mathbb{R}^m$ is a given source term. The initial conditions at time t_0 are given by y_0 in Equation (1.1.2). The flux function

$$\mathcal{F}\left(y, \nabla y\right) = \left(\mathcal{F}^c\left(y\right) - \mathcal{F}^v\left(y, \nabla y\right)\right) \tag{1.1.5}$$

is defined in terms of the convective flux $\mathcal{F}^c\left(y\right)$, which is only a function of the state y, and viscous flux $\mathcal{F}^v\left(y, \nabla y\right)$, which is a function of the state and the gradient, ∇y. Furthermore, the viscous flux can be written as

$$\mathcal{F}^v\left(y, \nabla y\right) = G\left(y\right) : \nabla y \tag{1.1.6}$$

where $G\left(y\right) = \mathcal{F}^v_{\nabla y}$ is its the partial linearization with respect to the gradient, ∇y, which is sometimes referred to as the homogeneity tensor [2].

The chemically reacting Navier-Stokes flow state variable is given by

$$y = \left(\rho v_1, \ldots, \rho v_d, \rho e_t, C_i, \ldots, C_{n_s}\right), \tag{1.1.7}$$

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where $m = d + n_s + 1$, n_s is the number of thermally perfect species, $\rho : \mathbb{R}^{n_s} \to \mathbb{R}$ is density, $(v_1, \ldots, v_d) : \mathbb{R}^m \to \mathbb{R}^d$ is the velocity, $e_t : \mathbb{R}^m \to \mathbb{R}$ is the specific total energy, and $C : \Omega \to \mathbb{R}^{n_s}$ are the species concentrations. The density is calculated from the concentrations as

$$\rho = \sum_{i=1}^{n_s} W_i C_i, \tag{1.1.8}$$

where W_i is the molecular weight of species i.

The k-th spatial convective flux component is given by

$$\mathcal{F}_k^c(y) = \left(\rho v_k v_1 + p\delta_{k1}, \ldots, \rho v_k v_d + p\delta_{kd}, v_k(\rho e_t + p), v_k C_1, \ldots, v_k C_{n_s}\right). \tag{1.1.9}$$

The pressure, $p : \mathbb{R}^m \to \mathbb{R}$, is calculated from the equation of state,

$$p = R^0 T \sum_{i=1}^{n_s} C_i, \tag{1.1.10}$$

where $T : \mathbb{R}^m \to \mathbb{R}$, is the temperature and $R^0 = 8314.4621\,\mathrm{JKmol}^{-1}\mathrm{K}^{-1}$ is the universal gas constant. The total energy, ρe_t, is given as the sum of the internal and kinetic and energies as

$$\rho e_t = \rho u + \frac{1}{2}\sum_{k=1}^{d} \rho v_k v_k, \tag{1.1.11}$$

where $\rho u : \mathbb{R}^m \to \mathbb{R}$ is the internal energy. The internal energy is also defined as the mass weighted sum of thermally perfect species specific internal energies that are n_p-order polynomials with respect to temperature,

$$\rho u = \sum_{i=1}^{n_s} W_i C_i \sum_{k=0}^{n_p} a_{ik} T^k. \tag{1.1.12}$$

In this work, all thermodynamic polynomials are continuous refits of the analytic form from NASA's polynomial representations [3].

The k-th spatial component of the viscous flux is given by

$$\mathcal{F}_k^v(y, \nabla y) = \left(\tau_{1k}, \ldots, \tau_{dk}, \sum_{j=1}^{d} \tau_{kj} v_j - W_i C_i h_i V_{ik} - q_k, C_1 V_{1k}, \ldots, C_{n_s} V_{n_s k}\right), \tag{1.1.13}$$

where $q : \mathbb{R}^m \times \mathbb{R}^{m\times d} \to \mathbb{R}^d$ is the thermal heat flux, $\tau : \mathbb{R}^m \times \mathbb{R}^{m\times d} \to \mathbb{R}^{d\times d}$ is the viscous stress tensor, $\left(h_1, \dots, h_{n_s}\right) : \mathbb{R}^m \to \mathbb{R}^{n_s}$ are the species specific enthalpies, and $\left(\left(V_{11}, \dots, V_{1d}\right), \dots, \left(V_{n_s 1}, \dots, V_{n_s d}\right)\right) : \mathbb{R}^m \times \mathbb{R}^{n_s\times d} \to \mathbb{R}^{n_s\times d}$ are the species diffusion velocities. The k-th spatial component of the viscous stress tensor is given by

$$\tau_k\left(y, \nabla y\right) = \mu\left(\frac{\partial v_1}{\partial x_k} + \frac{\partial v_k}{\partial x_1} - \delta_{k1}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial v_j}{\partial x_j}, \dots, \frac{\partial v_d}{\partial x_k} + \frac{\partial v_k}{\partial x_d} - \delta_{kd}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial v_j}{\partial x_j}\right), \tag{1.1.14}$$

where $\mu : \mathbb{R}^m \to \mathbb{R}$ is the dynamic viscosity. The k-th spatial component of the heat flux is given as

$$q_k\left(y, \nabla y\right) = -\lambda\frac{\partial T}{\partial x_k}.$$

where $\lambda : \mathbb{R}^m \to \mathbb{R}$ is the thermal conductivity.

