

Implementation of a Solver for Laminar Diffusion Flames into the Open Source Code OpenFOAM

Adhiraj Dasgupta

April 5, 2018

Contents

1	Governing Equations	1
1.1	The Equation of Continuity	1
1.2	The Species Mass Fraction Equations	1
1.3	The momentum equation	2
1.4	The energy equation	2
1.4.1	Sensible enthalpy	2
1.4.2	Sensible internal energy	3
1.5	Equations of state and other auxiliary relations	3
1.5.1	The species mass conservation equation	3
1.6	Thermodynamic properties	4
2	Compiling the libraries and applications	5
3	Setting up the case	6
3.1	The file <i>transportProperties</i>	6
3.1.1	<i>transportModel</i>	6
3.1.2	<i>mixtureAverageProperties</i>	6
3.1.3	<i>LewisNumberProperties</i>	7
3.1.4	<i>CHEMKINFile</i>	7
3.1.5	<i>CHEMKINThermoFile</i>	7
3.1.6	<i>CHEMKINTransportFile</i>	7
3.1.7	<i>Tmin, Tmax</i>	7
3.2	Fitting the transport properties	8
3.3	Modifications to the file <i>fvSchemes</i>	8
3.4	The keyword <i>pCorr</i>	8

Abstract

A general purpose CFD solver for simulating laminar diffusion flames has been developed based on the open source code `OpenFOAM`. This document provides a summary of the governing equations. A step-by-step method to run the simulation, with explanations for the various options are also provided.

Chapter 1

Governing Equations

The governing equations for a flame are essentially statements of conservation of mass, momentum and energy. There are multiple species present in a combustion system, and so each species has its own conservation equation. The equations are:

1. **The equation of continuity**, expressing the global mass conservation principle,
2. **The species mass fraction equations**, expressing the conservation for the individual species,
3. **The momentum equation**, which is a statement of the principle of conservation of momentum, and
4. **The energy equation**, which is obtained from the principle of conservation of energy.

In addition to these equations there are also **equations of state**, which help to close the system. Typically the energy equation is solved for the energy variable, and then the temperature is obtained from the caloric equation of state.

1.1 The Equation of Continuity

The equation of continuity can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0. \quad (1.1)$$

In the above equation, ρ is the gas-phase density and \mathbf{u} is the velocity.

1.2 The Species Mass Fraction Equations

The mass fraction of the gas-phase species k is governed by the following equation:

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) + \frac{\partial}{\partial x_i} (\rho V_{k,i} Y_k) = \dot{\omega}_k, \quad (1.2)$$

where Y_k is the mass fraction of species k , \mathbf{V}_k is the diffusion velocity of species k , and $\dot{\omega}_k$ is the rate of production of that species by chemical reactions.

Now in a mixture-averaged formulation, the diffusion velocity for species k is modeled as

$$V_{k,j} = \hat{V}_{k,j} + W_{k,j} + V_j^c,$$

where $\hat{V}_{k,j}$ is the contribution from Fickian diffusion, given by

$$\hat{V}_{k,j} = -\frac{D_{km}}{X_k} \frac{\partial X_k}{\partial x_j},$$

$W_{k,j}$ is the contribution from thermophoretic diffusion, given by

$$W_{k,i} = -\frac{D_{km}\Theta_k}{X_k} \frac{1}{T} \frac{\partial T}{\partial x_i},$$

and V_j^c is the correction velocity that ensures that the sum of the diffusive fluxes is zero. In these relations, X_k is the mole fraction of species k , D_{km} is the mass diffusion coefficient of species k into the rest of the mixture, and Θ_k is the thermal diffusion ratio for species k .

1.3 The momentum equation

The momentum equations are the Navier-Stokes equations for compressible flow:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i. \quad (1.3)$$

Here the stress tensor τ_{ij} is defined as

$$\tau_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3}\mu \frac{\partial u_m}{\partial x_m} \delta_{ij} = -p\delta_{ij} + \sigma_{ij},$$

where σ_{ij} is the deviatoric stress, \mathbf{g} is the acceleration due to gravity and p is the pressure.

1.4 The energy equation

The energy equation can be written in terms of the sensible enthalpy h_s , or the sensible internal energy e_s .

1.4.1 Sensible enthalpy

In terms of sensible enthalpy the energy equation can be written as

$$\begin{aligned} \frac{\partial(\rho h_s)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j h_s) + \frac{\partial(\rho K)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j K) \\ = \frac{\partial}{\partial x_j} \left(\rho \alpha \frac{\partial h_s}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left(\rho \alpha \sum_{k=1}^N h_{s,k} \frac{\partial Y_k}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,j} \right) \\ + \frac{\partial p}{\partial t} + \dot{Q} + \frac{\partial}{\partial x_j} (\sigma_{ij} u_i) + \rho u_i g_i - \sum_{k=1}^N \dot{\omega}_k \Delta h_{f,k}^\circ, \end{aligned} \quad (1.4)$$

where K is the kinetic energy of the flow, defined as $K \equiv \frac{1}{2} u_i u_i$, α is the thermal diffusivity of the mixture, defined as $\alpha \equiv \frac{\lambda}{\rho C_p}$, λ is the thermal conductivity of the mixture, C_p is its specific heat, $\Delta h_{f,k}^\circ$ is the formation enthalpy for species k , and \dot{Q} is the energy source, which may include radiation.

