The background of the slide features a wide-angle photograph of a sunset or sunrise over a calm lake or river. The sky is filled with dramatic, dark clouds through which bright, golden-yellow rays of light break through, creating a reflection on the water's surface. In the distance, a dark silhouette of a forest line is visible across the horizon.

Subgrid Models for Nonpremixed Combustion

CRSim Group Meeting
Feb 13, 2010

Challenges for Turbulent Combustion Modeling

📍 Spatial/Temporal Resolution

- In turbulent flow, length scales separate as $Re^{3/4} \Rightarrow Re^{9/4}$ (in 3D)
- Time scales scale with spatial scale ($Re^{3/4} \Rightarrow Re^3$)
- Chemical reaction (and diffusion) may further increase range of length/time scales
 - ▶ 10^{-9} sec ... 10^{-1} sec; 10^{-6} ... 10^{-3} m.
 - ▶ may couple with fluid dynamics length/time scales

📍 Number of equations

- Non-reacting flow / No species
 - ▶ Continuity (1), momentum (3), energy (1) \Rightarrow 5 PDEs.
- Reacting flow
 - ▶ $5 + \text{number of species.}$
 - ▶ Hydrogen/Air ~ 9 species, Methane/Air ~ 50 , Heptane/Air ~ 160 .
 - ▶ Highly nonlinear and stiff equations in general.

Length & Time Scales

(the “resolution” problem)



Direct Numerical Simulation (DNS)

- Solve governing equations directly, resolving all length & time scales
 - ▶ Highly accurate numerical algorithms (e.g. 4th order time, 8th order space).
- Limited to small, “simple” problems
 - ▶ Low Reynolds numbers, simple/trivial geometry.
 - ▶ Currently, $Re \approx 10^3$; “practical engineering” problems: $Re \approx 10^5-10^6$.
 - ▶ $10^6-10^9 \times$ compute power required for “practical” problems.



Large Eddy Simulation (LES)

- Filter “small” scales, and directly resolve “large” scales.
- Typically 2nd order time & space.
- Requires models for unclosed terms that result from filtering.



Reynolds-Averaged (RANS)

- Time-average the governing equations.
- Model all length and time scales.
- Workhorse for CFD modeling.

Computational Cost ↑

Degree of Modeling ↓

Thermochemistry Models

(the “number of species” problem)



Reaction Models

- In general, the thermochemical state for a single-phase system is determined by $\{T, p, y_i\}$
 - ▶ Reduce the number of degrees of freedom by making assumptions to (greatly) simplify the thermochemistry
 - ▶ Simplify chemical mechanisms (CSP, Manifold concepts)
 - ▶ Find parameterizing variables.



Mixing Models

- For LES and RANS, all length and time-scales are not resolved
- Thermochemical nonlinearity requires consideration (modeling) of subgrid heterogeneity
- Mixing models attempt to account for “unmixedness” in thermochemical variables.

A Few Deterministic Reaction Models

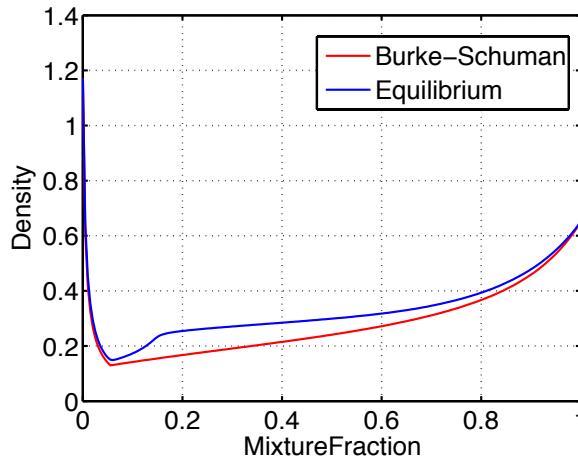
(Nonpremixed Combustion)

- 💡 **Burke-Schumann (flame-sheet) approximation.**
 - given local stoichiometry, assume complete combustion.
 - Linear relationship between mixture fraction & species.
 - Generally two flavors: adiabatic (1 parameter) and with heat loss (2 parameters).
- 💡 **Equilibrium**
 - Nonlinear (but unique) relationship between mixture fraction and species.
 - Two flavors: adiabatic (1 parameter) and with heat loss (2 parameters).
- 💡 **Steady Laminar Flamelet Model**
 - Solves a set of PDEs in mixture fraction space
 - Models effect of mixing rate (strain rate) on the flame
 - Can capture extinction, but not very well.
 - Two parameters: mixture fraction & scalar dissipation rate.

