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Modeling and Simulation of Refrigeration Systems with the Natural Refrigerant CO_2

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Abstract

This papers presents the current results of the development of a Modelica™ library for CO_2-Refrigeration systems based on the free Modelica library ThermoFluid.
The development of the library is carried out in a research project of EADS Airbus and the TUHH and is focused on the aim to get a library for detailed numerical investigations of refrigeration systems with the rediscovered, natural refrigerant carbon dioxid (CO_2).
A survey of the CO_2-Library is given and the modeling of CO_2-Heat exchangers is described in detail. A comparison with steady state results of heat exchangers is presented and results of a transient simulation run are discussed with respect to plausibility.

1 Introduction

The fact of climate changes due to ozone depletion and globale warming has been directed to significant research activities on the field of refrigeration and air-conditioning since the 1990s [7]. The objective of the investigations may yield to a long-term solution. Therefore so called natural, resp. alternative refrigerants with no Ozone Depleting Potential (ODP) and no or a very low Global Warming Potentail (GWP) are investigated and new technical developments are driven. Carbon dioxid (CO_2, R 744) as a natural refrigerant was rediscovered and has recently a very high potential to substitute currently used refrigerants in the area of mobile/automotive air-conditioning and refrigeration. This development is caused by the excellent thermodynamic, transport and environmental properties of CO_2. Due to the critical data of CO_2 the process must be realized as a transcritical cycle, which requires special control strategies.
In order to obtain a better understanding of the complex thermodynamic and hydraulic behaviour of CO_2-Refrigeration processes under steady and dynamic boundary conditions the modeling of components of a CO_2-System has been realized. A CO_2-Model library in Modelica™ was built up by using base classes of the free Modelica library ThermoFluid [14]. The scope of the CO_2-Library is the modeling of the system behaviour by consideration of the most important physical effects like compressible flow, heat transfer, pressure drop, large capacities and time delays.
The development of a CO_2-Library is carried out in a research project of European Aeronautic Defence and Space Company (EADS) Airbus and the Department of Technical Thermodynamics of the Technical University Hamburg–Harburg (TUHH). The main objective of the project is a proof of concept of a CO_2 based integrated cooling system on board of future airliners. For this purpose numerical and experimental investigations are in progress.

2 Carbon dioxid as refrigerant

Carbon dioxid was used as a refrigerant until the 1930s, but was then replaced by the synthetical refrigerants (HCFCs) that offered lower absolute pressures, simpler techniques and higher efficiencies in conventional vapor compression cycle. Due to the ODP and the GWP of the synthetical refrigerants substantial research activities on the field of refrigerants are initiated since the 1990s. Recent research on carbon dioxid is pushed for mobile, resp. automotive air-conditioning and refrigeration and has focused on the development of a transcritical cycle [2]. Figure 1 illustrates the GWP for the three refrigerants R 12, R 134a and CO_2; the use of R 12 is forbidden in europe since the be-

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ginning of 1990s. The refrigerant R 134a today is the most common refrigerant in mobile and automotive air-conditioning systems.

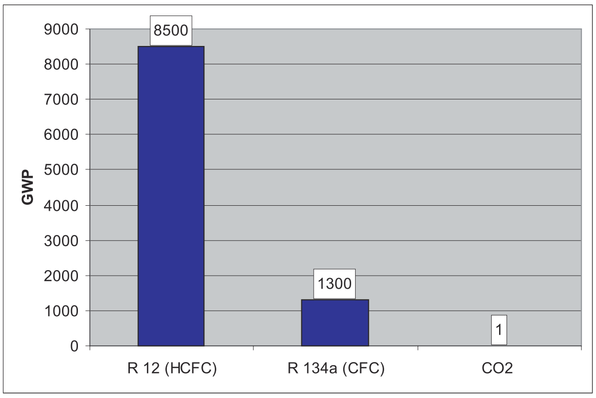

Figure 1: GWP of three different kind of refrigerants; GWP is standarised to 1 for CO_2

2.1 CO_2-Refrigeration cycle

The temperature and pressure at the critical point of CO_2 are 304,13 K and 73,77 bar. Therefore, the refrigerant cycle has to be operated transcritically when the ambient temperature is near or higher than the critical temperature. In this case the evaporation takes place at subcritical pressure and temperature and the heat rejection at supercritical state. At the supercritical status area pressure and temperature are not coupled anymore; so a CO_2-System has one more degree of freedom than conventional vapour compression cycles.