1.4.2 Sensible internal energy

In terms of the sensible internal energy the energy equation can be written as

$$\begin{aligned} \frac{\partial(\rho e_s)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e_s) + \frac{\partial(\rho K)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j K) \\ = \frac{\partial}{\partial x_j} \left(\rho \alpha_e \frac{\partial e_s}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left(\rho \alpha_e \sum_{k=1}^N e_{s,k} \frac{\partial Y_k}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,j} \right) \\ + \frac{\partial p u_i}{\partial x_i} + \dot{Q} + \frac{\partial}{\partial x_j} (\sigma_{ij} u_i) + \rho u_i g_i - \sum_{k=1}^N \dot{\omega}_k \Delta h_{f,k}^\circ, \end{aligned} \quad (1.5)$$

where

$$\alpha_e \equiv \frac{\lambda}{\rho C_v}.$$

1.5 Equations of state and other auxiliary relations

For our problems we assume that the gas-phase species behave as ideal gases. Thus the thermal equation of state becomes

$$p = \rho R_u T \sum_{k=1}^N \left(\frac{Y_k}{M_k} \right), \quad (1.6)$$

where M_k is the molecular weight of species k , and R_u is the universal gas constant.

The mole fractions X_k and the mass fractions Y_k are related by:

$$\begin{aligned} X_k &= \frac{Y_k \bar{M}}{M_k} \\ &= \frac{Y_k / M_k}{\sum_{l=1}^N (Y_l / M_l)}, \end{aligned}$$

where \bar{M} is the average molecular weight for the mixture, defined as

$$\bar{M} = \sum_{k=1}^N X_k M_k.$$

The temperature T is obtained from the caloric equation of state:

$$h_s = \int_{T_{std}}^T C_p dT,$$

where C_p is the specific heat of the mixture at constant pressure, and T_{std} is the standard temperature at which the formation enthalpies are defined. Typically T_{std} is taken to be 25° C (298.15 K).

1.5.1 The species mass conservation equation

Substituting the relation between Y_k and X_k in the equation for $\hat{V}_{k,i}$ and simplifying, we obtain the expression for the Fickian diffusion velocity as

$$\hat{V}_{k,j} = -\frac{D_{km}}{Y_k} \frac{\partial Y_k}{\partial x_j} - \frac{D_{km}}{\bar{M}} \frac{\partial \bar{M}}{\partial x_j}.$$

Thus the species mass fraction equation becomes

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) + \frac{\partial}{\partial x_i} (\rho W_{k,i} Y_k) + \frac{\partial}{\partial x_i} (\rho V_{k,i}^c Y_k) + \frac{\partial}{\partial x_i} (\rho V_{k,i}^W Y_k) = \frac{\partial}{\partial x_i} \left(\rho D_{km} \frac{\partial Y_k}{\partial x_i} \right) + \dot{\omega}_k, \quad (1.7)$$

where $V_{k,i}^W \equiv -\frac{D_{km}}{M} \frac{\partial \bar{M}}{\partial x_j}$.

1.6 Thermodynamic properties

For ideal gases, the standard-state thermodynamic properties are functions of temperature only. Thus the standard molar specific heat at constant pressure for species k is given by

$$\frac{C_{p,k}^\circ}{R_u} = \sum_{n=0}^4 a_{n,k} T^n, \quad (1.8)$$

where the superscript \circ denotes standard state. Similarly, for the standard-state values of the molar enthalpy H_k° and the standard-state molar entropy S_k° we have

$$\frac{H_k^\circ}{R_u T} = \sum_{n=0}^4 \frac{a_{n,k} T^n}{n+1} + \frac{a_{n,5}}{T}, \quad (1.9)$$

$$\frac{S_k^\circ}{R_u} = a_{0,k} \log(T) + \sum_{n=0}^4 \frac{a_{n,k} T^n}{n} + a_{6,k}. \quad (1.10)$$

Further, for ideal gases, the specific heats and the enthalpy are functions of temperature only; thus the superscript \circ can be dropped from $C_{p,k}^\circ$ and H_k° in Eqs. (1.8) and (1.9). The thermodynamic properties are evaluated as

$$\begin{aligned} \frac{C_{p,k}}{R_u} &= \sum_{n=0}^4 a_{n,k} T^n. \\ \frac{H_k}{R_u T} &= \sum_{n=0}^4 \frac{a_{n,k} T^n}{n+1} + \frac{a_{n,5}}{T}, \\ \frac{S_k^\circ}{R_u} &= a_{0,k} \log(T) + \sum_{n=0}^4 \frac{a_{n,k} T^n}{n} + a_{6,k}. \end{aligned}$$

The coefficients $a_{0,k}$ through $a_{6,k}$ for species k are obtained from the thermodynamic database that accompanies each mechanism.