The transport properties are calculated using mixture averaged properties. The k-th spatial component of the diffusion velocity for the i-th species is given as

$$V_{ik}^{\dagger} = \frac{\bar{D}_i}{C_i}\frac{\partial C_i}{\partial x_k} - \frac{\bar{D}_i}{\rho}\frac{\partial \rho}{\partial x_k}. \tag{1.1.15}$$

To ensure mass conservation, i.e. $\sum_{i=1}^{n_s} W_i C_i V_{ik} = 0$, a standard correction, see [4] and [5], is applied to the species diffusion velocity (1.1.15),

$$V_{ik} = V_{ik}^{\dagger} - \frac{\sum_{i=1}^{n_s} W_i C_i V_{ik}^{\dagger}}{\rho}. \tag{1.1.16}$$

The species mixture averaged diffusion coefficients $\left(\bar{D}_1, \dots, \bar{D}_{n_s}\right) : \mathbb{R}^m \to \mathbb{R}^{n_s}$, from [6], are defined for the i-th species as

$$\bar{D}_i = \frac{p_{atm}}{p\bar{W}}\frac{\sum_{j=1, j\neq i}^{n_s} X_j W_j}{\sum_{j=1, j\neq i}^{n_s} X_j / D_{ij}}, \tag{1.1.17}$$

where $p_{atm} = 101325$ Pa, X_j is the mole fraction of species j, D_{ij} is the diffusion coefficient of species i to species j, and $\bar{W} : \mathbb{R}^m \to \mathbb{R}$ is the mixture molecular weight, defined as

$$\bar{W} = \frac{\rho}{\sum_{i=1}^{n_s} C_i}. \tag{1.1.18}$$

and the mole fractions $\left(X_1, \dots, X_{n_s}\right) : \mathbb{R}^{n_s} \to \mathbb{R}^{n_s}$ can be calculated directly from concentrations,

$$X_i = \frac{C_i}{\sum_{i=1}^{n_s} C_i}. \tag{1.1.19}$$

The Wilke model [7] is used to calculate viscosity

$$\mu = \sum_{i=1}^{n_s} \frac{X_i \mu_i}{X_i + \sum_{i=1, i \neq j}^{n_s} \left(X_j \phi_{ij} \right)}, \tag{1.1.20}$$

where

$$\phi_{ij} = \frac{\left(1 + \left(\frac{W_j}{W_i} \right)^{1/4} \sqrt{\left(\frac{\mu_i}{\mu_j} \right)} \right)^2}{\sqrt{8 \left(1 + \frac{W_i}{W_j} \right)}},$$

and μ_i and μ_j are the species specific viscosities for species i and j, respectively. The Mathur model [8] is used to calculate conductivity,

$$\lambda = \frac{1}{2} \left(\sum_{i=1}^{n_s} X_i \lambda_i + \frac{1}{\sum_{i=1}^{n_s} \frac{X_i}{\lambda_i}} \right), \tag{1.1.21}$$

where λ_i is the conductivity of species i.

Finally, the source term, which includes the detailed chemical kinetics, is given by

$$\mathcal{S}(y) = \left(0, \ldots, 0, 0, \omega_1, \ldots, \omega_{n_s} \right), \tag{1.1.22}$$

where ω_i is the production rate of species i, which is the sum of the progress reaction rates from any arbitrary number of reactions and reaction types, cf. [9].

1.2 Nondimensionalization

We introduce nondimensionalization of a dimensional quantity, α, through the relationship

$$\alpha = \hat{\alpha} \alpha_{ref}, \tag{1.2.1}$$

where α_{ref} is the reference value of the same units as α and $\hat{\alpha}$ is the nondimensional quantity. This gives the state

$$y = \left(\rho \hat{v}_1 \left(\rho v\right)_{ref}, \ldots, \rho \hat{v}_d \left(\rho v\right)_{ref}, \rho \hat{e}_t \left(\rho e_t\right)_{ref}, \hat{C}_i \left(C\right)_{ref}, \ldots, \hat{C_{n_s}} \left(C\right)_{ref}\right), \tag{1.2.2}$$

establishing

$$y = \hat{y} \odot y_{ref}, \tag{1.2.3}$$

Where y_{ref} are the reference dimensional quantities and $\hat{y}$ is the nondimensional state. The objective is to derive an equivalent nondimensional form of the state that can be utilized within the formulation in order to reduce the potentially large disparity in magnitudes of the different components of the state. For instance, energy can be on the order of $10^5 J/m^3$ and concentrations can be on the order of $10^{-3} kmole/m^3$. This disparity can lead to poor conditioning of the linear systems associated with implicit time integration. We can arrive at the nondimensional conservation equation

$$\mathcal{F}_{ref}^{-1} \odot \left(\frac{\partial y}{\partial t} + \nabla \cdot \mathcal{F}\left(y, \nabla y\right) - \mathcal{S}\left(y\right)\right) = \frac{\partial \hat{y}}{\partial \hat{t}} + \hat{\nabla} \cdot \hat{\mathcal{F}}\left(\hat{y}, \hat{\nabla}\hat{y}\right) - \mathcal{S}\left(\hat{y}\right) = 0 \tag{1.2.4}$$

By inspection we found that following parameters can be set as free parameter reference quantities: p_{ref}, T_{ref}, ρ_{ref}, μ_{ref}, D_{ref}, λ_{ref}, and L_{ref}. The other reference quantities will be derived for simplification purposes.

