## Analysis of steam storage systems using Modelica

J. Buschle, W.D. Steinmann, R. Tamme German Aerospace Center (DLR), Institute of Technical Thermodynamics Pfaffenwaldring 38-40, 70569 Stuttgart, Gemany jochen.buschle@dlr.de

#### **Abstract**

Modelica is used for the analysis of steam accumulators used as energy storage systems in power plants and process industry. The analysis includes varying pressure accumulators and steam accumulators with latent heat technology. Physical models for the phase change material (PCM) and for the vertical discretisation of stacked volume elements are implemented in Modelica. Modelica is used for the analysis of new PCM enhanced steam accumulators which are not state of the art. The results of this analysis help to design these novel storage systems.

Keywords: thermal energy storage; steam accumulator; phase change material

#### 1 Introduction

Industrial process heat applications have been identified as a promising new area of application for thermal energy storage systems. Storage systems improve the efficiency by the reuse of energy in cyclic processes. The bulk of process heat applications require steam at pressures between 1 and 20 bar with corresponding saturation temperatures between 100°C and 210°C. While the application of phase change materials (PCMs) is straightforward for isothermal energy storage, no commercial system is available in this temperature range today.

Modelica is used to analyse different kinds of steam storage systems for applications in power plants and process industry. The analysis includes varying pressure steam accumulators, which are state of the art, and a novel kind of steam accumulator with a phase change material (PCM). For the various storage systems physical models are implemented in Modelica.

#### 2 Steam accumulator

Due to increasing costs for fossil energy, systems for thermal energy storage have become attractive for process heat applications. Especially in cyclic processes, energy storage systems offer an additional option for efficient energy usage. An example for such a cyclic process is the production of gas concrete. Here the produced stones are hardened under a steam atmosphere in an autoclave. During a hardening cycle, the pressure in the autoclave is raised to 15 bar for several hours. Between two production cycles, the steam is partially stored in varying-pressure accumulators (Figure 1), so called Ruths steam accumulators, which represent the current state-of-the-art technology in medium temperature thermal energy storage.

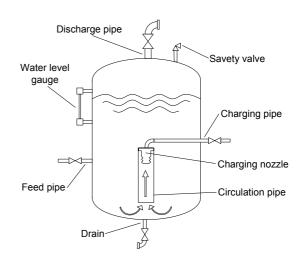


Figure 1: Varying pressure accumulator [1]

Varying-pressure accumulators use hot pressurised water as storage medium. Liquid and gas phases are in thermodynamic equilibrium. During the discharge process, the systems provides saturated steam at decreasing pressure.

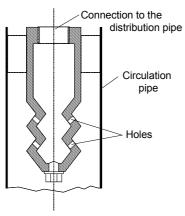


Figure 2: Charging nozzle with circulation pipe [1]

During the charging process, steam is blown into the liquid contained in the accumulator. The incoming steam bubbles condense in the liquid or pass into the steam space, depending on the thermodynamic equilibrium in the vessel. The bubbles which rise to the steam space increase the pressure and lead to a higher saturation temperature, so that the next bubble might condense. To use the entire storage content, the charging process requires circulation. Ruths invented a method that consists of nozzles (Figure 2) which turn the flow of steam upwards. The nozzles are surrounded by a circulation pipe, wherein the water flows upwards. The minimum temperature loss is composed of the difference between the steam space and the uppermost liquid layer as well as the difference between the saturation temperatures due to the additional pressure of the water at lower depths. Depending on the accumulator pressure and the steam intake, there is a certain depth for the nozzles which minimizes the overall temperature loss. [1]

### 3 MultiPhase Media Library

The Modelica.Media package provides a standardized interface to fluid media models and specific media models based on this interface. For the handling of multiphase applications, a general media package was developed based on the Modelica.Media package. An additional properties record called MultiPhasePropertiesRecord is used in the BaseProperties model to provide the thermodynamic properties of the different phases to the models using the Modelica.Media package.

```
replaceable record MultiPhasePropertiesRecord
  extends Modelica.Icons.Record;
  MassFraction x[nPhase];
  SpecificVolume v[nPhase];
  MassFraction[nPhase, nX] X;
  MassFraction[nPhase, nXi] Xi;
  SpecificEnthalpy h[nPhase];
  SpecificInternalEnergy u[nPhase];
  SpecificHeatCapacity R[nPhase];
  MolarMass MM[nPhase];
end MultiPhasePropertiesRecord;
```