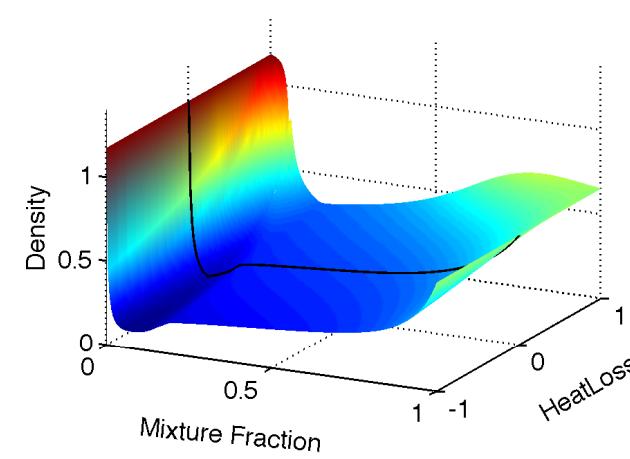
$$0 = \frac{\chi}{2} \frac{\partial^2 y_i}{\partial f^2} + \frac{s_i}{\rho}$$
$$0 = \frac{\chi}{2} \frac{\partial^2 T}{\partial f^2} - \frac{1}{\rho c_p} \sum_{j=1}^n h_j s_i$$

All of these models make assumptions about the interaction of the fluid dynamics and the chemistry.

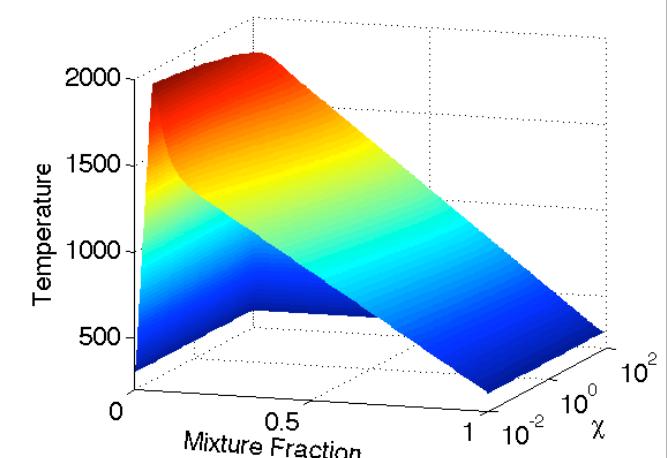
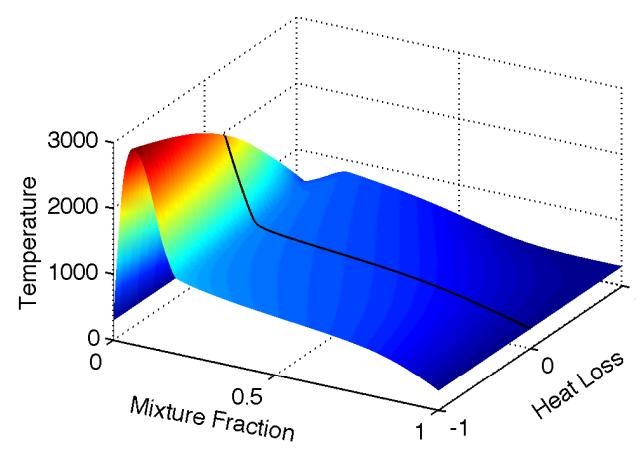
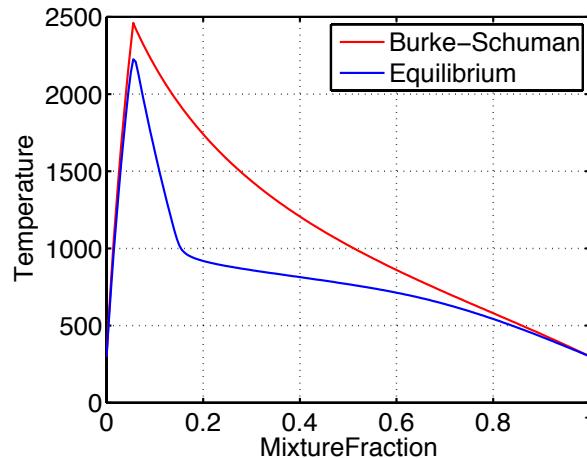
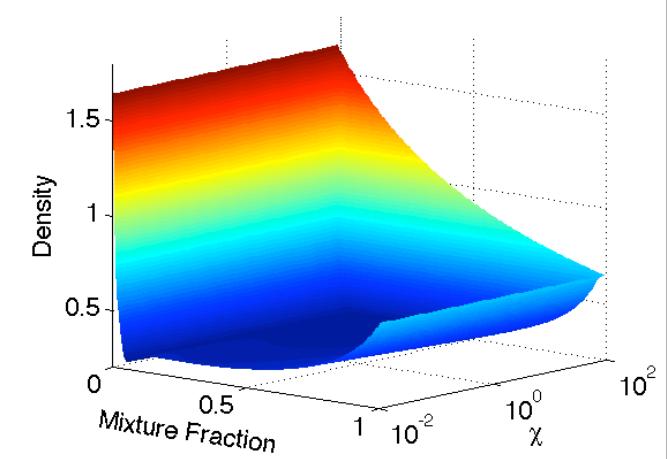
Mixture Fraction (adiabatic)