1.2.1 Momentum Equation

By first examining the momentum component, denoted as $|_{\rho v_i}$, of the conservation Equation (1.2.4) we can arrive at the velocity and time reference quantities and the nondimensional momentum equation,

$$\frac{\partial\left(\rho v_i\right)}{\partial t} + \nabla \cdot \left(\mathcal{F}_1|_{\rho v_i}, \ldots, \mathcal{F}_d|_{\rho v_i}\right) = 0 \text{ with } \mathcal{F}_k|_{\rho v_i} = \rho v_k v_i + p\delta_{ki} + \mu\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \delta_{1i}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial v_j}{\partial x_j}\right) \tag{1.2.5}$$

$$\frac{\partial\left(\hat{\rho}\rho_{ref}\hat{v}_i v_{ref}\right)}{\partial \hat{t} t_{ref}} + \frac{1}{L_{ref}}\hat{\nabla} \cdot \left(\mathcal{F}_1|_{\rho v_i}, \ldots, \mathcal{F}_d|_{\rho v_i}\right) = 0 \tag{1.2.6}$$

with

$$\mathcal{F}_k|_{\rho v_i} = \hat{\rho}\hat{v}_k\hat{v}_i v_{ref}^2 \rho_{ref} + \hat{p} p_{ref} \delta_{ki} + \hat{\mu}\mu_{ref} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} \frac{v_{ref}}{L_{ref}} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} \frac{v_{ref}}{L_{ref}} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \frac{v_{ref}}{L_{ref}} \right) \quad (1.2.7)$$

then

$$\frac{\partial \left(\hat{\rho}\hat{v}_i\right)}{\partial \hat{t}} \frac{\rho_{ref} v_{ref}}{t_{ref}} + \frac{1}{L_{ref}} \hat{\nabla} \cdot \left(\mathcal{F}_1|_{\rho v_i}, \ldots, \mathcal{F}_d|_{\rho v_i} \right) = 0 \quad (1.2.8)$$

with

$$\mathcal{F}_k|_{\rho v_i} = \hat{\rho}\hat{v}_k\hat{v}_i v_{ref}^2 \rho_{ref} + \hat{p} p_{ref} \delta_{ki} + \hat{\mu}\mu_{ref} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} \frac{v_{ref}}{L_{ref}} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} \frac{v_{ref}}{L_{ref}} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \frac{v_{ref}}{L_{ref}} \right) \quad (1.2.9)$$

then

$$\frac{\partial \left(\hat{\rho}\hat{v}_i\right)}{\partial \hat{t}} \frac{\rho_{ref} v_{ref}}{t_{ref}} + \frac{v_{ref}^2 \rho_{ref}}{L_{ref}} \hat{\nabla} \cdot \left(\mathcal{F}_1|_{\rho v_i}, \ldots, \mathcal{F}_d|_{\rho v_i} \right) = 0 \quad (1.2.10)$$

$$\mathcal{F}_k\hat{]}_{\rho v_i} = \hat{\rho}\hat{v}_k\hat{v}_i + \hat{p} \frac{p_{ref}}{v_{ref}^2 \rho_{ref}} \delta_{ki} + \hat{\mu} \frac{\mu_{ref}}{v_{ref} \rho_{ref} L_{ref}} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right) \quad (1.2.11)$$

with $p_{ref} = \rho v_{ref}^2$ and $t_{ref} = L_{ref}/v_{ref}$ we arrive on:

$$\frac{\partial \left(\hat{\rho}\hat{v}_i\right)}{\partial \hat{t}} \frac{v_{ref}^2 \rho_{ref}}{L_{ref}} + \frac{v_{ref}^2 \rho_{ref}}{L_{ref}} \hat{\nabla} \cdot \left(\mathcal{F}_1\hat{]}_{\rho v_i}, \ldots, \mathcal{F}_d\hat{]}_{\rho v_i} \right) = 0 \quad (1.2.12)$$

$$\mathcal{F}_k\hat{]}_{\rho v_i} = \left(\hat{\rho}\hat{v}_k\hat{v}_i + \hat{p}\delta_{ki} + \hat{\mu} \frac{1}{Re_{ref}} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right) \right), \quad (1.2.13)$$

where $Re_{ref} = \frac{\rho_{ref} v_{ref} L_{ref}}{\mu_{ref}}$, and then

$$\frac{\partial \left(\hat{\rho}\hat{v}_i\right)}{\partial \hat{t}} + \hat{\nabla} \cdot \left(\mathcal{F}_1 \hat{\rceil}_{\rho v_i}, \ldots, \mathcal{F}_d \hat{\rceil}_{\rho v_i} \right) = 0 \tag{1.2.14}$$

$$\mathcal{F}_k \hat{\rceil}_{\rho v_i} = \hat{\rho}\hat{v}_k \hat{v}_i + \hat{p}\delta_{ki} + \frac{\hat{\mu}}{Re_{ref}} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right). \tag{1.2.15}$$

This requires that $v_{ref} = \sqrt{p_{ref} / \rho_{ref}}$ and we select a reference viscosity, μ_{ref}.