In this record, the thermodynamic properties of the different phases of the medium are included. Compared to the **BasePropertiesRecord**, as defined in the **PartialMedium** package of the **Modelica.Media** library, the mass fraction of the different phases is added and the specific volume is used instead of the density. The **PartialMultiPhaseMedium** package extends the **PartialMedium** package of the **Modelica.Media** library. The **BaseProperties** model in the **PartialMultiPhaseMedium** package is extended in the following way.

```
redeclare replaceable partial model extends Base-
Properties
    "Base properties (p, d, T, h, u, R, MM and,
if applicable, X) of a medium"
  MultiPhasePropertiesRecord MultiPhase;
equation
d = 1/(MultiPhase.v*MultiPhase.x);
for i in 1:nX loop
  X[i] = MultiPhase.X[:, i] *MultiPhase.x;
end for;
for i in 1:nXi loop
  Xi[i] = MultiPhase.Xi[:, i] *MultiPhase.x;
end for:
h = MultiPhase.h*MultiPhase.x;
u = MultiPhase.u*MultiPhase.x;
R = MultiPhase.R*MultiPhase.x;
MM = MultiPhase.MM*MultiPhase.x;
end BaseProperties;
```

It is possible to use the **MultiPhase** medium models with single phase models. The required base properties are calculated as a mixture of the different phases.

#### 4 Downflow model

For the analysis of steam accumulators, a vertical discretisation of the storage vessel is elemental. Based on the **Modelica.Fluid** library, models for the simulation of multiphase flows are developed. The drainage and flooding of vessels can be reproduced as well as the vertical stacking of control volumes.

Between two volume elements stacked one above the other, two kinds of mass exchange mechanisms are identified. One type of mass exchange results from the pressure difference between these two elements and the other mass exchange occurs due to downflowing water and upflowing steam caused by the density difference of these two phases. The mass flow of the downflowing water is calculated in the following way:

The mass flow of the upflowing steam is not calculated separately. This mass transport mechanism is covered by the mass transport due to the pressure difference. The required volume fraction, y, can be calculated from the **MultiPhase Modelica.Media** models in the following way:

```
y = medium.MultiPhase.v[nPhase] *
    medium_u.MultiPhase.x[nPhase] '
    medium u.d;
```

#### 5 Simulation steam accumulator

In Figure 3 the simulation models for a Ruths accumulator and a single control volume are shown. They are connected to an ambience model by a control valve, an enthalpy flow rate sensor and a MultiPhase flange which ensures that only vapour is leaving the volumes. The enthalpy flow rate is integrated over time. The steam accumulator is dicretised in the vertical direction into control volumes. The water vapour exchange between the volume elements is calculated with the downflow model as presented in section 4.

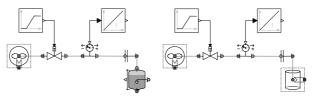
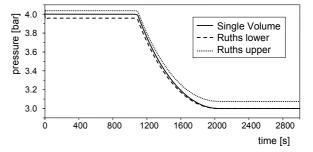


Figure 3: simulation models for Ruths accumulator and single control volume

The ambience model is initialized with a pressure of 3 bar. The volumes of the pressure vessel are initialized with a pressure of 4 bar and an enthalpy of 610 kJ / kg. The height of the pressure vessel is 3 m and the diameter is 1 m. The pressure vessel is filled up to 50 percent with water. The single control volume and steam accumulator model have the same dimensions. In the beginning, the control valve is closed. After 1000 seconds it is opened.

In Figure 4 the simulation results are presented. In the beginning the water is flowing down in the stacked volumes of the Ruths accumulator.



