Undergraduate Research

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Contents

[Rough Introduction, Probably going to have to be rewritten and reworked] [Basically wrote it to get a better understanding of all the things I have done so far] [will probably end up doing the introduction last as it is always usually the hardest part for me to write in papers]

1 Introduction

For the past 15 weeks I have been working under Dr. Paul Baumann doing undergraduate research. During this time I was able to learn many different skills,programs, and mathematically techniques to help solve different Problems. Over the Winter Break for this year, I worked on learning about the Finite Element Method, and Dr. Baumann's GRINS Program, which is a Multi-Physics Finite Element package, as well as learning just how to navigate and use the linux operating system, and what github was. By the end of the winter break I was able to formulate my very own Weak from of a 1-d Isobaric Premixed laminar flame problem. For the past 7 weeks I have been working on getting to know the GRINS Framework and learning Paraview to view and understand what was going on in some of the different GRINS examples. I also started learning Latex to write things like this. Since then I have been working on modifying one of the examples to run and model Methane combustion. Alot has gone in along with this, like learning about the GRI30 model for methane combustion, as well as the different types of NASA Glenn Coefficients(7 coefficients and 9 coefficients) and how they are used to calculate diferent Thermodynamic properties of individual chemical species. The lack of NASA 9 coefficients for a couple of species incorporated in the Methane combustion required an update to the antioch program that is used withing Grins to solve the reactions in Methane Combustion to incorporate NASA 7, During this I helped by making a file containing all of the species in Methane combustion and their NASA 7 coefficients, which were all obtained from GRI30 Thermodynamic data. This file was effentially then pulled and incorporated into the actual Antioch framework as a default file for NASA7. Along with this I had to obtain an xml file with the kinetics data as well as edit the default antioch chemical mixture data file to include the standard enthalpy of formation at 0 k for 5 or so species, which were obtained from atct.anl.gov/Thermochemical Data/version 1.118/species.

[This is the start of my Weak form formulation where i spent most of the Winter Break learning basic Finite Element Method to accomplish]
[Still Need to add all of my references into this section]

2 Weak Form of a One-Dimensional Isobaric Premixed Laminar Flame

After neglecting viscous effects, body forces, radioactive heat transfer, and the diffusion of heat due to concentration gradiants, we are able to reduce the three-dimensional governing equations quite dramatically into a set of one-dimensional differential equations.

2.1 Boundary Conditions

The boundary conditions for our one-dimensional premixed laminar flame contain information from the reactant stream and the hot stream. The Reactant stream boundary conditions are:

$$T(-\infty) = T_u \tag{1}$$
$$Y_k(-\infty) = \epsilon_k(\phi), \quad k = 1, .., N_{sp} \tag{2}$$

Here T_u is just the cold reactant stream temperature and $\epsilon_k(\phi)$ is the known incoming mass flux fraction of the kth species which depends on the reactant stream equivalaence ratio ϕ. In the hot stream:

$$T'(\infty) = 0 \tag{3}$$
$$Y_k`(\infty) = 0, \quad k = 1, .., N_{sp} \tag{4}$$

We also impose a temperature at the origin:

$$T(0) = T_i \tag{5}$$

Here the I apply the use of ' to signify a differentiation in x. We then choose a length L which is large enough to ensure vanishingly small derivatives above this length to decrease our space to $(-\infty, 0]$ and instead replace the Boundary conditions with:

$$T'(L) = 0 \tag{6}$$

$$Y_k`(L) = 0, \quad k = 1, .., N_{sp} \tag{7}$$

To eliminate the interval between $(-\infty, 0)$ we can integrate the species conservation equation between this interval and assume that T_i is small enough that the production terms for the species are negligable for T$\leq T_i$, we then obtain mixed boundary conditions for the species at the origin:

$$\dot{M}Y_k(0) + \rho(0)Y_k(0)u_k(0) = \dot{M}\epsilon_k(\phi), \quad k = 1, .., N_{sp} \tag{8}$$

Using Fick's law with mixture-averaged diffusion coefficients, we are able to remove the species diffusion velocities from the equation:

$$Y_k\mathbf{u}_k = -D_{km}\nabla Y_k \tag{9}$$

Here $-D_{km}$ is the effective average diffusion coefficient of species k into the mixture. After substituting for the species diffusion velocities and solving for Y_k' we obtain:

$$Y_k' = \frac{\dot{M}(Y_k(0) - \epsilon_k(\phi)}{\rho(0)D_{km}} \tag{10}$$

If we integrate the enthalpy conservation equation between $-\infty$ and 0 we obtain:

$$\begin{aligned} &\dot{M}\big(\sum_{k=1}^{N_{sp}} Y_k(0)u_k(0)h_k(T(0)) - \sum_{k=1}^{N_{sp}} \epsilon(\phi)h_k(T_u)\big) \\ &\quad + \rho(0)\sum_{k=1}^{N_{sp}} Y_k(0)u_k h_k(T(0)) - \lambda(0)T'(0) = 0 \end{aligned} \tag{11}$$

which when combined with (5) and (8) give for the boundary condition for T'(0):

$$T'(0) = \frac{\dot{M}}{\lambda(0)}\sum_{k=q}^{Nsp} \epsilon_k(\phi)(h_k(T(0)) - h_k(T_u)) \tag{12}$$