1.2.2 Species Conservation

The reference concentration can be found via

$$\hat{p} p_{ref} = \hat{R} R^0_{ref} \hat{T} T_{ref} \sum_{i=1}^{n_s} \hat{C}_i C_{ref}, \tag{1.2.16}$$

gives the nondimensional equation of state,

$$\hat{p} = \hat{R}\hat{T} \sum_{i=1}^{n_s} \hat{C}_i, \tag{1.2.17}$$

if

$$p_{ref} = R^0_{ref} T_{ref} C_{ref}, \tag{1.2.18}$$

We choose R^0_{ref} to be $8314 J/kmol/K$ and thus

$$C_{ref} = \frac{p_{ref}}{R^0_{ref} T_{ref}}. \tag{1.2.19}$$

We present the species conservation equation nondimensionalization prior to the energy equation as the latter relies on some realizations made from this section. The species conservation equation is,

$$\frac{\partial \left(C_i\right)}{\partial t} + \nabla \cdot \left(\mathcal{F}_1|_{C_i}, \ldots, \mathcal{F}_d|_{C_i} \right) - \omega_i = 0 \tag{1.2.20}$$

where

$$\mathcal{F}_k|_{C_i} = C_i v_k - C_i \left(\frac{\bar{D}_i}{C_i} \frac{\partial C_i}{\partial x_k} + \frac{\bar{D}_i}{\rho} \frac{\partial \rho}{\partial x_k} + \frac{\sum_{i=1}^{n_s} W_i C_i \hat{V_{ik}}}{\rho} \right). \tag{1.2.21}$$

Using the same approach as the previous section, we can arrive at the nondimensional species conservation equation,

$$\frac{\partial \left(\hat{C}_i\right)}{\partial \hat{t}} \frac{v_{ref} C_{\text{ref}}}{L_{ref}} + \frac{\hat{1}}{L_{ref}} \nabla \cdot \left(\mathcal{F}_1|_{C_i}, \ldots, \mathcal{F}_d|_{C_i} \right) - \hat{\omega}_i \frac{C_{ref}}{t_{ref}} = 0 \tag{1.2.22}$$

with

$$\mathcal{F}_k|_{C_i} = \hat{C}_i \hat{v}_k C_{ref} v_{ref} - \hat{C}_i C_{ref} \left(\frac{D_{ref}}{L_{ref}} \frac{\hat{\bar{D}}_i}{\hat{C}_i} \frac{\partial \hat{C}_i}{\partial \hat{x}_k} + \frac{D_{ref}}{L_{ref}} \frac{\hat{\bar{D}}_i}{\hat{\rho}} \frac{\partial \hat{\rho}}{\partial \hat{x}_k} + V_{ref} \frac{C_{ref} W_{ref} \sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V}_{ik}^{\dagger}}{\rho_{ref} \hat{\rho}} \right). \tag{1.2.23}$$

We set $\rho_{ref} = C_{ref} W_{ref}$ and $V_{ref} = D_{ref}/L_{ref}$

$$\frac{\partial \left(\hat{C}_i\right)}{\partial \hat{t}} + \frac{1}{v_{ref} C_{\text{ref}}} \hat{\nabla} \cdot \left(\mathcal{F}_1|_{C_i}, \ldots, \mathcal{F}_d|_{C_i} \right) - \hat{\omega}_i = 0 \tag{1.2.24}$$

$$\frac{1}{v_{ref} C_{\text{ref}}} \mathcal{F}_k|_{C_i} = \hat{C}_i \hat{v}_k - \hat{C}_i \frac{D_{ref}}{v_{ref} L_{ref}} \left(\frac{\hat{\bar{D}}_i}{\hat{C}_i} \frac{\partial \hat{C}_i}{\partial \hat{x}_k} + \frac{\hat{\bar{D}}_i}{\hat{\rho}} \frac{\partial \hat{\rho}}{\partial \hat{x}_k} + \frac{\sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V}_{ik}^{\dagger}}{\hat{\rho}} \right) \tag{1.2.25}$$

$$\frac{1}{v_{ref} C_{\text{ref}}} \mathcal{F}_k|_{C_i} = \hat{C}_i \hat{v}_k - \hat{C}_i \frac{1}{Sc} \frac{1}{Re} \left(\frac{\hat{\bar{D}}_i}{\hat{C}_i} \frac{\partial \hat{C}_i}{\partial \hat{x}_k} + \frac{\hat{\bar{D}}_i}{\hat{\rho}} \frac{\partial \hat{\rho}}{\partial \hat{x}_k} + \frac{\sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V}_{ik}^{\dagger}}{\hat{\rho}} \right) \tag{1.2.26}$$

$$\widehat{\mathcal{F}_k|}_{C_i} = \hat{C}_i \hat{v}_k - \hat{C}_i \frac{1}{Sc} \frac{1}{Re} \left(\frac{\hat{\bar{D}}_i}{\hat{C}_i} \frac{\partial \hat{C}_i}{\partial \hat{x}_k} + \frac{\hat{\bar{D}}_i}{\hat{\rho}} \frac{\partial \hat{\rho}}{\partial \hat{x}_k} + \frac{\sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V}_{ik}^{\dagger}}{\hat{\rho}} \right) \tag{1.2.27}$$

$$\frac{\partial \left(\hat{C}_i\right)}{\partial \hat{t}} + \hat{\nabla} \cdot \left(\widehat{\mathcal{F}_1|}_{C_i}, \ldots, \widehat{\mathcal{F}_d|}_{C_i} \right) - \hat{\omega}_i = 0 \tag{1.2.28}$$