Mixture Fraction & Heat Loss (Equilibrium)



Mixture Fraction & Scalar Dissipation Rate (SLFM)



Non-Deterministic Reaction Models

Concept:

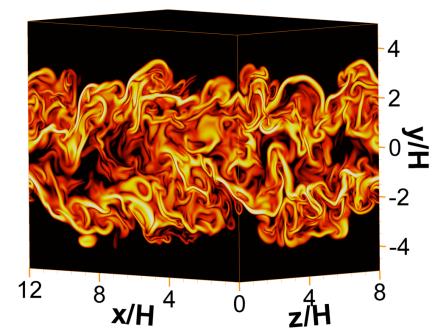
- Run a “high-fidelity” calculation near the conditions where you want to perform a simulation. (DNS or ODT)
 - ▶ use detailed chemistry, thermodynamics, etc.
- Extract data from the simulation & parameterize it by your favorite parameters
 - ▶ mixture fraction, heat loss, scalar dissipation rate, progress variables, etc...
 - ▶ You are limited only by your imagination - you can choose any parameter set...

Advantages:

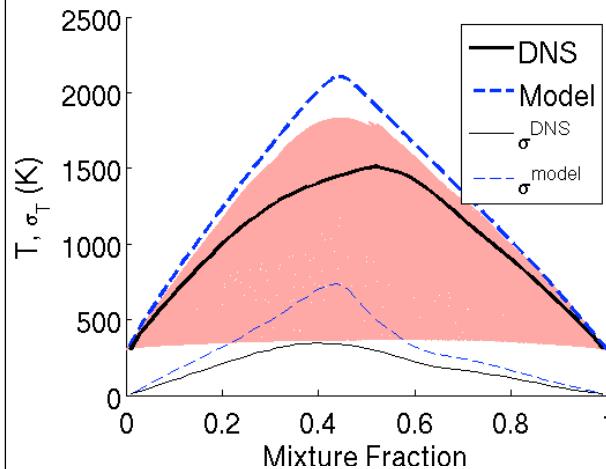
- Doesn’t require a priori assumptions regarding the interaction between mixing & reaction.
- Doesn’t require a priori assumptions regarding the appropriate parameters

Disadvantages:

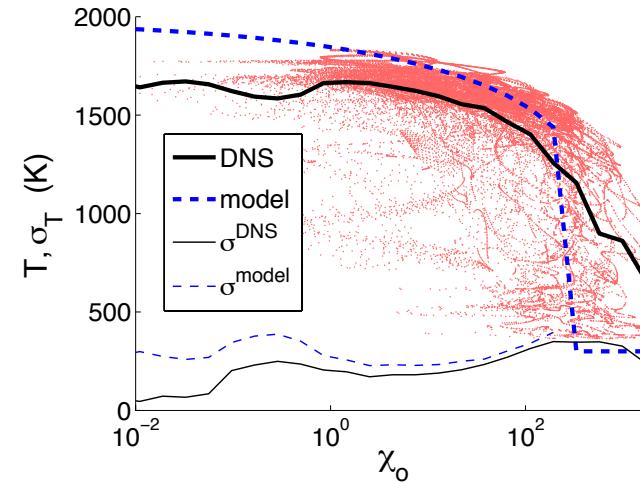
- can be quite costly relative to deterministic models
- how do you choose the best parameters?



DNS Temperature as a function of mixture fraction. Equilibrium model shown for comparison.



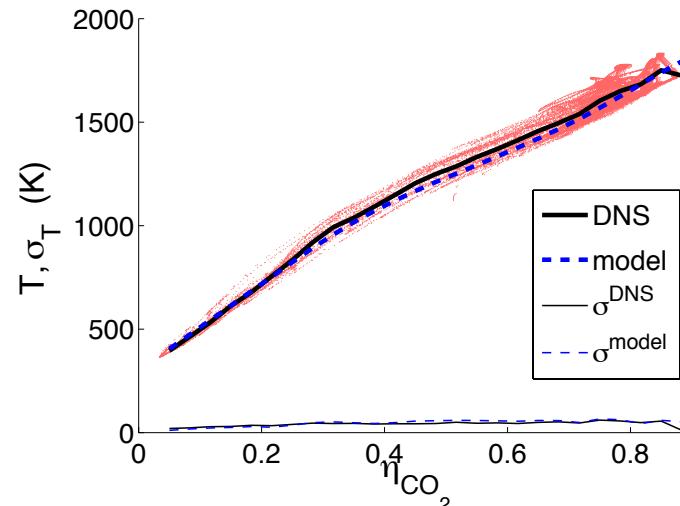
DNS Temperature as a function of χ at stoichiometric. SLFM model shown for comparison.



Tools:

- PCA - can help identify parameterizing variables
- MARS - multivariate adaptive regression splines - generates a functional form for $\phi(\eta)$.

DNS Temperature as a function of a CO₂ progress variable at stoichiometric. Newly proposed model shown for comparison.



Mixing Models

- In LES and RANS, we do not solve for fully resolved quantities.
- We solve for the reaction variables (e.g. mixture fraction) and we need to extract other variables (e.g. temperature) from that.
- Problem: $T = \mathcal{F}(f)$ but $\bar{T} \neq \mathcal{F}(\bar{f})$

$$\bar{\phi} = \int_{\eta_1} \cdots \int_{\eta_n} \phi(\eta_1, \dots, \eta_n) p(\eta_1, \dots, \eta_n) d\eta_1 \cdots d\eta_n$$

A HUGE challenge in combustion modeling!

If $\eta_1 \dots \eta_n$ are statistically independent, then

$$\bar{\phi} = \int_{\eta_1} \cdots \int_{\eta_n} \phi(\eta_1, \dots, \eta_n) p(\eta_1) \dots p(\eta_n) d\eta_1 \cdots d\eta_n$$

Presumed PDF Mixing Models

$$\bar{\phi} = \int_{\eta_1} \cdots \int_{\eta_n} \phi(\eta_1, \dots, \eta_n) p(\eta_1) \dots p(\eta_n) d\eta_1 \cdots d\eta_n$$

β -PDF

$$P(\varphi) = \varphi^{a-1} (1-\varphi)^{b-1} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}$$