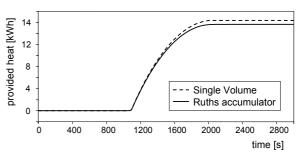


Figure 4: simulation results of pressure and provided heat for Ruths accumulator and single control volume

Because of the static pressure of the water column, the pressure in the lower volume element is increasing and the pressure in upper volume element is decreasing. After 1000 seconds, the control valve is opened and the pressure vessels are discharged to the ambience model. The pressure in the single control volume and in the upper volume of the Ruths accumulator is lowered to 3 bar. The pressure in the lower volume element of the Ruths accumulator re-

mains above 3 bar due to the static pressure. More heat is provided by the single control volume compared to the stacked volumes. The reason for this is the higher pressure in the lower volume elements of the Ruths accumulator which matches the real behavior of the varying-pressure accumulator.

#### 6 Phase change materials (PCM)

Isothermal energy storage increases the storage efficiency. This can be achieved by using a PCM as storage material. Due to the latent heat of melting thermal energy can be stored in a very small temperature range.

#### 6.1 Materials

For the temperature range of interest, various materials can be used as PCMs. Examples of inorganic materials are technical salts and eutectic mixtures of these salts such as: lithium nitrate (LiNO3), lithium chloride (LiCl), potassium nitrate (KNO3), potassium nitrite (KNO2), sodium nitrate (NaNO3), sodium nitrite (NaNO2) and calcium nitrate (Ca(NO3)2). In the group of organic PCMs an interesting material is Pentaerythritol. It undergoes a solid-solid transition at 189°C with an enthalpy of 269 kJ/kg [Benson, 1985]. The melting point of this plastic crystal is about 50 Kelvin above the solid-solid transition temperature.

#### 6.2 Calculation of enthalpy

Three ways to calculate the enthalpy in the **Modelica.Media** models are compared. The first method is the linear interpolation using If-, Elseif- and Elseclauses, the second method is the usage of the arc tangent function and the third method is the usage of the error function. Using the arc tangent method no If-clauses are needed. The arc tangent function can be calculated by series expansion as provided by Euler in the following way:

$$\arctan x = \frac{x}{1+x^2} + \frac{2}{3} \cdot \frac{x^3}{\left(1+x^2\right)^2} + \frac{2 \cdot 4}{3 \cdot 5} \cdot \frac{x^5}{\left(1+x^2\right)^3} + \dots$$

The error function is calculated according to W J Cody [3] as an approximation. In this implementation different approximations are combined by Ifclauses.

#### Linear interpolation method

The heat capacity in the liquid and in the solid state is assumed to be constant and increases from the onset temperature of phase change to a maximum at the transition temperature followed by a decrease until the constant value of the liquid state is reached at the final phase change temperature. In Figure 5 heat capacity and enthalpy are plotted against the temperature.

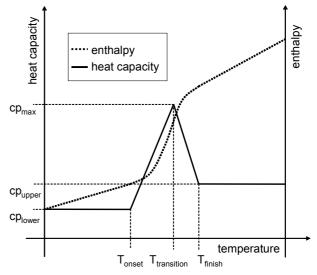


Figure 5: heat capacity and enthalpy plotted against temperature for the linear interpolation method

The latent heat of melting can be calculated in the following way:

$$\begin{split} &h_{trans} = c_{p,low} \cdot \left(T_{trans} - T_{ons}\right) + c_{p,up} \cdot \left(T_{fin} - T_{trans}\right) \\ &+ 0.5 \cdot \left(T_{trans} - T_{ons}\right) \cdot \left(c_{p,max} - c_{p,low}\right) \\ &+ 0.5 \cdot \left(T_{fin} - T_{trans}\right) \cdot \left(c_{p,max} - c_{p,up}\right) \\ &- c_{p,low} \cdot \left(T_{fin} - T_{ons}\right) - 0.5 \cdot \left(c_{p,up} - c_{p,low}\right) \cdot \left(T_{fin} - T_{ons}\right) \end{split}$$

