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Calculation of Thermophysical Properties in the Modelica Library TechThermo

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Abstract

Many physical models describing thermodynamic systems require correlations for thermophysical properties to complete the set of equations. A Modelica library like TechThermo which is intended for general application in technical thermodynamics must include also a set of models for calculation of thermophysical properties. Since the total number of models in TechThermo should be limited, the range of application for selected model must be as wide as possible. The models for calculation of thermophysical properties in TechThermo are based on general concepts which allow the introduction of new working media by modification of a few model parameters. Models for calculation of multiphase or multicomponent media are composed of models representing single phase behaviour and mixing models.

Keywords: thermodynamic system; thermophysical properties;

1 The TechThermo library

1.1 Aims of TechThermo

TechThermo is a basic library for engineering applications in thermodynamics. This basic library provides components which are relevant for the bulk of applications in this area. TechThermo is complemented by problem-specific libraries which include components relevant only for a limited scope of application (Figure1). There are different aspects how TechThermo can improve the efficiency of modelling activities:

- the library should allow a fast implementation of a model describing the simulation problem without generation of additional source code the detailing of the system may be limited, but this approach allows fast results and demands only limited knowledge of Modelica or numerical principles

- Experienced Modelica users should profit from TechThermo primarily by extending the models provided by the library thus minimizing the extent of work spent on implementation of trivial equations needed for describing a physical process.
- by standardization of interfaces the co-operation between model-developers is improved.
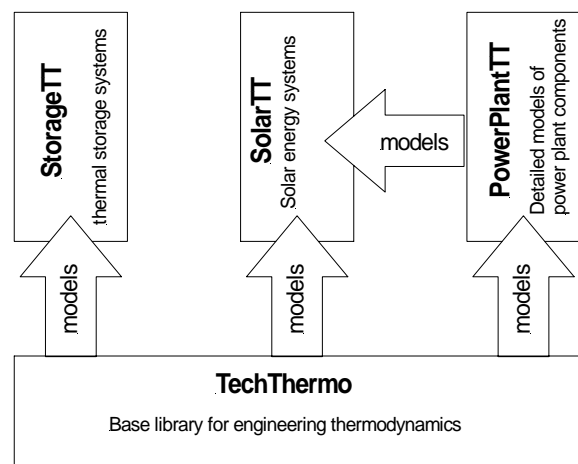
Figure 1: Application of basic library TechThermo in combination with problem-specific libraries

Although it would be comfortable to have a universal thermodynamic library which allows the modelling of any system by mere composition of basic models without input of further model equations, this approach was not chosen for TechThermo since the implementation of such a library seems not to be feasible in practice. Instead, the aim of TechThermo is to minimize the effort for supplementary models for a wide range of application.

1.2 Structure of TechThermo

Modelica-infrastructure:
Interface - definition of model interfaces
Source - models for imposing boundary conditions

Fundamentals of engineering thermodynamics:
Medium - thermophysical correlations for working media
Basis - descriptions of fundamental physical processes

Fundamentals of technical systems:
Component - models of basic technical units
Subsystem - simplified models of technical systems

Tab1: The structure of TechThermo

The models of TechThermo are organized in six main packages and an additional folder with examples. These six packages can be attributed to one of three different groups:

- package Interface and package Source include the models which are needed for the exchange of information between connected models and models for imposing boundary conditions. These two packages can be regarded as the infrastructure needed in any Modelica simulation
- package Medium and package Basis comprise models describing fundamental processes in thermodynamics and correlations for thermophysical properties of working media. These two packages can be regarded as the infrastructure needed for modelling thermodynamic processes.
- package Component and package Subsystem contain models describing basic technical components like turbines and

heat exchangers and models representing simplified systems like solar collectors or fuel cells. These two packages can be regarded as infrastructure for modelling technical systems.

The six main packages are stored in separate files; a subset of packages can be selected provided the hierarchy is regarded (Tab. 1): while package Interface demands no models from the other five packages, package Source demands package Interface, Medium demands Source and Interface and so on.

