Interfaces for thermodynamics calculations in material stream and holdup:

CalcTemperatureFromProperty
CalcPressureFromProperty

Interfaces for thermodynamics calculations in base unit:

CalcTemperatureFromProperty
CalcPressureFromProperty
HeatExchange

Implementation of temperature/pressure calculation

The main application of these functions is the calculation of a stream/holdup temperature from a given enthalpy value. Most of the times the enthalpy of a compound nonlinearly correlates with temperature. Thus for backward calculation of the temperature from an enthalpy value, one needs to solve a non-linear equation.

$$\boldsymbol{T = f^{-1}(H)}$$

This solving step is replaced by a lookup table functionality, i.e. temperature and enthalpy that are codepenedent, are precalculated for a certain range of values and stored in a table. This table can be used to determine temperature-enthalpy value pairs by interpolation between two neighboring points.

To add some more functionality these lookup tables can be called for every property, that has been defined in the materials database.

$$\boldsymbol{Val_{Prop,i}({}^{T}\!/_{p}) = f_i({}^{T}\!/_{p})}$$
$$\boldsymbol{f_{tot}({}^{T}\!/_{p}) = \sum_i w_i f_i({}^{T}\!/_{p})}$$
$$\boldsymbol{{}^{T}\!/_{p} = f_{tot}{}^{-1}(Val_{Prop,tot})}$$

The calculation of the temperature or pressure, e.g. pressure from saturation pressure, from different properties is then performed by the following steps:

1. Creation of tables of value pairs for each compound that is present in the system, i.e. temperature/pressure and respective dependent property value over a certain range of the temperature/pressure.
2. Combination of the compound-lookup tables by mass-weighted summation of the tables.
3. Read-out of temperature/pressure from the resulting lookup-table at a certain point of the property by interpolation between neighboring value pairs.

The functions in base unit are less time consuming than the stream/holdup-function and therefore are implemented for usage during solving process (i.e. CalculateResiduals-Function), if the composition of the holdup/stream varies in each iteration.

Units in library using thermodynamic calculations

Mixer, HeatExchanger

Interfaces in material stream and holdup

double CalcTemperatureFromProperty *(ECompoundTPProperties Property, double Time, double Value)*

Returns temperature of the stream/holdup for a specific value *Value* of the property *Property* at the time point *Time*. Possible properties are those defined in material database.

double CalcPressureFromProperty *(ECompoundTPProperties Property, double Time, double Value)*

Returns pressure of the stream/holdup for a specific value *Value* of the property *Property* at the time point *Time*. Possible properties are those defined in material database.

Interfaces in base unit

double CalcTemperatureFromProperty *(ECompoundTPProperties Property,vector<double>& CompoundFractions, double Value)*

Returns temperature of a generic system of composition *CompoundFractions* for a specific value *Value* of the property *Property*. Possible properties are those defined in material database.

double CalcPressureFromProperty *(ECompoundTPProperties Property,vector<double>& CompoundFractions, double Value)*

Returns pressure of a generic system of composition *CompoundFractions* for a specific value *Value* of the property *Property*. Possible properties are those defined in material database.

void HeatExchange(*CMaterialStream** Stream1, *CMaterialStream** Stream2, *double* Time, *double* Efficiency);

Performs a heat exchange between material streams *Stream1* and *Stream2* at specified time point with a specified efficiency (0 ≤ *Efficiency* ≤ 1).

$$|\dot{Q}| = \varepsilon|\dot{Q}_{\mathrm{ideal}}| =$$

$$= \varepsilon\left|\int_{T_1}^{T_{\mathrm{mix}}} \dot{m}_1 c_{\mathrm{p},1}(\theta)\, d\theta\right| = \varepsilon\left|\int_{T_2}^{T_{\mathrm{mix}}} \dot{m}_2 c_{\mathrm{p},2}(\theta)\, d\theta\right|$$