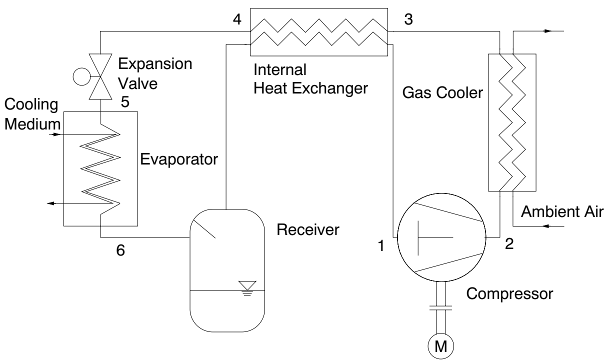

Figure 2: Schematic diagram of a CO_2-Refrigeration cycle

As shown in figure 2, the main components of a CO_2-Refrigeration cycle are compressor, gas cooler (instead of a condenser because of the supercritical heat rejection, that occurs sometimes), internal heat exchanger, expansion valve, evaporator and low-pressure receiver. The process path of a transcritical CO_2-Cycle is shown in figure 3. The path represented by **1-2-3-4-5-6** shows compression (1-2), isobaric heat rejection at gas cooler (2-3), isobaric cooling in the internal heat exchanger (3-4), adiabatic expansion (4-5), isobaric evaporation (5-6) and isobaric superheating at internal heat exchanger (6-1). In steady state the low-pressure receiver has no influence of the process. For more detailed explanation of the CO_2-Cycle see [6], [5].

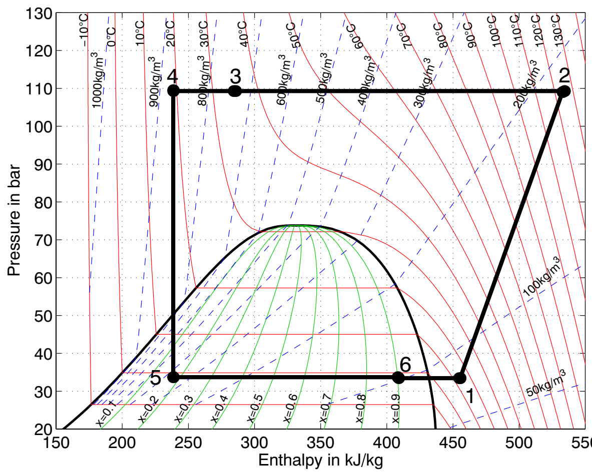

Figure 3: *p,h*-Diagram with states of a CO_2-Refrigeration cycle

3 CO_2-Library

The aim of the modeling is to create a library with physical based models of the above mentioned components. Such a library with models of these components and of additional components for testing, like sinks and sources, can be used for investigations of both, single components and complete refrigeration cycles. Furthermore it is of great interest to make dynamic simulation as well as steady state simulation of CO_2-Systems and single components, especially heat exchanger. Up to now, there is no commercial or free available simulation tool enabling dynamic and steady state simulation of CO_2-Cycle and -Components with only physical based models. There are some tools for steady state simulation but they need measured characteristics of the heat exchangers as an input.
The numerical investigation of heat exchanger components is of particular interest to find optimized heat exchangers for limited space. On the other hand the

concept of connectors in Modelica provides the opportunity using the same heat exchanger models for single component simulation as well as for a complex cycle simulation.

There are different backgrounds for modeling and simulation of complex, closed CO_2-Refrigeration cycles. The first aim is a better understanding of the complex, coupled thermodynamic, fluidmechanic and heat transfer effects in a transcritical operating CO_2-System. Here the influence of some typical system parameters like compressor speed, heat exchanger and receiver geometry and refrigerant filling can be tested. Furthermore aspects of the control of the system should be investigated. Finally, the library is used for simulation and evaluating of different system design in various applications.