2 Models including correlations for thermophysical properties

2.1 Relevance of correlations between variables describing thermodynamic systems

Thermodynamic systems can be described by various variables. The most common state variables for technical systems are

- spec. enthalpy
- pressure
- density
- spec. entropy
- temperature
- spec. internal energy
- steam quality
- vector with mass fractions

The minimal number of independent variables needed to define the state of a system depends on the number of phases and components, for a pure substance only two variables are needed. Depending on the physical process various combinations of variables may be used in a model. Mathematical correlations between state variables are needed if different sets of variables are used. These correlations must ensure that all sets of variables define the identical thermal state.

2.2 Representation of thermal state information in TechThermo

The connectors in the TechThermo library transfer information between models as energy flows. Three different kinds of energy flows are defined:

- combined heat and mass transfer

- heat transfer (without mass transfer), defined by heat flow rate q_dot and temperature t

- pure exergy, defined by exergy flow rate exergy_dot

While the selection of connector variables defining heat transfer and pure exergy flow is obvious, various sets of variables listed in section 2.1 can be used. The connector for combined heat and mass transfer in TechThermo is defined by

- mass flow rate m_dot

- pressure p

- spec. enthalpy h

- composition vector x_i[n_comp]

Pressure and spec. enthalpy represent a minimal set of state variables. If models include physical processes described by other variables, these variables must be calculated from pressure and spec. enthalpy. One basic concept of TechThermo is the separation of models including correlations for thermophysical properties from the other parts of a model. A fourth connector for thermal state information is defined including all variables listed in section 2.1. This concept should be demonstrated here by the model AirCompressor representing an adiabatic compressor for air. The physical process is shown in Figure 2. Assuming an isentropic efficiency eta_isentrop the spec. enthalpy h_out at the outlet is

```
h_out=h_in+(State2.h-h_in) /
       eta_isentrop
```

Variable State2.h is the spec. enthalpy after an isentropic compression form pressure p_in to pressure p_out. The entropy after the isentropic compression is identical to the entropy for inlet enthalpy h_in and pressure p_in. The models demands two thermophysical correlations:

1. spec. entropy s_in at inlet enthalpy h_in and pressure p_in

2. spec. enthalpy State2.h for entropy s_in and pressure p_out.

Figure 3 shows the diagram layer of AirCompressor. The model CompressorNoProp1 represents the compressor model without specification of the working fluid. By addition of two models AirPerfectGasCaloric including the thermophysical property correlations for air the model is completed. Thermal state connectors are used to link CompressorNoProp1 and the two AirPerfectGasCaloric models. By exchanging the

property models the compressor can be adapted to other working fluids. AirCompressor also includes two models NotUsedVariables; these models are used to define the remaining variables of the thermal state connectors by parameters to complete the set of equations.
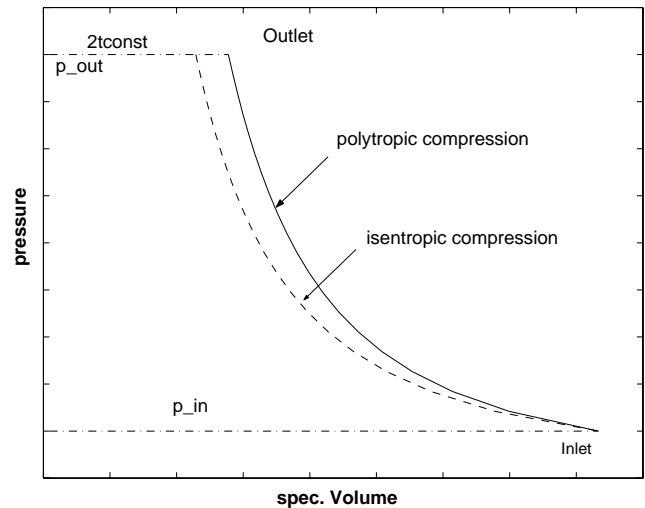