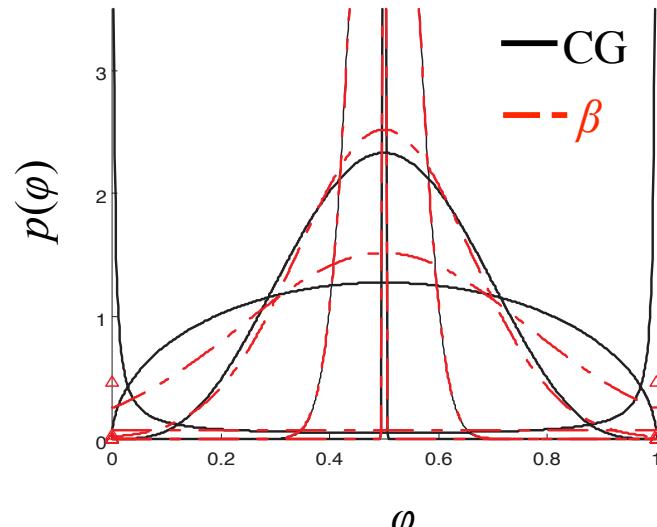
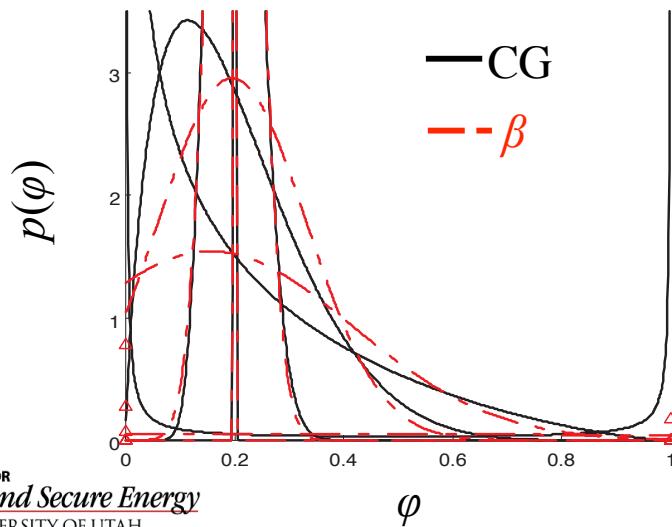
$$a = \bar{\varphi} \left[\frac{\bar{\varphi}(1-\bar{\varphi})}{\sigma_\varphi^2} - 1 \right] = \bar{\varphi} \left[\sigma_{\max}^2 / \sigma_\varphi^2 - 1 \right]$$