The library is based on free Modelica library ThermoFluid. The ThermoFluid library, especially the base classes and partial components, is in regard to the implementation of the three balance equations (energy, mass, momentum) and the method of discretization (finite volume) very well suited for modeling of CO_2-Systems. In cooperation with the developers of ThermoFluid a high accuracy medium model for CO_2 based on an equation of state was implemented for the whole fluid region [9].

3.1 Survey of CO_2-Library

So far, the following models and classes have been implemented:

- **Heat transfer and pressure loss relations for the whole fluid region:**
  This constitutive equations are used for the calculation of heat flux and pressure drop due to friction, which are added to the balance equations of energy and momentum [10], [11].

- **Models for the air side of heat exchangers:**
  The balance equation of energy is implemented by the finite volume method [8]; well suited heat transfer correlations for the air side have been implemented [4].

- **Pipes and heat exchangers:**
  Based on the medium model, classes of ThermoFluid, the heat transfer and pessure drop correlations and the air side models pipes and heat exchangers have been modelled. The pipes are modelled with discretized parameters.

- **Compressor:**
  The model is made for a reciprocating compressor. Therefore, the mass flow is calculated by the general equation of a reciprocating compressor and enthalpy change is calculated according to the isentropic efficiency. The compressor is modelled with lumped parameters.

- **Expansion valve:**
  The throttling process is treated as isenthalpic and the pressure drop is calculated according to the flow coefficient of the valve [1]. The flow coefficient results by the specific valve contruction and the opening ratio of the valve. Therefore, the flow characteristic of the valve has to be known and the model has to be parameterized with the corresponding values. For the valve model lumped parameters are used.

- **Receiver:**
  Up to now, a simple receiver model is implemented. The model seperates the incoming two phase flow into its vapour and liquid phase. As long as the liquid level of the receiver is lower than the outlet height saturated vapour leaves; if the liquid level reaches the outlet height a two phase flow leaves up to a height only liquid leaves. Due to the sophesticated construction of CO_2-Receivers in most of the operating modes a two phase flow leaves the receiver even if the liquid level is much lower the outlet height. It seems to be not easy to model this components with physical correlations; so the modelling is in progress.

- **Flow splits and junctions:**
  For this models classes of ThermoFluid are used; for the pressure drop in the momentum equation special correlations for splits and junctions have been implemented taking the ratio of mass flow into account [3]. The change of mass flow direction is taken under account in the implementation.

4 Examples of Modeling

4.1 Modeling of heat exchangers

So far, available heat exchangers for CO_2-Refrigeration systems are compact prototype components from the automotive application, see figure 4. The heat exchangers are built up as follows: The CO_2-Flow is splitted in different streams through so called Flat-Tubes (or Multiport-Micro-Tubes), see figure 5. The Flat-Tubes consists of a number of parallel bores in which the CO_2 flows. The refrigerant is splitted and collected at the feeder and manifold of the heat exchangers. Outside the heat exchanger air passes over slitted fins enhancing the air side heat transfer area and heat transfer coefficient, see figure 6.

Figure 4: CO_2-Gas cooler

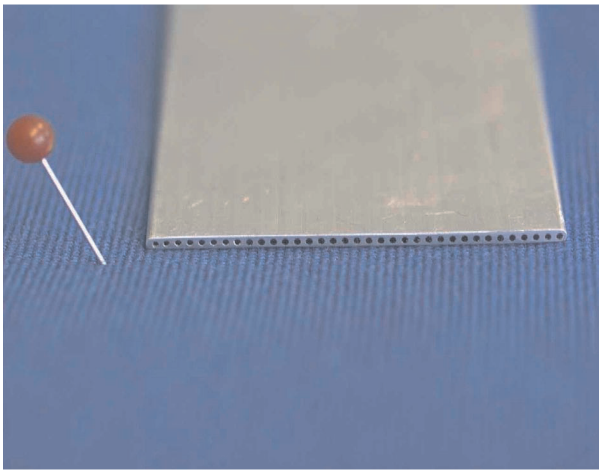

Figure 5: Cross section of a Flat-Tube

In a heat exchanger different flow pathes for the CO_2 are possible; usually gas coolers are constructed as crossflow and evaporators are built up as cross-counterflow heat exchangers. In figure 7 the schematic flow path of CO_2 through a crossflow heat exchanger is shown; e.g. here the CO_2has three transits through the heat exchanger. At every transit the CO_2-Flow is splitted in a number of parallel Flat-Tubes, the bores of every Flat-Tube are flowed through concurrent.