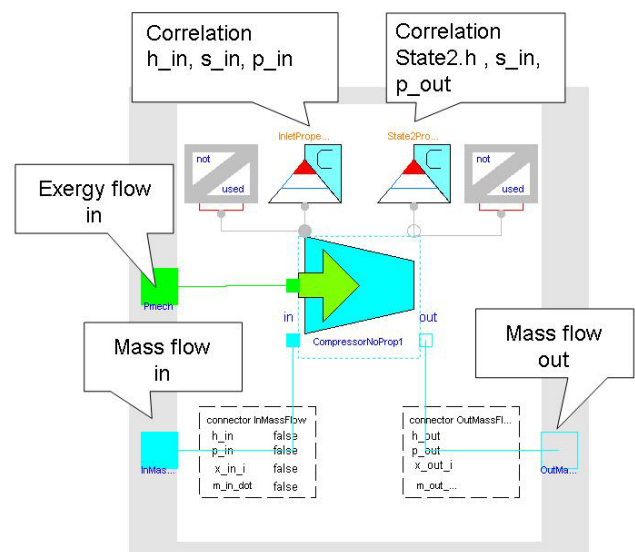Figure 2: p-v diagram of adiabatic compression

Figure 3: Diagram layer of the compressor model AirCompressor including two models for calculation of thermophysical properties of the working fluid.

3 The main package Medium in TechThermo

3.1 Selection of model describing property data

TechThermo is intended as a basis library for applications in technical thermodynamics. The models included should be used in a wide range of applications. Concerning the models for thermophysical correlations included in the main package Medium of TechThermo there are two basic aspects:

– only models based on general concepts are contained; these models can be adapted to various media by modification of a small number of parameters

– TechThermo does not include large multiparameter equations of state which are only available for a limited number of media.

The accuracy of general models usually is limited; if the models offered by TechThermo don't fulfil the demands, additional models are provided by problem-specific model libraries.

Mathematical models for thermodynamic property data are available within a wide range of complexity and accuracy. Criteria for selection of algorithms can be

– accuracy compared to reference values

– consistency; especially interesting near to phase transitions

– dependence on selected variables; many multiparameter equations of state can't be inverted and demand iterative solution if the set of independent variables changes

– numerical aspects like stability and required calculation time

The selection of the property models strongly influences the behaviour of the model. The choice should always be adapted to the specific simulation problem. Aspects that should be considered are

- the extend of variation for a state variable within a model; if the variation is limited, the application of simple linear property models may be sufficient without introducing significant errors; e.g. if a simulation deals with a gas at room temperature at ambient pressure the application of the ideal gas law is often sufficient, using real

gas property routines does not provide different results

- the accuracy of the property model should correspond to the accuracy of the other physical models; e.g. in two phase flow the results provided by models for pressure loss or heat transfer coefficients often show errors within the range of 30-50%, using complex models for calculating the density of the medium is not efficient in combination with models of limited accuracy.

- in dynamic simulations the assumption of thermal equilibrium in the working fluid may be not valid; the application of high accuracy property routines describing steady state systems does not improve the quality of the model compared to the real world.

Using high precision property routines does not necessarily improve the quality of simulation results; on the other side, the complex high precision property routine make the finding of a solution more difficult from a numerical point of view. The choice of the adequate level of complexity of property routines is essential for effective modelling and simulation.
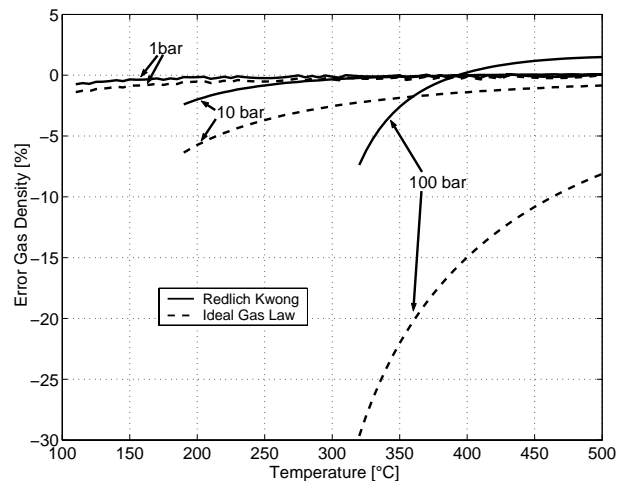
Figure 4: Accuracy of the results for density of steam provided by the Ideal Gas model and the Redlich-Kwong equation of different pressure levels.

