User Guide

Contents

5.2 Thermophysical models

Thermophysical models are used to describe cases where the thermal energy, compressibility or mass transfer is important.

OpenFOAM allows thermophysical properties to be constant, or functions of temperature, pressure and composition. Thermal energy can be described in form of enthalpy or internal energy. The $p-v-T$ relation can be described with various equations of state or as isobaric system.

The thermophysicalProperties dictionary is read by any solver that uses the thermophysical model library. A thermophysical model is constructed in OpenFOAM as a pressure-temperature $p-T$ system from which other properties are computed. There is one compulsory dictionary entry called `thermoType` which specifies the complete thermophysical model that is used in the simulation. The thermophysical modelling starts with a layer that defines the basic equation of state and then adds further layers for the thermodynamic, transport and mixture modelling, as listed in Table **5.1**.

Equation of State — equationOfState	
icoPolynomial	Incompressible polynomial equation of state, *e.g.* for liquids
perfectGas	Perfect gas equation of state
Basic thermophysical properties — thermo	
eConstThermo	Constant specific heat c_p model with evaluation of internal energy e and entropy s
hConstThermo	Constant specific heat c_p model with evaluation of enthalpy h and entropy s
hPolynomialThermo	c_p evaluated by a function with coefficients from polynomials, from which h, s are evaluated
janafThermo	c_p evaluated by a function with coefficients from JANAF thermodynamic tables, from which h, s are evaluated
Derived thermophysical properties — specieThermo	
specieThermo	Thermophysical properties of species, derived from c_p, h and/or s
Transport properties — transport	
constTransport	Constant transport properties
polynomialTransport	Polynomial based temperature-dependent transport properties
sutherlandTransport	Sutherland’s formula for temperature-dependent transport properties
Mixture properties — mixture	
pureMixture	General thermophysical model calculation for passive gas mixtures
homogeneousMixture	Combustion mixture based on normalised fuel mass fraction b
inhomogeneousMixture	Combustion mixture based on b and total fuel mass fraction f_t
veryInhomogeneousMixture	Combustion mixture based on b, f_t and unburnt fuel mass fraction f_u
dieselMixture	Combustion mixture based on f_t and f_u
basicMultiComponentMixture	Basic mixture based on multiple components
multiComponentMixture	Derived mixture based on multiple components
reactingMixture	Combustion mixture using thermodynamics and reaction schemes
egrMixture	Exhaust gas recirculation mixture
Thermophysical model — thermoModel	
hePsiThermo	General thermophysical model calculation based on enthalpy h or internal energy e, and compressibility ψ
heRhoThermo	General thermophysical model calculation based on enthalpy h or internal energy e, and density ρ
hePsiMixtureThermo	Calculates enthalpy for combustion mixture based on enthalpy h or internal energy e, and ψ
heRhoMixtureThermo	Calculates enthalpy for combustion mixture based on enthalpy h or internal energy e, and ρ
heheuMixtureThermo	Calculates enthalpy h or internal energy e for unburnt u gas and combustion mixture

Table 5.1: Layers of thermophysical modelling.

Various combinations are available as ‘packages’, specified using, *e.g.*

```

thermoType
{
    type            heRhoThermo;
    mixture         pureMixture;
    transport       const;
    thermo          hConst;
    equationOfState perfectGas;
```

```
    specie                  specie;
    energy                  sensibleEnthalpy;
}

mixture
{
    specie
    {
        molWeight           28.96;
    }
    thermodynamics
    {
        Cp                  1004.4;
        Hf                  0;
    }
    transport
    {
        mu                  1.831e-05;
        Pr                  0.705;
    }
}


// ************************************************************************* //
```

Only certain combinations are predefined. One method to identify the possible combinations from Table **5.1** is to use a nonexistent setting for one of the entries, *e.g.* `banana` and execute the solver. OpenFOAM will issue an error message and list all possible combinations to the terminal.