For the modeling of the CO_2-Flow a homogenous distribution of the flow is supposed. By this assumption the flow is modelled by one single pipe. The

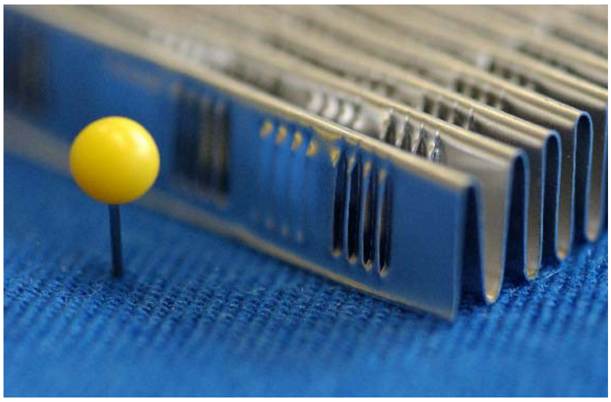

Figure 6: Slitted fins

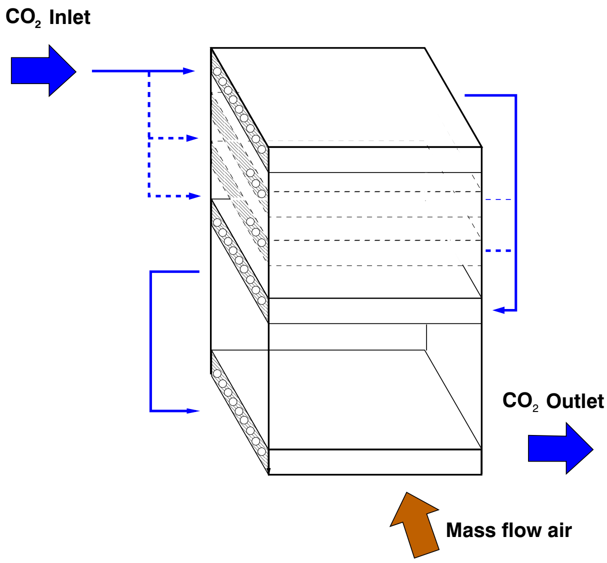

Figure 7: Flow path through a cross flow heat exchanger

heat transfer area and the flow cross section are determined by the geometry and the number of all concurrent flowed pipes; whereas the heat transfer coefficient and the pressure loss is calculated with the mass flow rate and the geometry of a single bore.

The assumption of homogenous mass flow and temperature distribution is also made for the air side. Therefore, it is possible to model the air flow through one air channel. In the modeling can be assumed that the slitted fins and the Flat-Tubes create a triangular channel, see figure 6. So the total mass flow of air is scaled down to the mass flow through one channel by division through the total number of air channels of the heat exchanger. At the air side only the energy balance equation is implemented by the finite volume method. The medium properties are introduced by polynomi-