$$b = a \frac{(1-\bar{\varphi})}{\bar{\varphi}}$$

Clipped-Gaussian PDF

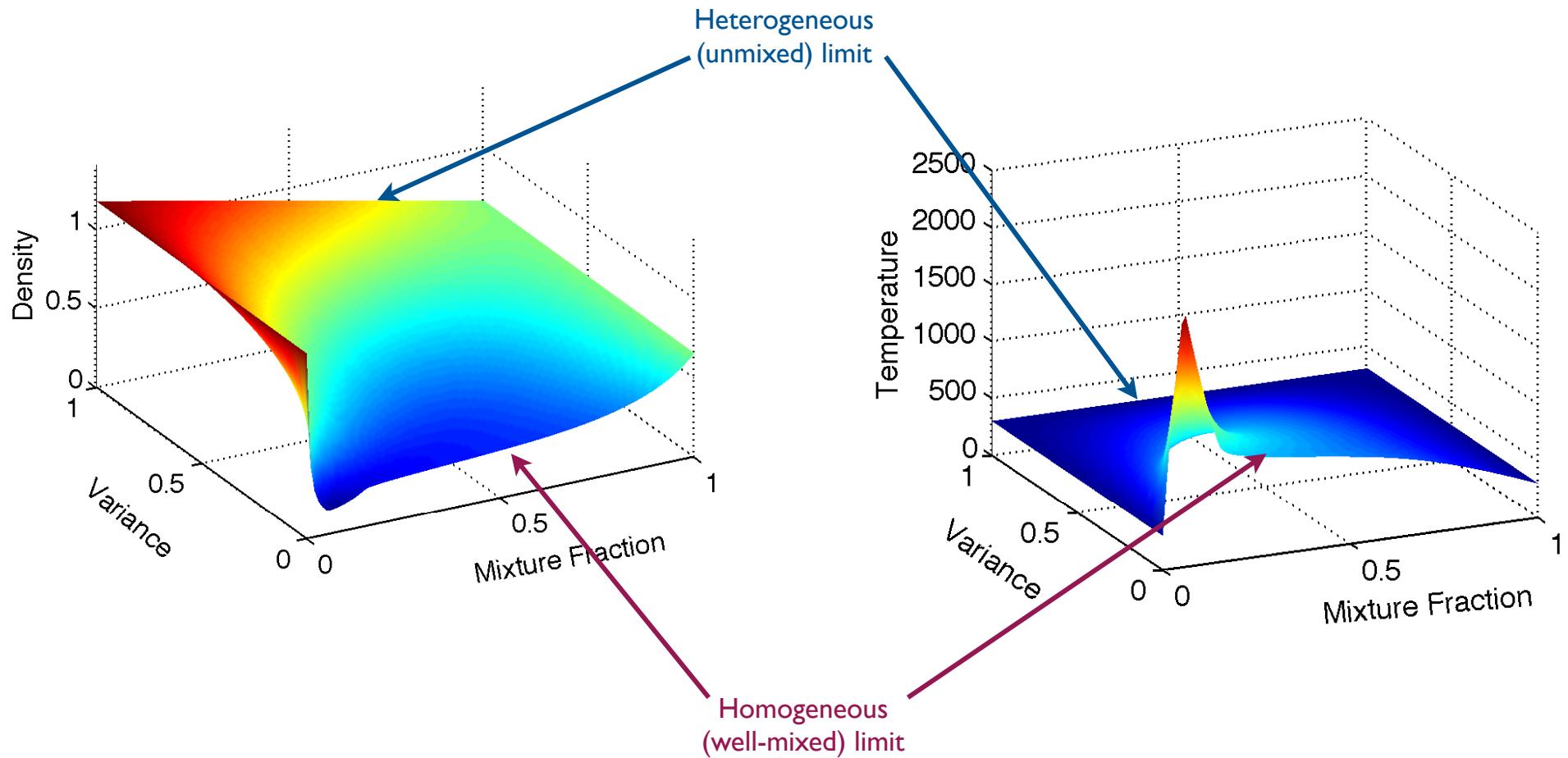
$$P(\varphi) = \begin{cases} \alpha_0 & \varphi = 0 \\ \frac{1}{\sqrt{2\pi G_\Phi}} \exp\left[\frac{-(\varphi-\Phi)^2}{2G_\Phi}\right] & 0 < \varphi < 1 \\ \alpha_1 & \varphi = 1 \end{cases} .$$

α_1 and α_2 are non-trivial functions
of the mean and variance.



Presumed PDF Example

Adiabatic equilibrium model with clipped-gaussian mixing model



TabProps

An Approach to Tabulating Mixing & Reaction Models

Motivation - What we Need

- ✓ A standard format to express $\phi=F(\eta)$ in a generic way.
Different models mean different F .
- ✓ A common way to express all reaction models
- ✓ The ability to calculate an extensible (and arbitrary) set of properties ϕ .
- ✓ A simple means of constructing models with presumed PDF.

TabProps Approach

Uses B-Splines to create interpolants of arbitrary order in up to five independent variables. Write an “importer” to get your favorite model into TabProps

All reaction models must provide T, p, Y_i as functions of an arbitrary set of independent variables.

Cantera is used for most property evaluation. There is a fairly simple mechanism to extend the properties that can be evaluated.

Built-in support for β -PDF and Clipped-Gaussian PDF models with Gauss-Kronrod adaptive integrators.

The β -PDF is inherently difficult to integrate accurately, and TabProps suffers from inaccuracies when using the β -PDF.

Some Features

- ➊ Several “built-in” reaction models
 - Non-reacting stream mixing
 - Burke-Schumann (flame-sheet) chemistry (adiabatic & with heat loss)
 - Equilibrium chemistry (adiabatic & with heat loss)
- ➋ Extensible support for other more complex reaction models
 - Currently only James’ flamelet code...
- ➌ Support for both table creation and table read-up / querying.
 - convenient interface for CFD codes.
- ➍ Table post-processing & visualization
 - dumps out Matlab or TecPlot files for visualization (this is how I made the plots I showed here)
- ➎ Robust file formats - HDF5 format
 - Store spline coefficients, not a tabular dataset. This is more compact.
- ➏ Input-file driven (though a little tricky at first)
 - easy to implement several models at once.
 - workflow automates generation of mixing models from reaction models.