1.2.3 Energy Equation

$$\frac{\partial\left(\rho e_t\right)}{\partial t}+\nabla\cdot\left(\mathcal{F}_1|_{\rho e_t},\ldots,\mathcal{F}_d|_{\rho e_t}\right)=0 \tag{1.2.29}$$

$$\mathcal{F}_k|_{\rho e_t}=v_k\left(\rho e_t+p\right)+\sum_{j=1}^{d}\tau_{kj}v_j-W_iC_ih_iV_{ik}+\lambda\frac{\partial T}{\partial x_k} \tag{1.2.30}$$

with $e_{t,ref}=v_{ref}^2$

$$\frac{\partial\left(\hat{\rho}\hat{e}_t\right)}{\partial\hat{t}}+\frac{1}{\rho v_{ref}^3}\hat{\nabla}\cdot\left(\mathcal{F}_1|_{\rho e_t},\ldots,\mathcal{F}_d|_{\rho e_t}\right)=0 \tag{1.2.31}$$

$$\begin{aligned}\mathcal{F}_k|_{\rho e_t}=\;&\rho v_{ref}^3\hat{v}_k\left(\hat{\rho}\hat{e}_t+\hat{p}\right)+\frac{\mu_{ref}v_{ref}^2}{L_{ref}}\sum_{j=1}^{d}\hat{\mu}\left(\frac{\partial\hat{v}_i}{\partial\hat{x}_k}+\frac{\partial\hat{v}_k}{\partial\hat{x}_i}-\delta_{ki}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial\hat{v_j}}{\partial\hat{x_j}}\right)\hat{v}_j\\&-\rho_{ref}h_{ref}\frac{D_{ref}}{L_{ref}}\hat{W}_i\hat{C}_i\hat{h}_i\hat{V}_{ik}+\lambda_{ref}\frac{T_{ref}}{L_{ref}}\hat{\lambda}\frac{\partial\hat{T}}{\partial\hat{x}_k}\end{aligned} \tag{1.2.32}$$

We set $e_{t,ref}=h_{ref}=c_{p,ref}T_{ref}=v_{ref}^2$ which gives $T_{ref}=v_{ref}^2/c_{p,ref}$. Then the following can be done

$$\begin{aligned}\mathcal{F}_k|_{\rho e_t}=\;&\rho_{ref}v_{ref}^3\hat{v}_k\left(\hat{\rho}\hat{e}_t+\hat{p}\right)+\frac{\mu_{ref}v_{ref}^2}{L_{ref}}\sum_{j=1}^{d}\hat{\mu}\left(\frac{\partial\hat{v}_i}{\partial\hat{x}_k}+\frac{\partial\hat{v}_k}{\partial\hat{x}_i}-\delta_{ki}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial\hat{v_j}}{\partial\hat{x_j}}\right)\hat{v}_j\\&-\rho_{ref}h_{ref}\frac{D_{ref}}{L_{ref}}\hat{W}_i\hat{C}_i\hat{h}_i\hat{V}_{ik}+\frac{\lambda_{ref}v_{ref}^2}{c_{p,ref}L_{ref}}\hat{\lambda}\frac{\partial\hat{T}}{\partial\hat{x}_k}\end{aligned} \tag{1.2.33}$$

$$\begin{aligned}\mathcal{F}_k|_{\rho e_t}=\;&\rho_{ref}v_{ref}^3\left(\hat{v}_k\left(\hat{\rho}\hat{e}_t+\hat{p}\right)+\frac{\mu_{ref}}{\rho_{ref}v_{ref}L_{ref}}\sum_{j=1}^{d}\hat{\mu}\left(\frac{\partial\hat{v}_i}{\partial\hat{x}_k}+\frac{\partial\hat{v}_k}{\partial\hat{x}_i}-\delta_{ki}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial\hat{v_j}}{\partial\hat{x_j}}\right)\hat{v}_j\right.\\&\left.-\frac{D_{ref}}{v_{ref}L_{ref}}\hat{W}_i\hat{C}_i\hat{h}_i\hat{V}_{ik}+\frac{\lambda_{ref}}{v_{ref}c_{p,ref}L_{ref}}\hat{\lambda}\frac{\partial\hat{T}}{\partial\hat{x}_k}\right)\end{aligned} \tag{1.2.34}$$

$$\mathcal{F}_k|_{\rho e_t} = \rho_{ref} v_{ref}^3 \left(\hat{v}_k \left(\hat{\rho}\hat{e}_t + \hat{p}\right) + \frac{\mu_{ref}}{\rho_{ref} v_{ref} L_{ref}} \sum_{j=1}^{d} \hat{\mu} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right) \hat{v}_j - \frac{D_{ref}}{v_{ref} L_{ref}} \hat{W}_i \hat{C}_i \hat{h}_i \hat{V}_{ik} + \frac{\lambda_{ref}}{v_{ref} c_{p,ref} L_{ref}} \hat{\lambda} \frac{\partial \hat{T}}{\partial \hat{x}_k} \right) \tag{1.2.35}$$

Using $Pr_{ref} = \frac{\mu_{ref} c_{p,ref}}{\lambda_{ref}}$ with $\frac{1}{Re_{ref}} \frac{1}{Pr_{ref}} = \frac{\lambda_{ref}}{v_{ref} c_{p,ref} L_{ref}}$ then we arrive at the nondimensional energy equation

$$\mathcal{F}_k|_{\rho e_t} = \rho_{ref} v_{ref}^3 \left(\hat{v}_k \left(\hat{\rho}\hat{e}_t + \hat{p}\right) + \frac{1}{Re_{ref}} \sum_{j=1}^{d} \hat{\mu} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right) \hat{v}_j - \frac{1}{Sc_{ref}} \frac{1}{Re_{ref}} \hat{W}_i \hat{C}_i \hat{h}_i \hat{V}_{ik} + \frac{1}{Re_{ref}} \frac{1}{Pr_{ref}} \hat{\lambda} \frac{\partial \hat{T}}{\partial \hat{x}_k} \right) \tag{1.2.36}$$