Figure 4 shows the deviation from the reference values for the density of superheated steam provided by the Ideal Gas law and the Redlich Kwong correlation. Depending on temperature and pressure range the difference in accuracy changes significantly: at low temperatures, the simple Ideal Gas law model shows almost the same quality like the Redlich-Kwong equation. For applications at high pressure levels the differences become significant, using the Ideal Gas law here probably is not acceptable.

3.2 Organisation of property models

The main package Medium includes six sub-packages with property models:

- Gas
- Liquid
- Solid
- MultiPhase
- MultiComponent

Two additional sub-packages (MediumSpecificData, MathTool) supply fundamental constants for various substances and mathematical tools like cubic equation solvers.

Property model can be separated into two groups:

- single phase models for pure substances
- multiphase and/or multicomponent models

In TechThermo, models describing a multiphase / multicomponent system are composed of basic single phase models for pure substances. Depending on the variables included in the models, these basic models can be divided into three groups:

- volumetric properties including pressure, temperature and density
- caloric properties including spec. enthalpy, heat of evaporation, spec. entropy and spec. internal energy
- transport properties like viscosity and heat conductivity

3.3 Basic concepts for Implementation of property models

Basic concepts for the implementation of property models should be demonstrated here by the example of the perfect gas law. The perfect gas is described by the ideal gas correlation between density rho, temperature t and pressure p and a correlation between the caloric variables spec. enthalpy, spec. internal energy and entropy assuming a constant spec. heat capacity.

3.3.1 Definition of substances by record with fundamental constants

The Ideal Gas correlation is implemented in the model IdealGasVolumetricNoProp:

```
model IdealGasVolumetricNoProp "p/rho=RT"
extends TTInterface.ThermalState.PropertyPort;


replaceable TTMedium.MediumSpecificData.
Data.MediumThermoFundamentalConstants
SpecificConstants "record with medium specific
constants";

SIunits.SpecificHeatCapacity r_gas
"spec. gas constant";

parameter Boolean switch_r_gas_const=true
"if switch_r_gas_const==true then specific gas
constant r_gas is defined by
parameter molar mass SpecificConstants.m_mol";

equation

if switch_r_gas_const==true then
  r_gas = GeneralCon-

stants.R/SpecificConstants.m_mol;
end if;


StateCut.p = r_gas*(StateCut.t + 273.15)*

StateCut.rho;


end IdealGasVolumetricNoProp;
```

The medium is defined by the spec. gas constant which is calculated from the molar mass m_mol and the general gas constant. R. If the molar mass remains constant during the simulation (switch_r_gas_const is true) the value for the molar mass is taken from the record SpecificConstants which includes the fundamental constants of a medium. SpecificConstants is a record of type MediumThermoFundamentalConstants:

```
record MediumThermoFundamentalConstants
"record defining reference state for
thermophyscial properties TTcode:CfD1"

parameter SIunits.MolarMass m_mol "mo-
lar mass";
parameter SIunits.
ThermodynamicTemperature t_critical
"critical temperature";
parameter SIunits.Pressure p_critical
"critical pressure";
parameter SIunits.Density rho_critical
"critical density";
parameter SIunits.SpecificHeatCapacity
r_gas=GeneralConstants.R/m_mol "spe-
cific gas constant";
parameter Real omega_acentric "acentric
factor";
end MediumThermoFundamentalConstants;
```

This record contains the molar mass and the state variables in the critical point. These constants are easily available for many substances. In the Tech-

Thermo library models are preferred which require only these fundamental constants for the specification of the substance.

The model model `AirIdealGasVolumetric` calculates the volumetric properties of dry air assuming the ideal gas law:

```
model AirIdealGasVolumetric
"p/rho=RT for Air TTcode:Cal"
      extends TTMedium.Gas.Support.
      IdealGasVolumetricNoProp
      (redeclare TTMedium.
      MediumSpecficData.Data.
      AirThermoFundamentalConstants
      SpecificConstants);
```

`AirIdealGasVolumetric` extends the general model `IdealGasVolumetricNoProp` and defines the medium by the record `AirThermoFundamentalConstants`.

