

# Chapter 1

## Table Generation

### 1.1 B-Splines

#### 1.1.1 L-U Factorization

### 1.2 HDF5 Databases

### 1.3 Software API

#### 1.3.1 Table Generation

#### 1.3.2 B-Splines

##### 1-D Splines

##### 2-D Splines

##### Higher-Dimensional Splines



## Chapter 2

# Reaction Models

Given a single-phase reacting system with  $N_s$  species, one must specify  $N_s + 1$  variables (*e.g.*,  $N_s - 1$  mass fractions, temperature and pressure) to uniquely specify the entire thermochemical state,  $\phi$ , of the system [1, 2, 3]. Reaction models parameterize  $\phi$  by  $N_\eta \ll N_s + 1$  parameters called *reaction variables*, which we represent collectively as  $\eta$ . A reaction model then provides a unique mapping from  $\eta$  to  $\phi$ , *i.e.*, each  $\phi_i$  is represented by an  $N_\eta$ -dimensional surface in  $\eta$ -space.

We define a reaction model as a mapping between thermochemical state variables and reaction variables,

$$\phi = \phi(\eta). \quad (2.1)$$

### 2.1 The Mixture Fraction

As many of the results will use the mixture fraction as a reaction variable, it is briefly defined here. Elemental mass fractions,  $Z_\ell$ , may be defined in terms of the species mass fractions,  $Y_i$ , as

$$Z_\ell = \sum_{i=1}^{N_s} \frac{a_{\ell,i} W_\ell}{W_i} Y_i, \quad (2.2)$$

where  $N_s$  is the number of species,  $a_{\ell,i}$  is the number of atoms of element  $\ell$  in species  $i$ ,  $W_\ell$  is the molecular weight of element  $\ell$ , and  $W_i$  is the molecular weight of species  $i$ . The mixture fraction,  $f$ , may be written in terms of coupling functions,  $\beta$ , as [1]

$$f = \frac{\beta - \beta_0}{\beta_1 - \beta_0}, \quad (2.3)$$

where  $\beta_1$  and  $\beta_0$  are constants evaluated in the fuel and oxidizer streams, respectively. The coupling function,  $\beta$ , is defined in terms of the elemental mass

fractions as

$$\beta = \sum_{\ell=1}^{N_e} \gamma_{\ell} Z_{\ell} = \sum_{\ell=1}^{N_e} \gamma_{\ell} \sum_{i=1}^{N_s} \frac{a_{\ell,i} W_{\ell} Y_i}{W_i}, \quad (2.4)$$

where  $\gamma_{\ell}$  are weighting factors. The  $\gamma_{\ell}$  are not unique; for this study Bilger's definition [4] of the mixture fraction is adopted, for which  $\gamma_C = 2/W_C$ ,  $\gamma_H = 1/(2W_H)$ ,  $\gamma_O = 1/W_O$ ,  $\gamma_N = 0$ . The stoichiometric mixture fraction,  $f_{st}$ , is determined from equation (2.3) with  $\beta = 0$ . The dissipation rate is defined as  $\chi = 2D\nabla f \cdot \nabla f$ , with  $D$  obtained from  $Le = \lambda/(\rho c_p D)$ . In this study, the Lewis number of the mixture fraction was assumed to be unity.

## 2.2 Effects of Heat Loss

Heat loss is an important aspect of combustion modeling, and may occur through radiation or conduction/convection. We define the fractional heat loss,  $\gamma$  as

$$\gamma = \frac{h_a - h}{h_a - h_c} = \frac{h_a - h}{h_{a,s}} \quad (2.5)$$

$$h_{a,s} \equiv \sum_{i=1}^{N_s} Y_i h_{a,i} - h_i^o$$

with

$$c_p = \sum_{i=1}^{N_s} Y_i c_{p,i}, \quad (2.6)$$

$$h = \sum_{i=1}^{N_s} Y_i h_i, \quad (2.7)$$

$$h_i = h_i^o + \int_{T_o}^T c_{p,i} dT, \quad (2.8)$$

where  $h_i$  is the enthalpy of species  $i$ ,  $h_i^o$  is the enthalpy of formation of species  $i$  at temperature  $T_o$ , and  $c_p$  is the isobaric heat capacity.

## 2.3 Burke-Schuman Model

Burke-Schuman chemistry assumes infinitely fast, irreversible, and complete reaction. Thus, composition is a piece-wise linear function of mixture fraction. The enthalpy is determined from the composition and equation (2.7). For the adiabatic case, all state variables are unique functions of the mixture fraction,  $\phi = \phi(f)$ .

### 2.3.1 Heat Loss

## 2.4 Equilibrium Model

The chemical equilibrium model is valid when chemistry is infinitely fast and reversible. For an adiabatic two-stream mixing problem, the thermochemical state is uniquely parameterized by the mixture fraction,  $\phi = \phi(f)$ .

### 2.4.1 Heat Loss



## Chapter 3

# Mixing Models

In a Reynolds-Averaged Navier-Stokes (RANS) or Large-Eddy Simulation (LES) calculation, mean or filtered state variables are needed as functions of the mean (or filtered) reaction variables. This is typically achieved through

$$\bar{\phi}_i = \int_{\eta_{N_\eta}} \cdots \int_{\eta_1} \phi_i^*(\boldsymbol{\eta}) P(\eta_1 \cdots \eta_{N_\eta}) d\eta_1 \cdots d\eta_{N_\eta}, \quad (3.1)$$

where  $\phi_i^*(\boldsymbol{\eta})$  is the reaction model, which provides state variables,  $\phi$ , as unique functions of the set of reaction variables,  $\boldsymbol{\eta}$ , and  $P(\eta_1 \cdots \eta_{N_\eta})$  is the joint probability density function (PDF) of all reaction variables. Clearly, in a RANS or LES computation, the error in  $\bar{\phi}$  has contributions from the reaction model as well as the model used to approximate the joint PDF. This study examines only the error due to the reaction model,  $\phi_i(\boldsymbol{\eta})$ .





## Chapter 4

# User-Interface

### 4.1 The Parser

### 4.2 Line Commands



# Bibliography

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