$$\hat{\mathcal{F}}_k\Big|_{\rho e_t} = \left(\hat{v}_k \left(\hat{\rho}\hat{e}_t + \hat{p}\right) + \frac{1}{Re_{ref}} \sum_{j=1}^{d} \hat{\mu} \left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki} \frac{2}{3} \sum_{j=1}^{d} \frac{\partial \hat{v_j}}{\partial \hat{x_j}} \right) \hat{v}_j - \frac{1}{Sc_{ref}} \frac{1}{Re_{ref}} \hat{W}_i \hat{C}_i \hat{h}_i \hat{V}_{ik} + \frac{1}{Re_{ref}} \frac{1}{Pr_{ref}} \hat{\lambda} \frac{\partial \hat{T}}{\partial \hat{x}_k} \right). \tag{1.2.37}$$

$$\frac{\partial \left(\hat{\rho}\hat{e}_t\right)}{\partial \hat{t}} + \hat{\nabla} \cdot \left(\hat{\mathcal{F}}_1\Big|_{\rho e_t}, \ldots, \hat{\mathcal{F}}_d\Big|_{\rho e_t} \right) = 0 \tag{1.2.38}$$

1.2.4 The Reference Flux and Collection of Nondimensional Fluxes

From the previous sections we have deduced that the reference flux is:

$$\mathcal{F}_{ref}^{-1} = \left(\underbrace{\left(\frac{\rho_{ref} v_{ref}^2}{L_{ref}}\right)^{-1}, \ldots, \left(\frac{\rho_{ref} v_{ref}^2}{L_{ref}}\right)^{-1}}_{\text{repeats } m\text{-dimensional times}}, \left(\frac{\rho_{ref} v_{ref}^3}{L_{ref}}\right)^{-1}, \underbrace{\left(\frac{v_{ref} C_{\text{ref}}}{L_{ref}}\right)^{-1}, \ldots, \left(\frac{v_{ref} C_{\text{ref}}}{L_{ref}}\right)^{-1}}_{\text{repeats } n_s \text{ times}} \right) \tag{1.2.39}$$

$$
\begin{aligned}
\hat{\mathcal{F}_k}\Big|_{\rho v_i} &= \hat{\rho}\hat{v}_k\hat{v}_i + \hat{p}\delta_{ki} + \frac{\hat{\mu}}{Re_f}\left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial \hat{v_j}}{\partial \hat{x_j}}\right) \\
\hat{\mathcal{F}}_k\Big|_{\rho e_t} &= \hat{v}_k\left(\hat{\rho}\hat{e}_t + \hat{p}\right) + \frac{1}{Re_{ref}}\sum_{j=1}^{d}\hat{\mu}\left(\frac{\partial \hat{v}_i}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_i} - \delta_{ki}\frac{2}{3}\sum_{j=1}^{d}\frac{\partial \hat{v_j}}{\partial \hat{x_j}}\right)\hat{v}_j \\
&\quad - \frac{1}{Sc_{ref}}\frac{1}{Re_{ref}}\hat{W}_i\hat{C}_i\hat{h}_i\hat{V}_{ik} + \frac{1}{Re_{ref}}\frac{1}{Pr_{ref}}\hat{\lambda}\frac{\partial \hat{T}}{\partial \hat{x}_k} \\
\hat{\mathcal{F}_k}\Big|_{C_i} &= \hat{C}_i\hat{v}_k - \hat{C}_i\frac{1}{Sc}\frac{1}{Re}\left(\frac{\hat{\mathcal{D}}_i}{\hat{C}_i}\frac{\partial \hat{C}_i}{\partial \hat{x}_k} + \frac{\hat{\mathcal{D}}_i}{\hat{\rho}}\frac{\partial \hat{\rho}}{\partial \hat{x}_k} + \frac{\sum_{i=1}^{n_s}\hat{W}_i\hat{C}_i\hat{V}_{ik}^{\dagger}}{\hat{\rho}}\right)
\end{aligned}
\tag{1.2.40}
$$

1.2.5 Other Relationships

Here we derive the nondimensional relationships used for equations outside the conservation equations as well as present further considerations for nondimensionalization.

Transport and Thermodynamic Quantities

Species dependent quantities, such as the species diffusion coefficient, we describe in a thermally perfect gas as functions of temperature. Quantities such as diffusion coefficients have $n_s \times n_s$ functions of temperature, $D_{ij} = f_{ij}(T)$, whereas quantities such as species viscosity have n_s functions of temperature, $\mu_i = f_i(T)$. Regardless, the functions of temperature are assumed to be smooth functions that can be represented by a n_p-order polynomial, $\psi = \sum_{k=0}^{n_p} a_k T^k$. Currently we re-fit the polynomial so we utilize a change of coordinates of $T \to \hat{T}$ to determine approximate $\hat{a}_k$ but the coefficients, $\hat{a}_k$ can also be adapted directly from known polynomials via

$$
\hat{\psi} = \sum_{k=0}^{n_p} \hat{a}_k \hat{T}^k \text{ where } \hat{a}_k = \frac{a_k T_{ref}^k}{\psi_{ref}}. \tag{1.2.41}
$$