nales fitting the properties well in the temperature intervall of 253.15 K to 342.15 K. Because the air side heat transfer is much lower than on the refrigerant side, a detailed physical model based on characteristic numbers and geometry parameters and validated on experimental investigation has been found by a literature review and is implemented [4].
The wall model is taken from the ThermoFluid library. It is modeled as a capacitive, cylindric wall.
This specific models of CO_2-Pipe, wall and air have to be connected in the right way to get a reasonable model of a heat exchanger. For the connection the heat connectors of ThermoFluid can be used; the conneting variables are temperature and heat flux. The implementation, especially the connection is as follows: First the same number of air channel objects is created like the dicscretization number of the pipe and wall. The air channel model itself can be discretized in air flow direction with another number. At the connection to the air side the calculation of the heat flux for one single air channel has to be taken into consideration. Therefore it has to be scaled up by a factor of the numbers of total air channels and the discretization number. In the modeling a class is programmed where the air channel objects are declared and where the scaling is programmed. Furthermore, every air channel object is connected with the wall temperature of the equivalent, discretized wall element. So every volume of a discretized air channel gets the same wall surface temperature. The following code example shows this implementation; here *geoHX.pipe_n* means the discretization of pipe and wall and *geoHX.AC* means the discretization of air flow:

```
model AirChannelDCrossFlow
    ....
    Co2Flow.Air.DiscAirChannelDDry
    AirChannels[geoHX.pipe_n] ;
    ThermoFluid.Interfaces.HeatTransfer.HeatFlowD
    AirHT(n=geoHX.pipe_n) "Heat connector";
equation
    for ac in 1:geoHX.pipe_n loop
        for i in 1:geoHX.AC_n loop
            AirChannels[ac].T_W[i] = AirHT.T[ac];
\\ Air surface temp. connected
\\ with heat connector
        end for;
      ...
      AirHT.q[ac] = AirChannels[ac].Q_dot_total*
               geoHX.total_channels/geoHX.pipe_n;
      \\ Heat flow at the connector is scaled
    end for;
     ....
end AirChannelDCrossFlow;
```

A schematic illustration of the modeling idea and the connections is shown in figure 8. The implementation of a heat exchanger in Modelica is shown in figure 9 as the graphical representation in the modeling and simulation tool Dymola™.
The implementation of a cross counter heat exchanger can be realized now easily. Only the connections of temperature and heat flow have to change in the class *AirChannelDCrossFlow* in a specific way.

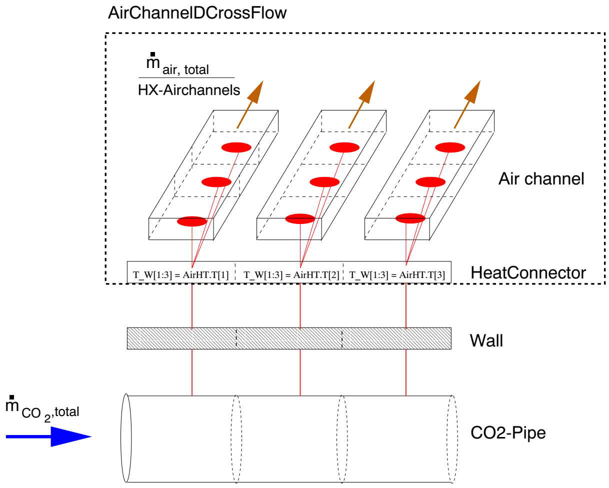

Figure 8: Schematic illustration of the modeling of heat exchangers

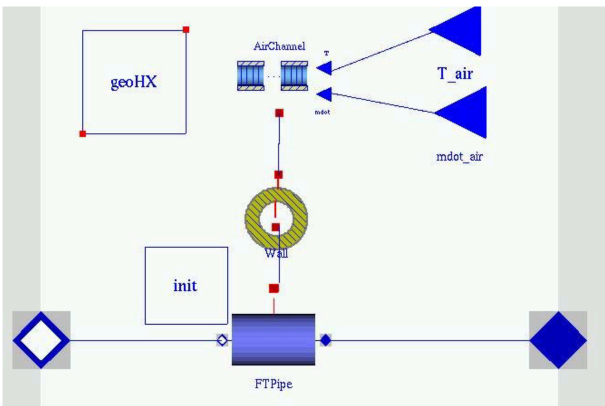

Figure 9: Graphical representation of the heat exchanger model

4.1.1 Comparison of steady state simulation and measurement

With these models simulations in a test configuration have been run. The test configuration consists of a source providing pressure and enthalpy at the heat exchanger inlet and a mass flow sink generating a defined mass flow at the outlet. The source and sink are used to set the boundary conditions resulting from the measured data at the component.

The following comparison is made for a crossflow gas cooler and cross-counter flow evaporator from the CO_2-Experimental system built up at the Department of Aircraft Systems Engineering of the TUHH. The geometry parameters of the components are known. In the tables 1 and 2 the measured data and the results of the simulations at the point of steady state are shown.

The comparison of experimental data and simulation results shows a very good correspondence, especially if you take under account that the printed experimental data are taken as is. The tolerance of the sensors has not been taken into account, yet.