We now have boundary conditions for T' and Y_k' on the space [0,L]

2.2 Conservation of energy equation

The conservation of energy equation for a one-dimensional premixed laminar flame reduces down to:

$$c_p\dot{M}T' = (\lambda T')' - \sum_{k=1}^{N_{sp}} \rho Y_k u_k c_{p,k} T' - \sum_{k=1}^{N_{sp}} \dot{w}_k h_k W_k \tag{13}$$

Inserting Fick's law into the energy equation we obtain:

$$c_p\dot{M}T' = (\lambda T')' + \sum_{k=1}^{N_{sp}} \rho D_{km} Y_k' c_{p,k} T' - \sum_{k=1}^{N_{sp}} \dot{w}_k h_k W_k \tag{14}$$

To then obtain the weak form of this equation we integrate over our whole space and multiply by a test function σ :

$$\int_0^L [c_p\dot{M}T'\sigma - (\lambda T')'\sigma - \sum_{k=1}^{N_{sp}} \rho D_{km} Y_k' c_{p,k} T'\sigma + \sum_{k=1}^{N_{sp}} \dot{w}_k h_k W_k \sigma] dx = 0 \tag{15}$$

We then use integration by parts and insert our boundary conditions to obtain:

$$\int_0^L [c_p\dot{M}T'\sigma + \lambda T'\sigma' - \sum_{k=1}^{N_{sp}} \rho D_{km} Y_k' c_{p,k} T'\sigma + \sum_{k=1}^{N_{sp}} \dot{w}_k h_k W_k \sigma] dx$$
$$+\sigma(0)\dot{M} \sum_{k=1}^{N_{sp}} \epsilon_k(\phi)(h_k(T(0)) - h_k(T_u)) = 0 \tag{16}$$

2.3 Species Mass Equation

The Balancing of the individual species mass for the premixed laminar flame in one dimenstion boils down to, after application of Fick's law once again:

$$\dot{M}Y_k' = (\rho Y_k' D_{km})' + \dot{w}_k W_k, \quad k = 1, .., N_{sp} \tag{17}$$

We then multiply by our test function γ_k and integrate over our whole space to obtain a weak form of the equation:

$$\int_0^L [\dot{M}Y_k'\gamma_k - (\rho Y_k' D_{km})'\gamma_k - \dot{w}_k W_k \gamma_k] dx = 0, \quad k = 1, .., N_{sp} \tag{18}$$

once again we integrate by parts and apply our boundary conditions to obtain:

$$\int_0^L [\dot{M}Y_k'\gamma_k + (\rho Y_k' D_{km})\gamma_k' - \dot{w}_k W_k \gamma_k] dx + \dot{M}(Y_k(0) - \epsilon_k(\phi))\gamma_k = 0, \quad k = 1, .., N_{sp} \tag{19}$$

2.4 Conservation of Mass Equation

The Conservation of the total mass in the system allows us to conclude that for the whole system:

$$\dot{M} = \rho u = \text{constant} \tag{20}$$

to convert this into a weak form equation we can just use the method of lagrange multipliers and multiply our residual by the scalar test function ψ

$$\psi(\dot{M} - \rho u) = 0 \tag{21}$$

2.5 Other Constraint equation

Along with the conservation of Mass equation, we also include the ideal gas law to constrain our system of equations:

$$\rho = \frac{P\bar{W}}{RT} \tag{22}$$

2.6 Weak statement form of our problem

Overall, the weak statement of our problem is to find a $\mathbf{u}$=$(T, Y_k, \dot{M})$ and a $\mathbf{v}$=(σ, γ, ψ) that is a solution to

$$\begin{aligned}
&\int_0^L [c_p\dot{M}T'\sigma + \lambda T'\sigma' - \sum_{k=1}^{N_{sp}} \rho D_{km} Y_k' c_{p,k} T'\sigma + \sum_{k=1}^{N_{sp}} \dot{w}_k h_k W_k \sigma]dx \\
&\qquad + \sigma(0)\dot{M} \sum_{k=1}^{N_{sp}} \epsilon_k(\phi)(h_k(T(0)) - h_k(T_u)) = 0 \\
&\int_0^L [\dot{M}Y_k'\gamma_k + (\rho Y_k' D_{km})\gamma_k' - \dot{w}_k W_k \gamma_k]dx + \dot{M}(Y_k(0) - \epsilon_k(\phi))\gamma_k = 0, \quad k = 1, .., N_{sp} \\
&\qquad \psi(\dot{M} - \rho u) = 0 \\
&\qquad \rho = \frac{P\bar{W}}{RT}
\end{aligned}$$