If the transition temperature, the onset temperature of phase change, the final temperature of phase change, the heat capacity in the liquid state, the heat capacity in the solid state and the latent heat of melting are known, the maximum heat capacity can be calculated from the latent heat of melting.

$$\begin{split} c_{p,max} &= \frac{2 \cdot h_{trans} - c_{p,low} \cdot \left(T_{trans} - T_{ons}\right) - c_{p,up} \cdot \left(T_{fin} - T_{trans}\right)}{T_{fin} - T_{ons}} \\ &+ c_{p,low} + c_{p,up} \end{split}$$

The calculation of the enthalpy in the **Modelica.Media** package is implemented with if, elseif and else clauses in the following way:

```
if noEvent(T < T_{onset}) then
  h = c_{p,lower}*(T - T0);
elseif noEvent(T > T_{finish}) then
  h = c_{p,lower} * (T_{onset} - T0) + h_{transition} + c_{p,upper} * (T - T_{finish});
else
  if noEvent(T < T_{transition}) then
      h = c_{p,lower} * (T_{onset} - T0) + c_{p,lower} *
           (T - T_{onset}) + 0.5*(c_{p,max} - c_{p,lower})*
           (T - T_{onset})^2/(T_{transition} - T_{onset});
      h = c_{p,lower} * (T_{onset} - T0) + c_{p,lower} *
           (T_{transition}-T_{onset})+0.5*(C_{p,max}-C_{p,lower})*
           (T<sub>transition</sub>-T<sub>onset</sub>)+C<sub>p,max</sub>* (T-T<sub>transition</sub>)-0.5*
           (Cp,max - Cp,upper) * (T-Ttransition) ^2/
           (Tfinish-Ttransition);
   end if;
end if;
```

#### Arc tangent method

The arc tangent function is used to reproduce the behavior of the PCM's enthalpy at the melting point.

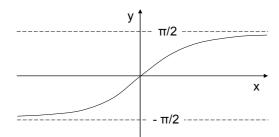


Figure 6: arc tangent curve

For the calculation of the enthalpy curve the arc tangent function is standardized to one and moved in y direction by 0.5 and in the x direction by the melting temperature,  $T_{transition}$ . The resulting curve is multiplied with the latent heat of melting,  $h_{transition}$ . The sensible heat,  $c_p^*$ , is added in the second term. The melting range coefficient,  $C_{MR}$ , is used to adjust the width of the melting range.

$$\begin{split} h &= h_{transition} \cdot \left[ \frac{arctan(\!\left(T - T_{transition}\right) \cdot C_{MR}\right)}{\pi} + 0.5 \right] \\ &+ c_{_{D}} * \cdot \! \left(T - T_{_{0}}\right) \end{split}$$

The effective heat capacity is calculated by differentiating the enthalpy function.

$$c_p = \frac{h_{transition}}{\pi \cdot (((T - T_{transition}) \cdot C_{MR})^2 + 1)} + c_p *$$

In Figure 7 enthalpy and heat capacity calculated with the arc tangent method are plotted against temperature. The thermodynamic properties of an eutectic mixture of potassium nitrate, sodium nitrate and sodium nitrite are used. The latent heat of melting, h<sub>transition</sub>, is 83 kJ/kg, the melting temperature ,T<sub>transition</sub>, is 415 Kelvin, the heat capacity ,cp, is 1.5 kJ/(kg K) and the reference temperature ,T<sub>0</sub>,is 273 Kelvin. The melting range coefficient ,C<sub>MR</sub>,is 2.

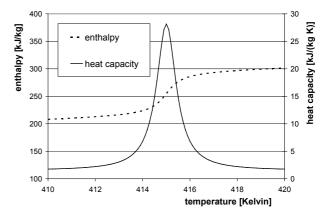


Figure 7: enthalpy and heat capacity calculated with the arc tangent method plotted against temperature

#### Error function method

The Gauss error distribution curve is used to reproduce the behavior of the heat capacity of the PCM at the melting point.