Table 1: Comparison of measured data at a gas cooler with simulation results in steady state

Boundary conditions from measured data					
$\dot{m}_{air}$	$\dot{m}_{CO2}$	$\bar{p}_{CO2}$	$T_{CO2,in}$	$h_{CO2,in}$	$T_{air,in}$
[kg/s]	[kg/s]	[bar]	[K]	[kJ/kg]	[K]
0,605	0,013	96,0	395,4	538,5	308,9
0,593	0,032	87,5	355,0	487,2	312,9
0,598	0,036	88,3	373,4	513,8	312,9
Measured data			Simulation		
$T_{CO2,out}$	$T_{air,out}$	$\dot{Q}_{CO2}$	$T_{CO2,out}$	$T_{air,out}$	$\dot{Q}_{CO2}$
[K]	[K]	[kW]	[K]	[K]	[kW]
309,5	315,7	-3,02	312,7	313,5	-2,85
314,7	320,2	-3,45	316,2	318,0	-3,14
315,3	323,3	-4,99	317,4	320,0	-4,37

Table 2: Comparison of measured data at an evaporator with simulation results in steady state

Boundary conditions from measured data					
$\dot{m}_{air}$	$\dot{m}_{CO2}$	$\bar{p}_{CO2}$	$T_{CO2,in}$	$h_{CO2,in}$	$T_{air,in}$
[kg/s]	[kg/s]	[bar]	[K]	[kJ/kg]	[K]
0,21	0,032	49,1	286,7	295,3	301,6
0,21	0,036	40,3	278,7	281,3	294,7
0,21	0,013	34,6	272,9	222,1	285,2
Measured data			Simulation		
$h_{CO2,out}$	$T_{air,out}$	$\dot{Q}_{air}$	$h_{CO2,out}$	$T_{air,out}$	$\dot{Q}_{CO2}$
[kJ/kg]	[K]	[kW]	[kJ/kg]	[K]	[kW]
372,8	289,85	-2,48	374,8	289,6	2,54
357,4	281,95	-2,74	357,4	282,0	2,75
378,2	277,65	-2,03	380,3	275,6	2,04

4.2 Implementation of constitutive equations

In order to obtain a most physical modeling of CO_2 flow through pipes and any kind of heat exchangers constitutive equations for pressure drop and heat transfer for the whole fluid region are implemented according to [11], [10]. A comparison of implemented relations with experimental data from the SINTEF [12] shows a good correspondence [13]. The pressure drop and heat transfer correlations are empirical equations which only are exactly valid for steady state. Due to the fact that such correlations for dynamic state are not available it seems to be the best and a very common method for describing these effects in a dynamic simulation.

The correlations have been implemented with regard to numerical robustness and simulation time. At the foldover between laminar and turbulent flow the describing empirical equations of heat transfer and pressure drop have no steady transition. By avoiding event iterations in this case a function for the smooth transition has been implemented. The unsteady transition of the pressure drop coefficient at a Reynolds number of *2300* is shown in figure 10 with a solid line. The dashed line between Reynolds numbers of *2000* and *3000* shows the run of the interpolated pressure drop coefficient. The interpolation function fullfills the following requirments:

- The gradient inbetween the limits of validity is always smaller than infinity.
- The gradient near the limits of the intervall is nearly zero.
- Exactly at the limits of validity the interpolation function calculates the exact value of the current function.

The interpolation function is implemented by using the *tanh*- and the *tan*-function as follows:

```
function Stepsmoother
//Interpolationsfunction to avoid event iterations
   input Real func;
//value, where function value becomes 100%
   input Real nofunc;
//value, where function value becomes 0%
   input Real x;
//Variable generating the event
   output Real result;
protected
   Real m;
   Real b;
algorithm
    m := Pi/(func - nofunc);
```

```
    b := -Pi/2 - m*nofunc;
    result := (tanh(tan(m*x + b)) + 1)/2;
  end Stepsmoother;
```