A Sample Input File

```
# Activate some reaction models. Note that you can have multiple entries, but
# you must only have a single "REACTION MODEL" line. Also, a model may be
# turned off by removing it from this list, even if it is in the rest of the input file.
REACTION MODEL = AdiabaticEquilibrium

# specify the name of the input file for cantera, as well as
# the name of the gas mixture from the cantera input file
AdiabaticEquilibrium.CanteraInputFile      = gri30.cti
AdiabaticEquilibrium.CanteraGroupName = gri30

# specify the composition and temperature of the fuel stream
AdiabaticEquilibrium.FuelComposition.MoleFraction.CH4 = 1.0
AdiabaticEquilibrium.FuelTemperature = 300.0

# specify the composition and temperature of the oxidizer stream
AdiabaticEquilibrium.OxidizerComposition.MoleFraction.O2 = 0.21
AdiabaticEquilibrium.OxidizerComposition.MoleFraction.N2 = 0.79
AdiabaticEquilibrium.OxidizerTemperature = 300.0

# specify the variables for output from the reaction model.
# all of these variables will be put through the mixing model.
AdiabaticEquilibrium.SelectForOutput = temperature density viscosity
AdiabaticEquilibrium.SelectSpeciesForOutput = CO CO2 H2O OH
AdiabaticEquilibrium.nfps = 200
```

REACTION MODEL = AdiabaticFastChem AdiabaticEquilibrium Equilibrium

#-- The AdiabaticFastChem model specification

```
AdiabaticFastChem.CanteraInputFile = gri30.cti
AdiabaticFastChem.CanteraGroupName = gri30
AdiabaticFastChem.FuelComposition.MoleFraction.CH4 = 1.0
AdiabaticFastChem.FuelTemperature = 300
AdiabaticFastChem.OxidizerTemperature = 300
AdiabaticFastChem.OxidizerComposition.MoleFraction.O2 = 0.21
AdiabaticFastChem.OxidizerComposition.MoleFraction.N2 = 0.79
AdiabaticFastChem.nfps = 201
AdiabaticFastChem.SelectForOutput = temperature density viscosity
AdiabaticFastChem.SelectSpeciesForOutput = CO CO2 H2O OH
```

#-- The AdiabaticEquilibrium Model Specification

```
AdiabaticEquilibrium.CanteraInputFile = gri30.cti
AdiabaticEquilibrium.CanteraGroupName = gri30
AdiabaticEquilibrium.FuelComposition.MoleFraction.CH4 = 1.0
AdiabaticEquilibrium.FuelTemperature = 300.0
AdiabaticEquilibrium.OxidizerComposition.MoleFraction.O2 = 0.21
AdiabaticEquilibrium.OxidizerComposition.MoleFraction.N2 = 0.79
AdiabaticEquilibrium.OxidizerTemperature = 300.0
AdiabaticEquilibrium.SelectForOutput = temperature density viscosity
AdiabaticEquilibrium.SelectSpeciesForOutput = CO CO2 H2O OH
AdiabaticEquilibrium.nfps = 200
```

#-- The Equilibrium Model Specification

```
Equilibrium.CanteraInputFile = gri30.cti
Equilibrium.CanteraGroupName = gri30
Equilibrium.FuelComposition.MoleFraction.CH4 = 1.0
Equilibrium.FuelTemperature = 300
Equilibrium.OxidizerTemperature = 300
Equilibrium.OxidizerComposition.MoleFraction.O2 = 0.21
Equilibrium.OxidizerComposition.MoleFraction.N2 = 0.79
Equilibrium.nfps = 201
Equilibrium.GridStretchFactor = 4.0
Equilibrium.NHeatLossPts = 50
Equilibrium.SelectForOutput = temperature density viscosity
Equilibrium.SelectSpeciesForOutput = CO CO2 H2O OH
```