3.3.2   Flexible choice of used state variables

The correlations between the caloric variables are provided by the model `PerfectGasCaloricNoProp`.

assuming a constant specific heat.
There are various correlations for spec. enthalpy h and spec. internal energy u:

    1   $h = cp * (t-t0) + h0$
        $u = cv *(t-t0) + u0$
    2   $h = u + p / rho$

There are also different options for the calculation of the spec. entropy:

    1   $s = cv * \log(T / T0) + R\_gas * \log(rho0 /.rho) + s0$
    2   $s = cp * \log T / T0) + R\_gas * \log(p /.p0) + s0$

Depending on the application, different formulation might be advantageous. The user can select options by structural parameters. Many property models in TechThermo offer alternative formulations for the calculation of material properties.

3.3.3   Icon representation of property models

The icons of the property model should provide first information about the included correlations. The basic icon is shown in Figure 5. The range of validity, the included variables and the substance is indicated in the corresponding areas of the icon.
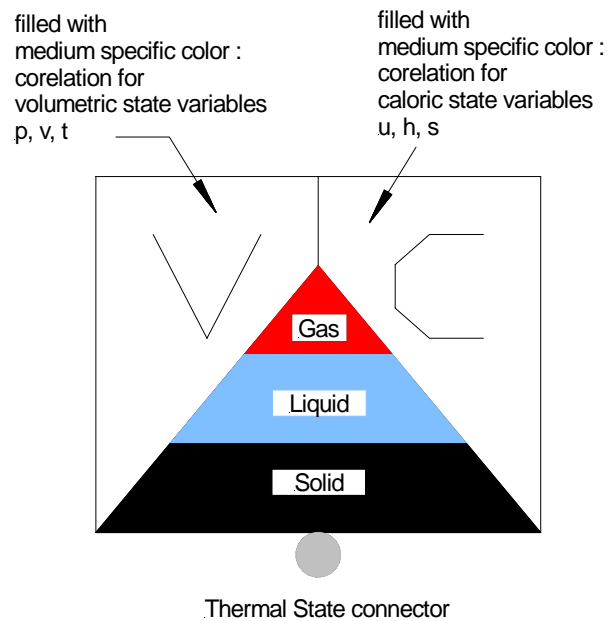

Figure 5: Icon used for models containing thermo-physical property correlations.

Figure 6 shows the icon of the AirPerfectGasCalVol. This model is composed of `IdealGasVolumetric` and a model `PerfectGasCaloric` as shown in Figure 7
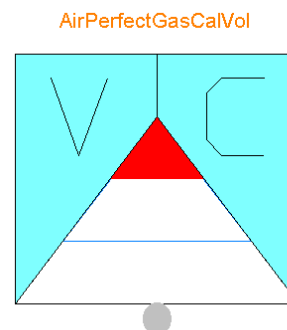

Figure 6: Icon for `AirPerfectGasCalVol` providing correlations for both caloric and volumetric state variables of dry air
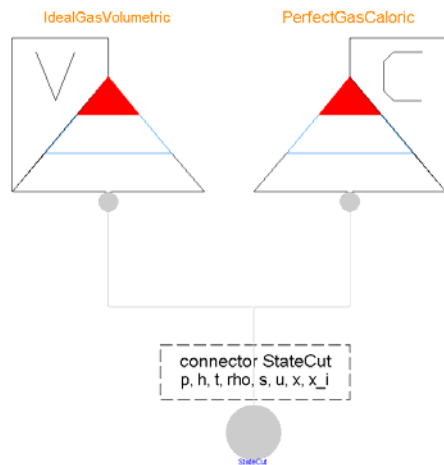
Figure 7: Diagram layer of `AirPerfectGas-CalVol`; combination of model `IdealGas-Volumetric` and model `PerfectGasCaloric`

3.3.4   Composed models

`AirPerfectGasCalVol` represents a simple form of a composed model; two basic models are joined to offer the complete set of state variables. The concept of composed models becomes especially interesting for multiphase models which a composed of models representing the separate phases. For wet steam with steam quality x the thermal state variables can be calculated from the properties of the liquid and the gas phase:

- h = h' + x * (h''-h')
- u = u' + x * (u''-u')
- s = s' + x * (s''-s')
- rho = 1/rho' + x * (1/rho'' – 1/rho')

h', u', s', rho' are the properties of the saturated liquid, h'', u'', s'', rho'' are the properties of the saturated steam. Additional correlations are:

- Δh = h'' – h'
- s'' – s' = Δh / (t$_{sat}$ + 273.15)
- h = u + p / rho

with heat of vaporization Δh and t$_{sat}$ saturation temperature. Model `WetSteamV01NoProp` is composed of five models to calculate the properties of wet steam:

- `TSatPSatAntoineNoProp` provides the correlation between saturation temperature and saturation pressure
- `HeatVaporizationNoProp` calculates the heat of vaporization dependent on the saturation temperature
- `VariableRhoCalVolNoProp` calculates the properties for the liquid phase for saturation pressure and saturation temperature
- `IdealGasVolumetricNoProp` calculates the properties for the gas phase assuming saturation pressure and saturation temperature
- `TwoPhaseMix` calculates the properties of wet steam from the information provided by the other four models

`WetSteamV01NoProp` can be specified for any substance provided the following constants for the substance are available:

- state variables in the critical point
- two constants needed for the Antoine correlation for saturation pressure /saturation temperature
- a single value for the heat of vaporization dependent on saturation temperature

The modular approach is advantageous regarding the consistancy at the transition between different regions. Since the properties of the two phases of the wet steam are calculated using single phase property models there are no discontinuities at the transitions between the two phase region and the single phase regions.
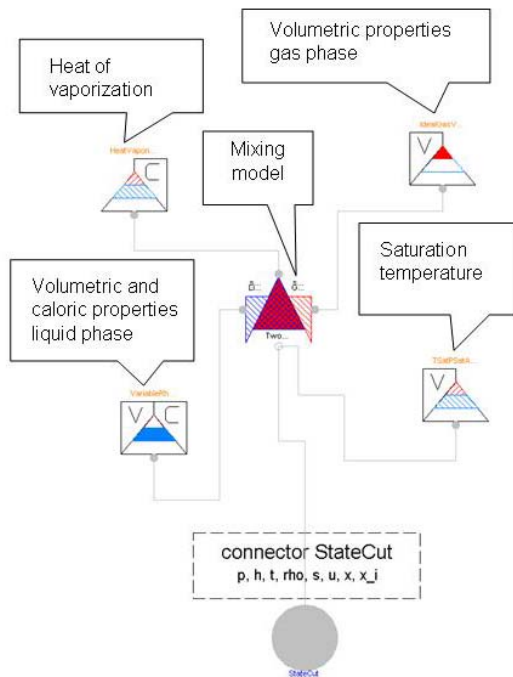
Figure 9: Diagram layer of `WetSteamV01NoProp` for calculation of properties of wet steam.

3.3.5   Alternative formulation for non-linear correlations

The convergence behaviour of a model is influenced by the formulation of non-linear property correlations. Which variable is chosen as dependent might affect the numerical performance of a model. If possible, TechThermo offers for the non-linear property model various formulations. One example is the Redlich-Kwong equation for the volumetric properties of gases:

$$p = \frac{RT}{\dfrac{1}{rho} - b} - \frac{a}{T^{0,5} \dfrac{1}{rho}\left(\dfrac{1}{rho} + b\right)}$$

coefficients a and b are calculated from values for the critical state.

As already shown in Figure 4, this cubic algorithm provides better results as linear correlations like the ideal gas law. The model `RealGasVolumetric-NoProp` offers three different options:

1   acausal formulation
2   temperature t as function of pressure p and density rho
3   density rho as function of pressure p and temperature t

The user can select one of these three options by a structural parameter. For options 2 and 3 a cubic equation solver is used.

Conclusions and Outlook

The TechThermo library includes a basic set of models with correlations for thermophysical properties. These models have been selected considering the range of application, so only models which can be used for many different substances are included. The property models in TechThermo should allow complete descriptions of a thermodynamic system in the initial phase of model developing. Since property models are separated from the other parts of a model by a thermal state connector, a quick exchange of property models is possible.

Further development aims at implementing property models which are more efficient regarding numerical aspects. These models should offer flexibility in the selection of the dependent variable and should optimize the calculation time / accuracy ratio. One approach here includes the transformation of state variables and the application of cubic equation solvers.

References

[1]   Reid, R.C., Prausnitz, J.M., Poling, B.E. : "*The Properties of Gases & Liquids*", 4th edition, McGraw-Hill Book Company, 1988