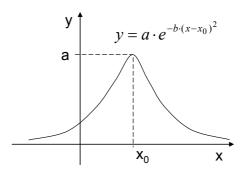


Figure 8: Gauss error distribution curve

For the calculation of the heat capacity curve the coefficients of the Gauss error distribution curve are adapted. The coefficient a is the maximum heat capacity,  $c_{p,max}$ , at the melting temperature,  $x_0$  is the melting temperature  $T_{transition}$  and b is the melting range coefficient,  $C_{MR}$ , which is used to adjust the width of the melting range. The sensible heat,  $c_p^*$ , is added in the second term.

$$\mathbf{c}_{\mathrm{p}} = \mathbf{c}_{\mathrm{p}_{\mathrm{max}}} \cdot \exp[-\mathbf{C}_{\mathrm{MR}} \cdot (\mathbf{T} - \mathbf{T}_{\mathrm{transition}})] + c_{p}^{-*}$$

The enthalpy is calculated by integrating the heat capacity function.

$$h = h_{transition} \cdot \frac{erf\left[\sqrt{C_{MR}} \cdot \left(T - T_{transition}\right)\right] + 1}{2} + c_p * \cdot \left(T - T_0\right)$$

The error function is implemented according to W J Cody [3]. The heat capacity  $c_{p,max}$  in the melting point can be found with the following equation.

$$cp_{max} = h_{transition} \cdot \sqrt{\frac{C_{MR}}{\pi}}$$

In Figure 8 the enthalpy and the heat capacity calculated with the error function method are plotted against temperature. The thermodynamic properties of the eutectic salt mixture, as presented in the arc tangent method, are used. The melting range coefficient  $C_{MR}$  is 1.

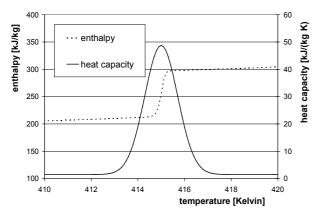


Figure 8: enthalpy and heat capacity calculated with the error function method plotted against temperature

#### Comparsion enthalpy methods

For the comparison of the three suggested methods the thermal behaviour of a cylinder of PCM is simulated. The cylinder is discretised into 100 radial layers. The inner diameter is 1cm and the outer diameter is 2cm. The prescribed temperature at the inner side of the cylinder is switched between 440 and 400 Kelvin every 1000 seconds. Again the thermodynamic properties of the eutectic salt mixture, as presented in the arc tangent method, are used. The resulting temperature profile is plotted in Figure 9. Volume 1 is the PCM layer at the inner side of the tube and Volume 100 is the PCM layer at the outer side of the tube.

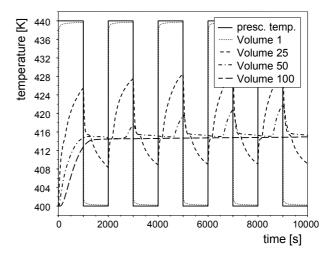


Figure 9: temperature profile of radial discretised cylinder

The results of simulation time of the three methods to calculate the enthalpy of the PCM are presented in the following table:

	Arc tangent	Linear interpol.	Error function
CPU-time for integration [s]	40,7	179	1250
CPU-time for one GRID interval [ms]	81,4	358	2500
Number of (successful) steps	197444	28846	25471

The arc tangent method is 4.5 times faster than the linear interpolation method and more than 30 times faster than the error function method.

# 7 Simulation PCM enhanced steam accumulator

A concept to increase the energy efficiency of an existing varying-pressure steam accumulator is to connect a tube register with externally arranged PCM to the pressure vessel (Figure 10). A pump assures the circulation between the tube register and pressure vessel. The charging and discharging operations are the same as for a varying pressure accumulator, as presented in section 2. With the PCM the capacity of the storage system can be increased. The same amount of thermal energy can now be stored in a smaller temperature range. The heat transport inside of the PCM is a limiting factor to the power of the storage system.