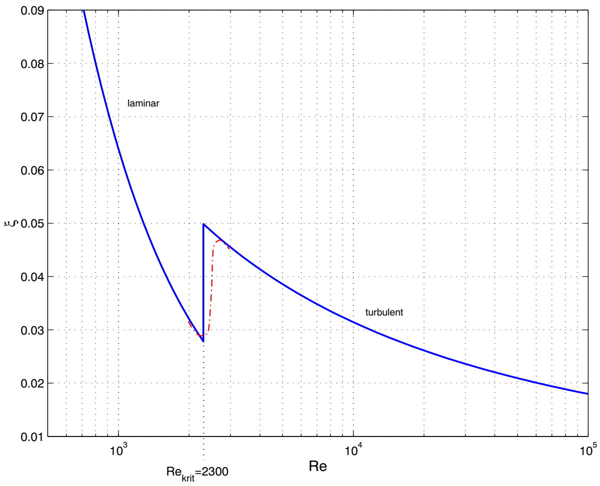

Figure 10: Example for the unsteady transition of the pressure drop coefficient (solid line) and the implemented interpolation function (dashed line)

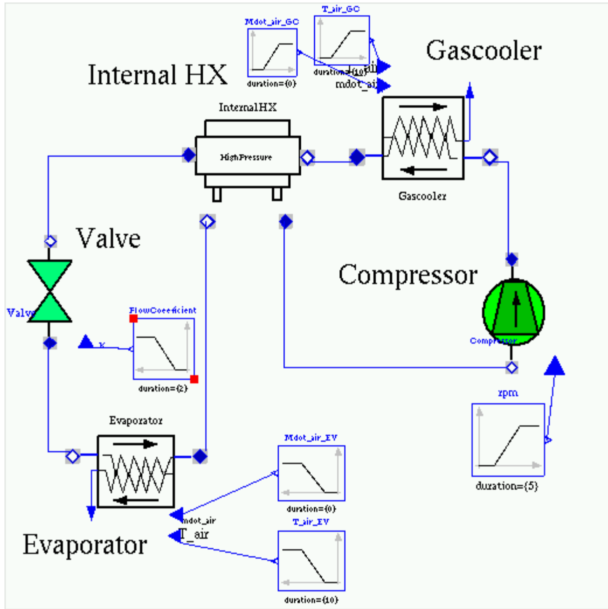

Figure 11: Object diagram of simulated CO_2-Cycle

Table 3: Boundary conditions and initial values of the simulation run

Compressor	$\lambda = 0.75$, $\eta_{is} = 0.75$
Gas cooler	$\dot{m}_{air} = 3200$ kg/h, $T_{air,in} = 305$ K
Evaporator	$\dot{m}_{air} = 580$ kg/h, $T_{air,in} = 305$ K
System volume	$V_{tot} = 1.13$ l
Refrigerant filling	200 kg/m^3
Initial value	$p_0 = 66$ bar, $h_0 = 420$ kJ/kg

5 Simulation results of a CO_2-System

In the following simulation results of the start up of a CO_2-System are presented. The results are discussed with respect to plausibility since reliable data of transient processes from a test rig are only available for a few weeks. The simulated model is shown in object diagram in figure 11. This configuration does not consits a receiver since the receiver model is not implemented in the right way, see subsection 3.1.

In table 3 the boundary conditions and initial values are listed. The following boundary conditions are changed during the simulation run:

- Start up of compressor speed $n = 120 \rightarrow 1000$ rpm in 2 seconds;
- Variation of flow coefficient $K_v = 0.03 \rightarrow 0.02 m^3/h$ in 0,1 seconds starting at 60 seconds simulation time.

5.1 Results

In figure 12 the pressure at compressor inlet and outlet is plotted versus time. What can be seen from the results is the divergent run of the pressures and a typicall overshoot, resp. undershoot at the beginning. This system behaviour is plausible as well as the divergent run of pressure after changing the flow coefficient of the valve. This can be made clear by looking at the mass flow rates at the compressor and the expansion valve in figure 13. At the beginning the compressor mass flow rate is much higher than the mass flow at the valve. The compressor mass flow increases proportional with the compressor speed, whereas the flow rate at the valve just increases with the increasing pressure difference at the valve. The difference between both mass flows effects a shifting of refrigerant mass from the low pressure section to the high pressure section of the system. The decreasing density of the sucked refrigerant at the compressor causes in the strong decreasing of the compressor mass flow after 2 seconds. The valve mass flow rate is mostly affected by the pressure difference, so the mass flow does not decrease; the system time delay causes a higher valve flow rate for a few seconds resulting in the shown over- and undershooting of pressures. The same effect of displaced mass explains the divergent run of the pressures after changing the flow coefficient.

