Cantera Energy Equation

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1 Introduction

The current energy equation that is implemented in Cantera's 1D solver has the temperature as the dependent variable. The form of the equation also has ideal gas assumptions baked into it. This document will cover a derivation of the energy equation that does not make ideal gas assumptions. The energy equation will also stay in the form of enthalpy instead of temperature. Cantera's 0D reactor energy equation uses a total enthalpy form, so here we seek to also use a form to allow for consistency between the 1D and 0D solvers..

First start with Kee's general energy equation. This is an energy equation for enthalpy(sensible + chemical)

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \nabla \cdot (\lambda \nabla T) - \sum_{k=1}^{K} \nabla \cdot h_k \vec{j}_k + \Phi \tag{1}$$

For the 1D solver, we choose to ignore the viscous heating term(Φ), and assume the pressure to not vary across the domain(low speed). The pressure material derivative term is assumed to be zero. Under these assumptions, the governing enthalpy equation.

$$\rho \frac{Dh}{Dt} = \nabla \cdot (\lambda \nabla T) - \sum_{k=1}^{K} \nabla \cdot h_k \vec{j}_k \tag{2}$$

Expanding the expression for the total enthalpy, and assuming 1-dimensionality.

$$\rho \frac{\partial h}{\partial t} = -\rho u \frac{\partial h}{\partial z} + \frac{\partial}{\partial z}(\lambda \frac{\partial T}{\partial z}) - \sum_{k=1}^{K} \frac{\partial}{\partial z}(h_k j_k) \tag{3}$$

An upwinding discretization scheme is used for the convective terms, and a central differencing scheme is used for the diffusive terms.

Convective Terms: if $u_j > 0$:

$$\left(\frac{dh}{dz}\right)_j = \frac{h_j - h_{j-1}}{z_j - z_{j-1}} \tag{4}$$

else,

$$\left(\frac{dh}{dz}\right)_j = \frac{h_{j+1} - h_j}{z_{j+1} - z_j} \tag{5}$$

The diffusive term in the energy equation is expressed as a function of the temperature. For the new energy equation, the dependent variable is enthalpy, and temperature is computed from enthalpy using an equation of state. I don't know what would be more preferable in the coding: Have a temperature vector computed once reference that or to have a temperature function(called T) that is called when necessary and it inverts the EOS using enthalpy at the point and the pressure + species mass fractions to get the temperature.

The diffusive term(with one-sided stencils for the inner derivative term used that point to wards the point of interest:

$$\frac{\partial}{\partial z}(\lambda \frac{\partial T}{\partial z}) = \tag{6}$$