For mixture averaged quantities, $\hat{\mu}$, $\hat{\lambda}$, and $\hat{\hat{\mathcal{D}}}_i$, no extra steps need to be taken other than replacing the dimensional quantities with the nondimensional as can be seen via inspection that they are contracted with X_i, which are dimensionless quantities. It is also beneficial that the dimensionless variables, Re, Pr, and Sc, can be incorporated into the mixture averaged evaluations

$$
\underline{\hat{\lambda}} = \frac{1}{Re_{ref}}\frac{1}{Pr_{ref}}\hat{\lambda} = \frac{1}{Re_{ref}}\frac{\lambda_{ref}}{\mu_{ref}\, c_{p,ref}}\frac{\lambda}{\lambda_{ref}} = \frac{1}{Re_{ref}}\frac{1}{\mu_{ref}\, v_{ref}^2}\lambda \tag{1.2.42}
$$

thus replacing the $\frac{1}{Re_{ref}}\frac{1}{Pr_{ref}}\hat{\lambda}\frac{\partial \hat{T}}{\partial \hat{x}_k}$ term in Equation (1.2.37) with $\underline{\hat{\lambda}}\frac{\partial \hat{T}}{\partial \hat{x}_k}$. The same can be done for the viscous and diffusion velocity terms in Equations (1.2.26) and (1.2.15).

Species Diffusion Velocity

Equation (1.1.15) in nondimensional form is

$$V_{ik}^{\dagger} = \frac{D_{ref}}{L_{ref}} \left(\frac{\hat{D}_i}{\hat{C}_i} \frac{\partial \hat{C}_i}{\partial \hat{x}_k} - \frac{\hat{D}_i}{\hat{\rho}} \frac{\partial \hat{\rho}}{\partial \hat{x}_k} \right) \rightarrow V_{ik}^{\dagger} = V_{ref} \hat{V_{ik}^{\dagger}} = \frac{D_{ref}}{L_{ref}} \hat{V_{ik}^{\dagger}} \tag{1.2.43}$$

To ensure mass conservation we still apply $\sum_{i=1}^{n_s} W_i C_i V_{ik} = \rho_{ref} V_{ref} \sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V_{ik}} = 0 \rightarrow \sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V_{ik}} = 0$ which gives the same correction in nondimensional form

$$\hat{V_{ik}} = \hat{V_{ik}^{\dagger}} - \frac{\sum_{i=1}^{n_s} \hat{W}_i \hat{C}_i \hat{V_{ik}^{\dagger}}}{\hat{\rho}}. \tag{1.2.44}$$

Reaction Rate Evaluation

The evaluation of reaction rates can be cumbersome when transitioning between units. The source term is

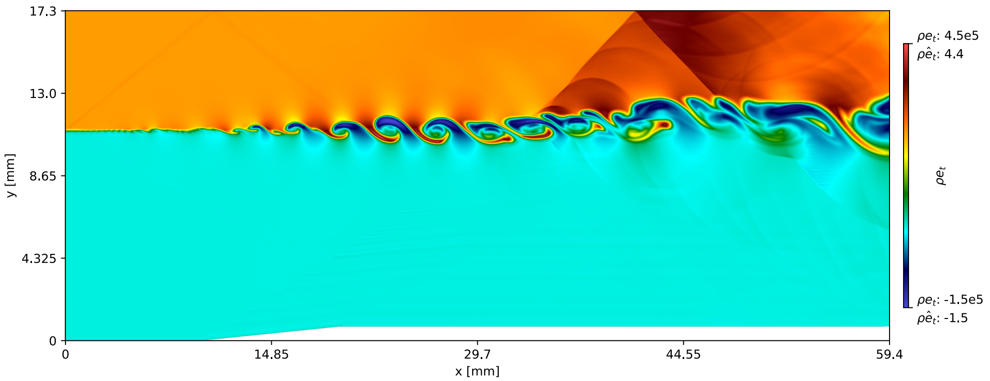
$$\mathcal{S}(y) = \left(0, \ldots, 0, 0, \omega_1, \ldots, \omega_{n_s}\right), \tag{1.2.45}$$

where ω_i is the production rate of the ith species. Instead of nondimensionalizing all terms necessary to calculate the reaction rates, we dimensionalize species and temperature for the evaluation of ω_i and nondimensionlize when applying to the conservation equations,

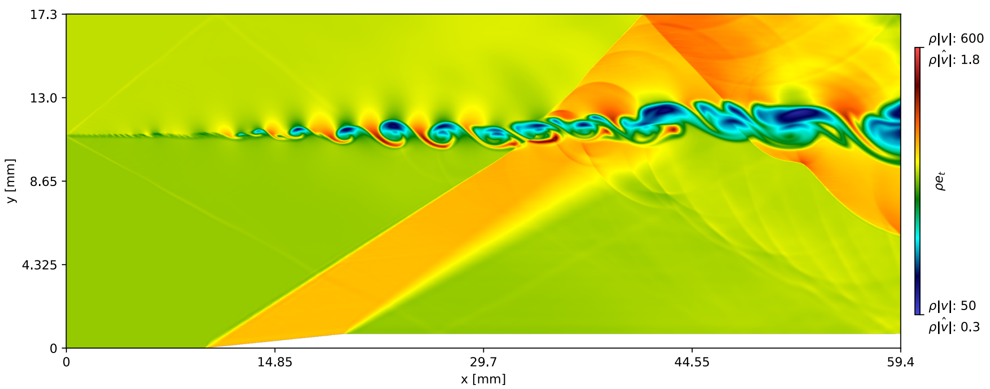
$$\hat{\omega}_i = \frac{\omega_i\left(C_i, T\right)}{\omega_{ref}} = \frac{\omega_i\left(C_i, T\right) L_{ref}}{C_{ref} v_{ref}}. \tag{1.2.46}$$