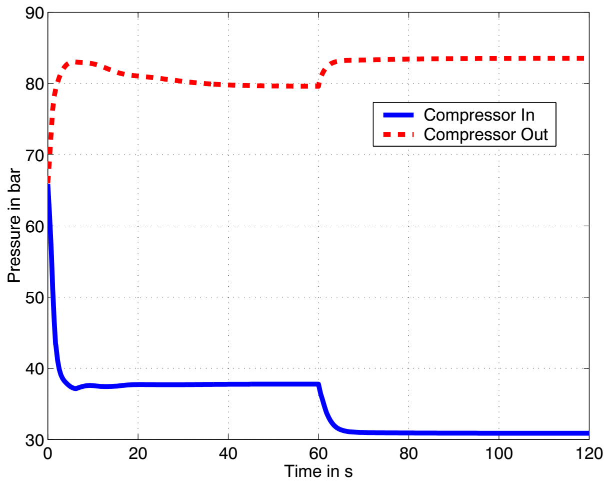

Figure 12: Pressure run at compressor in- and outlet

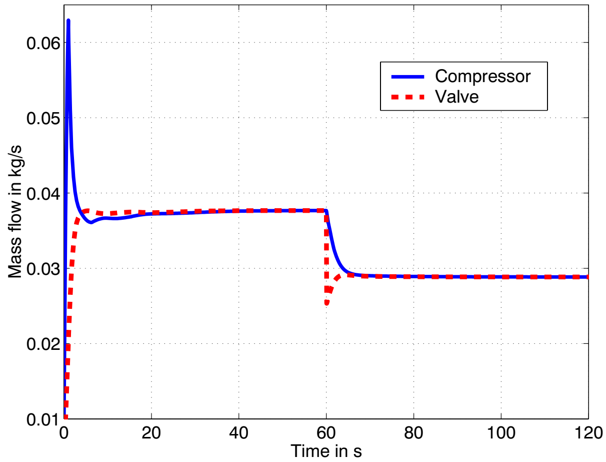

Figure 13: Mass flow rate at valve and compressor

This model contains about 2600 nontrivial scalar equations. The simulating of the start up and the changing of flow coefficient was performed on a PC with a Pentium 1000 MHz and 256 MB of main memory and took 5 minutes. The length of time of simulation is very sensitive due to the initial values. To realize a simulation of 5 minutes for this model you have to provide very suitable initial values; furthermore up to now the initialization in the two phase region needs wide experience. To get suitable initial values for the gas region we are using matlab^{TM} based script to predict the steady state pressure drop for the initalized mass flow rate. Starting a simulation with a mass flow rate of zero and equal pressure in every object increases the executing time extremely or generates a termination of simulation.

Nevertheless, the simulation results show that Modelica, the free Modelica library ThermoFluid and the CO_2-Library are very well qualified for the simulation of the complex processes in a CO_2-Refrigeration cycle.

6 Conclusion

A developed CO_2-Library based on free Modelica library ThermoFluid was presented, which contains models for all important components of a CO_2-Refrigeration system. The intention is to create a library for the simulation of single components and complete cycles. Such a library can be used to get a better understanding of the thermodynamic, fluid-mechanic and heat transfer effects in a CO_2-System. Furthermore, it can be used for the optimization of specific heat exchangers, for the evaluating of optimal system configuration and for the layout and optimization of the system control.

The presented simulation results for the steady state of two different types of CO_2-Heat exchangers show a very correspondence with measured datas. The results of transient simulation show a plausible system behaviour due to the thermodynamic and hydraulic effects. Up to now a validation with transient measured datas was not possible since an available CO_2-Test rig operates just for a few weeks.

Future work contains the validation of the models and the improvement of the initialization due to new features in Modelica. If the models are verified the control of the system will implemented.

6.1 Acknowledgement

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