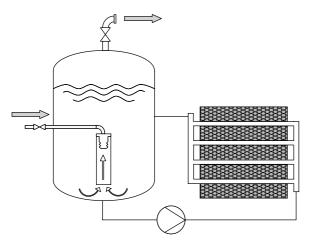


Figure 10: PCM enhanced steam accumulator

In Figure 11 the model of the PCM enhanced steam accumulator is shown as it is implemented in Modelica. The ambience model is initialized with a pressure of 3 bar. The volumes of the pressure vessel are initialized with a pressure of 4 bar and an enthalpy of 610 kJ / kg. The height of the pressure vessel is 3 m and the diameter is 1 m. The pressure vessel is filled up to 50 percent with water. The inner diameter of the 10 tubes connected to the pressure vessel is 20 mm and the outer diameter is 25 mm. The outer diameter of the PCM layer is 100 mm. The tubes have a length of 5 meter. The thermodynamic properties of the eutectic salt mixture, as presented in section 6.2, are used. The temperature of the PCM is initialized to 416 Kelvin. This means that the PCM is completely molten.

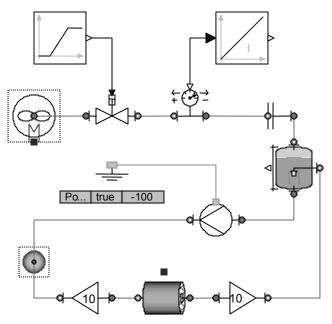


Figure 11: simulation model PCM enhanced steam accumulator

In the beginning, the control valve is closed. After 1000 seconds it is opened and the storage vessel is discharged. The pump is switched on all the time.

In Figure 12 simulation results of pressure and provided heat are plotted against time. The pressure in the upper part of the storage vessel is decreasing after the control valve is opened to 3 bar. The provided heat is higher compared to the simulation results of the varying-pressure accumulator in section 5.

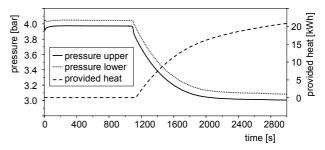


Figure 12: simulation results of pressure and provided heat for the PCM enhanced steam accumulator

In Figure 13 the temperature in the lower part of the storage vessel and in the PCM layer around the tubes is plotted against time. Only parts of the PCM are solidified after 2000 seconds of discharging. The melting temperature is 415 Kelvin.

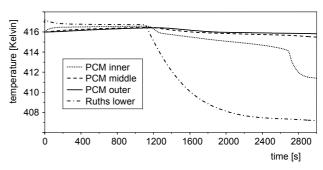


Figure 13: simulation results of the temperature in the lower control volume of the pressure vessel and the temperatures in the PCM cylinders around the tube register

#### 8 Conclusions

With the simulation models presented in this work, PCM steam storage concepts can be analyzed. Simulation results of a PCM steam accumulator with a tube register and externally arranged PCM are presented. In the next step, different simulation models will be developed for comparison. These simulation models will focus on using macro-encapsulation of

the storage material, composite materials and the integration of layers made of materials showing a high thermal conductivity to increase the power of the storage system. Further validation of the models will be done using laboratory scale experiments. Using a tube register with externally arranged PCM, the number of tubes and their distance has to be defined, depending on the steam process the accumulator is integrated into. The aim of the work is to provide a dimensioning tool that enables to design the thermal behavior of the steam accumulator.

#### References

- [1] Goldstern, Walter Steam storage installations. Springer-Verlag OHG, Berling / Göttingen / Heidelberg, 1970.
- [2] Steinmann, W.D., Buschle, J. Analysis of thermal storage systems using Modelica. Proceedings of the 4th International Modelica Conference, Hamburg, March 7-8, pp 331-337, 2005.
- [3] Cody, W. J. Rational Chebyshev approximations for the error function, Mathematics of Computation, pages 631-638, 1969.
- [4] Benson, D.K., Burrows, R.W., Webb, J.D. Solid state phase transitions in Pentaerythritol and related polyhydric alcohols. Solar Energy Materials 13, pp 133-152, 1985.