1.3 Demonstration Case

Using the following parameters $\rho_{ref} = 1\ kg/m^3$, $T_{ref} = 1000\ K$, $p_{ref} = 101325\ Pa$, $L_{ref} = 1\ m$, and $\rho_{ref} = 1\ \frac{kg}{m^3}$ gives $v_{ref} = 318.315\ \frac{m}{s}$ and $e_{ref} = 101325\ Pa$. We demonstrate here with an instantaneous solution from a hydrogen-air chemically reacting shear layer case developed by [10] simulated using the JENRE® Multiphysics Framework [1, 11]. The detailed reaction mechanism from Westbrook [12] was used to calculate the developed solution presented here, which includes minor species, H_2O_2 that are critical fo the solution and exist in small concentrations on the order of $1e-7\ kmol/m^3$. Figures 1.3.1-1.3.2 display the instantaneous results for the demonstration case for the conserved variables: total energy, ρe_t, momentum magnitude $\rho|v|$, H_2O_2 concentrations, and H_2O concentrations. The ratio in scales found here for maximum values of the conservation variables changed from max $\left(\rho e_t / C_{H_2O_2}\right) \approx 1e12$ to max $\left(\hat{\rho e_t} / \hat{C_{H_2O_2}}\right) \approx 1e5$.

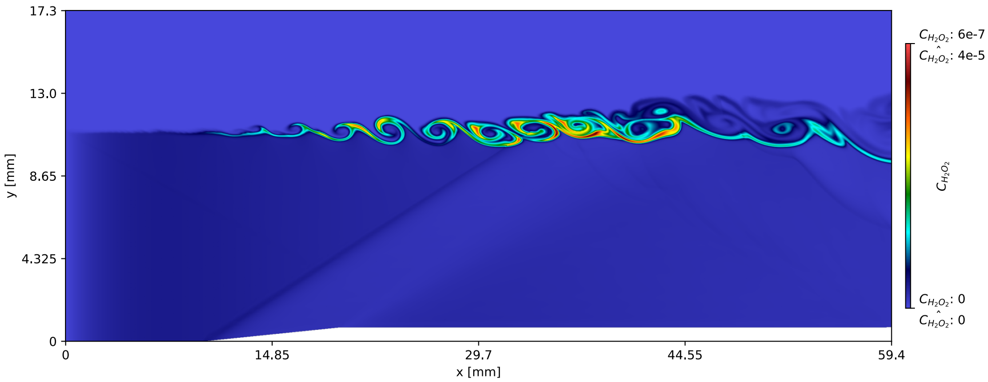


(a) Stagnation energy, ρe_t, the dimensional values are in the range $(-1.5e5, 4.5e5)$ J/m^3 whereas the nondimensional range is $(-1.5, 4.4)$.

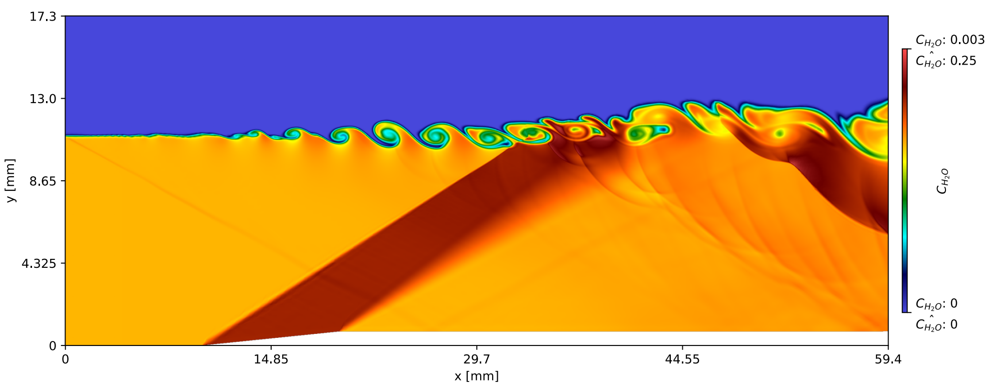


(b) Momentum magnitude, $\rho|v|$, the dimensional values are in the range $(50, 600)$ $kg/\left(s \cdot m^2\right)$ whereas the nondimensional range is $(0.27, 1.75)$.

Fig. 1.3.1— Results for a chemically reacting hydrogen-air shear layer solution demonstrating the variety of scales found in the conservation variables for chemically reacting flow simulations. The ratio in scales found here for maximum values of the conservation variables changed from max $\left(\rho e_t / C_{H_2O_2}\right) \approx 1e12$ to max $\left(\rho \hat{e}_t / \hat{C_{H_2O_2}}\right) \approx 1e5$.



(a) $C_{H_2O_2}$ the dimensional values are in the range $(0, 6e-7)$ $kmole/\left(m^3\right)$ whereas the nondimensional range is $(0, 4e-5)$.



(b) C_{H_2O} the dimensional values are in the range $(0, 0.003)$ $kmole/\left(m^3\right)$ whereas the nondimensional range is $(0, 0.25)$.

Fig. 1.3.2— Results for a chemically reacting hydrogen-air shear layer solution demonstrating the variety of scales found in the conservation variables for chemically reacting flow simulations. The ratio in scales found here for maximum values of the conservation variables changed from max $\left(\rho e_t / C_{H_2O_2}\right) \approx 1e12$ to max $\left(\hat{\rho e_t} / \hat{C_{H_2O_2}}\right) \approx 1e5$.

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