CFD with OpenSource software

A course at Chalmers University of Technology
Taught by Håkan Nilsson

Study questions and answers for:

Project work:

Implementation of a mass flux term with thermodiffusion mass transport into the species transport equation in a compressible solver

Author:
J. Lorenzo Alejandro Barba-Piña

Peer reviewed by:
Pradip Aryal
Xiaoan Mao
Mohammad H. Arabnejad-Khanouki

Disclaimer: This is a student project work, done as part of a course where OpenFOAM and some other OpenSource software are introduced to the students. Any reader should be aware that it might not be free of errors. Still, it might be useful for someone who would like learn some details similar to the ones presented in the report and in the accompanying files. The material has gone through a review process. The role of the reviewer is to go through the tutorial and make sure that it works, that it is possible to follow, and to some extent correct the writing. The reviewer has no responsibility for the contents.

January 19, 2020

Study questions and answers

1. How do temperature gradients affect mass diffusivity in binary gas mixtures?
   Answer:

   When a two component mixture is under the effects of temperature changes, there is a diffusive process that depends on the temperature gradients and can cause the separation of the mixture. This process is caused by the effect that temperature has on the kinetic properties of molecules of different sizes and shapes. In the case of a binary mixture of fluids, the total mass flux of the reference component is equal to the sum of the Fickian mass diffusivity and the diffusion caused by temperature gradients, also known as thermophoresis or thermodiffusion term. The following expression represents the mass flux equality for a reference component a of a binary mixture,

   $$J_a(x, y, z, C_a, T, \rho) = \rho \left[D_{ab} \nabla C_a + D_T C_{a0} (1 - C_{a0}) \nabla T \right] \tag{1}$$

2. What is the thermodiffusion ratio? How is it related to mass diffusivity processes?
   Answer:

   The thermodiffusion ratio is a dimensionlees quantity formed by the product of the temperature of the system, with the ratio of thermodiffusion coefficient and mass diffusivity. This quantity is used to determine the effects of thermodiffusion in a mixture of fluids, such as the direction of the reference component concentration flux, and the influence that thermodiffusion has over regular mass diffusion. Thermodiffusion ratio equation, can be expressed as follows,

   $$K_T = T \frac{D_T}{D_{ab}} \tag{2}$$

3. Describe briefly the structure of the *thermophysicalModels* library, how are the thermophysical properties of a fluid obtained/calculated when running a simulation case?
   Answer:

   The *thermophysicalModels* library is structured with a central base thermophysical model that works as the base class that contains all the data members that are used for the different submodels that form the whole structure of the library. The base model determines the physics of the system (e.g. rhoThermo, psiThermo, fluidThermo, etc.) and submodels are used for calculations of thermophysical properties such as transport, mixture, thermodynamics and equation of state terms.

   If a simulation case requires the usage of the *thermophysicalModels* library, it is necessary to include a dictionary file called *thermophysicalProperties* dictionary, inside the *constant* folder of the case. In this file the user will set the required initial values by the mentioned submodels to then start the calculations of the energy, momentum, and in some cases, the species transport equation.

4. In the *thermophysicalModels* code context, why is it necessary to declare the data members and member functions of a transport model in a base thermophysical model? (it can also be

a thermodynamic or state equation model).
Answer:

To implement a new transport model in the *thermophysicalModels* library it is necessary to create a base class that serves as a core for the data members and member functions of that transport model. Since there are several data members that are shared for all the thermophysical sub-models (e.g. ρ, μ, Cp, α, etc.). The base thermophysical model will provide an abstract class where some of the data members are defined as a virtual member functions (That is the reason to call it an abstract class). This is used for the derivation of sub-classes (Derived classes) that inherit the data members that are common to whole structure of the library.

5. In a solver code where thermophysical models are required, how are thermophysical models declared? Which file contains that declaration?
Answer:

A thermophysical model is called inside the *createFields.H* file by pointing to the thermophysical model class with an *autoPtr* pointer *pThermo*. Then data members and member functions can be accessed by the *thermo* reference to *pThermo.*

```
Info<< "Reading thermophysical properties\n" << endl;

autoPtr<rhoThermo> pThermo
(
    rhoThermo::New(mesh)
);
rhoThermo& thermo = pThermo();
thermo.validate(args.executable(), "h", "e");
```

6. Explain briefly the entries of the *thermophysicalProperties* dictionary (this is related with the structure of *thermophysicalModels* library).
Answer:

This question can be answered witht the help of a *thermophysicalProperties* dictionary example. The properties and meaning of each entry will be mentioned with comment lines:

```
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      thermophysicalProperties;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

thermoType  //- The thermophysical model is constructed with the following entries.
{
    type            thermoDiffheRhoThermo; //- Select the thermophysical base model.
    mixture         pureMixture;   //- Select the mixture type
    transport       thermoDiffconst; //- Select the model for transport calculations
    thermo          hConst;   //- Select the thermodynamic energy model
    equationOfState perfectGas;  //- Select the equation of state.
    specie          specie;  //- Select the specie model.
```

```
    energy          sensibleEnthalpy; //- Select the energy variable model.
}

mixture //- The mixture model is constructed
{       // with the initial values of the following models.
    specie   //- Defines a specie with the average mole weight of the mixture
    {
       molWeight   7.00125; //- He-N2 50-50 mole weight mixture
    }
    thermodynamics            //- Defines the thermodynamics
    {                         // of the mixture with thermodynamic
       Cp          3112.452;  // constant values of Cp and enthalpy of formation.
       Hf          0;
    }
    transport
    {
       mu          1.969e-05; //- Defines the transport calculations, in this case, the
       Pr          0.45;      // values are entries of a constant transport model, but
       Dab         7.5e-5;    // in general the entries are initial values or coefficients
       KT          20.3;      // of a variable transport model.
    }
}
```