5.2.1 Thermophysical property data

The basic thermophysical properties are specified for each species from input data. Data entries must contain the name of the specie as the keyword, *e.g.* `O2`, `H2O`, `mixture`, followed by sub-dictionaries of coefficients, including:

`specie`
: containing *i.e.* number of moles, `nMoles`, of the specie, and molecular weight, `molWeight` in units of g/mol;

`thermo`
: containing coefficients for the chosen thermodynamic model (see below);

`transport`
: containing coefficients for the chosen transport model (see below).

The thermodynamic coefficients are ostensibly concerned with evaluating the specific heat c_p from which other properties are derived. The current thermo models are described as follows:

hConstThermo
: assumes a constant c_p and a heat of fusion H_f which is simply specified by a two values c_p H_f, given by keywords `Cp` and `Hf`.

eConstThermo
: assumes a constant c_v and a heat of fusion H_f which is simply specified by a two values c_v H_f, given by keywords `Cv` and `Hf`.

janafThermo
: calculates c_p as a function of temperature T from a set of coefficients taken from JANAF tables of thermodynamics. The ordered list of coefficients is given in Table **5.2**. The function is valid between a lower and upper limit in temperature T_l and T_h respectively. Two sets of coefficients are specified, the first set for temperatures above a common temperature T_c (and below T_h, the second for temperatures below T_c (and above T_l). The function relating c_p to temperature is:

$$c_p = R((((a_4T + a_3)T + a_2)T + a_1)T + a_0) \qquad (5.1)$$

In addition, there are constants of integration, a_5 and a_6, both at high and low temperature, used to evaluating h and s respectively.

hPolynomialThermo
: calculates C_p as a function of temperature by a polynomial of any order. The following case provides an example of its use: $FOAM_TUTORIALS/lagrangian/porousExplicitSourceReactingParcelFoam/filter

Description	Entry	Keyword
Lower temperature limit	T_l (K)	`Tlow`
Upper temperature limit	T_h (K)	`Thigh`
Common temperature	T_c (K)	`Tcommon`
High temperature coefficients	$a_0 \dots a_4$	`highCpCoeffs (a0 a1 a2 a3 a4...`

High temperature enthalpy offset	a_5	`a5...`
High temperature entropy offset	a_6	`a6)`
Low temperature coefficients	$a_0 \dots a_4$	`lowCpCoeffs (a0 a1 a2 a3 a4...`
Low temperature enthalpy offset	a_5	`a5...`
Low temperature entropy offset	a_6	`a6)`

Table 5.2: JANAF thermodynamics coefficients.

The transport coefficients are used to to evaluate dynamic viscosity μ, thermal conductivity κ and laminar thermal conductivity (for enthalpy equation) α. The current transport models are described as follows:

constTransport
: assumes a constant μ and Prandtl number $Pr = c_p\mu/\kappa$ which is simply specified by a two keywords, `mu` and `Pr`, respectively.

sutherlandTransport
: calculates μ as a function of temperature T from a Sutherland coefficient A_s and Sutherland temperature T_s, specified by keywords `As` and `Ts`; μ is calculated according to:

$$\mu = \frac{A_s\sqrt{T}}{1 + T_s/T} \qquad (5.2)$$

polynomialTransport
: calculates μ and κ as a function of temperature T from a polynomial of any order.

The following is an example entry for a specie named `fuel` modelled using sutherlandTransport and janafThermo:

```
fuel
{
        specie
        {
                nMoles              1;
                molWeight        16.0428;
        }
        thermodynamics
        {
                Tlow                   200;
                Thigh                 6000;
                Tcommon            1000;
                highCpCoeffs  (1.63543  0.0100844  -3.36924e-06  5.34973e-10
                                            -3.15528e-14  -10005.6  9.9937);
                lowCpCoeffs    (5.14988  -0.013671  4.91801e-05  -4.84744e-08
                                            1.66694e-11  -10246.6  -4.64132);
        }
        transport
        {
                As                      1.67212e-06;
                Ts                      170.672;
        }
}
```

The following is an example entry for a specie named `air` modelled using constTransport and hConstThermo:

```
air
{
        specie
        {
                nMoles                    1;
                molWeight              28.96;
        }
        thermodynamics
        {
                Cp                             1004.5;
                Hf                             2.544e+06;
        }
        transport
        {
                mu                             1.8e-05;
                Pr                             0.7;
        }
}
```