Thus we have a fully determinable system from which we can solve for the flow field and also for the temperature and composition of the gas mixture.

Chapter 2

Compiling the libraries and applications

The transport model library depends on the mole fraction library for some calculations, and so the latter must be built first. The easiest way to do that is to copy the `moleFractions` directory to the user's directory and issuing the command `wmake libso` in the terminal.

Once the mole fraction library is successfully built, the transport library may be built. The user may need to modify the provided options file in order to specify the location of the user's source code and the user's libraries. Then the command `wmake libso` should work.

If all goes well, as they should, at this stage the libraries have been built successfully; it remains now to build the applications that use the libraries. The transport fitting program must be built before any solvers can be built. This utility is called `fitTransport`, and it has the GNU Scientific Library (<https://www.gnu.org/software/gsl>) as a dependency. If GSL is installed in the standard locations, as would be the case if it is built using the default options, the provided options file should work. Issuing the command `wmake` at the command prompt should install the fitting program.

The solver is called `laminarReactingFoam`. A sample options file is provided, and the user may need to change it to include the locations of the user's code and libraries. Then the solver may be built by issuing the command `wmake`.

Chapter 3

Setting up the case

Setting up a case for use with the solver is almost identical to the way the same case would be set up for `reactingFoam`, with a few minor differences, as explained next:

1. A *transportProperties* file is added under the *constant* directory of the case.
2. The fits to the transport properties saved as four files in the *constant* directory:
 - *viscosityProperties*,
 - *conductivityProperties*,
 - *diffusivityProperties*, and
 - *thermophoreticProperties*.
3. The file *fvSchemes* that resides in the *system* directory of the case must be modified to account for a set of new equations.
4. Optionally, a keyword `pCorr` may added to the *thermoPhysicalProperties* file.

These features are explained in the following sections.

3.1 The file *transportProperties*

The *transportProperties* file has the following entries:

3.1.1 `transportModel`

This option tells the code which transport model to use. The available options are

- `mixtureAverage`, and
- `LewisNumber`.

Depending on which of these transport models is used, a corresponding subdictionary must be added to the file. The name of the subdictionary is formed by appending the word `Properties` to the name of the transport model.

3.1.2 `mixtureAverageProperties`

As the name suggests, this is the subdictionary that is used to specify the settings for the mixture-averaged transport model. The following settings are available:

gradX

In the original formulation for Fickian diffusion velocities, the flux is taken to be proportional to the gradient of the mole fraction, and given as

$$\begin{aligned}\hat{V}_{k,j} &= -\frac{D_{km}}{X_k} \frac{\partial X_k}{\partial x_j} \\ &= -\frac{D_{km}}{Y_k} \frac{\partial Y_k}{\partial x_j} - \frac{D_{km}}{\bar{M}} \frac{\partial \bar{M}}{\partial x_j}.\end{aligned}$$

If this option is set to on, the above equation is used to calculate the diffusion velocity. However, if it is set to be off, the flux is taken to be proportional to the gradient of the mass fraction,

$$\hat{V}_{k,j} = -\frac{D_{km}}{Y_k} \frac{\partial Y_k}{\partial x_j}.$$

By default this options is set to be on.

thermophoresis

This option indicates whether thermophoresis will be included for light species. By default this is set to off.

CutOff

This is the molecular weight below which thermophoresis will be computed. The default value is 5.

3.1.3 LewisNumberProperties

This subdictionary is used to set up a simulation with the Lewis number-based transport model. A subdictionary named `Le` must be included here, even though all the entries are optional. The Lewis numbers for the species are prescribed here.

By default all species are assumed to have a Lewis number of unity.

3.1.4 CHEMKINFile

This is the path to the kinetics file in Chemkin format.

3.1.5 CHEMKINThermoFile

This is the path to the thermo data in Chemkin format.

3.1.6 CHEMKINTransportFile

This is the path to the transport database in Chemkin format.

3.1.7 Tmin, Tmax

The transport properties are fitted between these two temperatures. By default they are taken to be 300 and 3000.

3.2 Fitting the transport properties

The utility `fitTransport` generates fits to the transport properties. The coefficients for the fits are written to the following files in the *constant* directory of the case: *conductivityProperties*, *diffusivityProperties*, *thermophoreticProperties*, and *viscosityProperties*. For each species, these files contain the fit coefficients, and the fitting error.

In addition, the molecular parameters read from the transport database are summarized in the file *transportData* in the constant directory. Also, the transport properties are written out as a function of temperature in a new directory called *transport*.

3.3 Modifications to the file *fvSchemes*

The new entries are all added to the `divSchemes` section. The new keywords are

1. `div(phi,Yi)`,
2. `div((mu*dev2(T(grad(U)))))`,
3. `div(JHs)`,
4. `div(Hconduction)` or `div(Econduction)`, and
5. `div(phi,he)`.

3.4 The keyword `pCorr`

The implementation of the pressure equation in `OpenFOAM` contains an extra flux term, likely for added stability. This term can cause problems in some cases. In this code the user has the option of disabling or enabling this extra term through the keyword `pCorr` in the file *thermoPhysicalProperties*.

By default the term is dropped.