Thermodynamic Simulation of Rotary Displacement Machines

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Abstract

The thermodynamic simulation of rotary compressors by means of a chamber model is an accepted method for the development and analysis of these machines.

The paper presents an improved method for modelling rotary compressors, which allows the simulation of the steady or transient operation of any rotary displacement machine. Also any gases, liquids or composites of both are possible as working fluids. The functionality is demonstrated on the basis of an adiabatic Root's type compressor.

The implementation is based on object-orientated paradigms. The modularity of the simulation program gives good transparency, maintenance and extensibility.

1 Introduction and motivation

The simulation of technical processes and the associated machines is nowadays an accepted means for the analysis, evaluation and development of machines or methods. An advantage for empirical research is the ability to examine new machines even before prototyping. Even the examination itself may be easier than a corresponding experiment because every part of the simulation model is accessible at any time and the simulation can be frozen in any state to have a more detailed look at it. This is often impossible in an experiment.

The core of a program system for the simulation of the operating behaviour of rotary displacement machines is the calculation of the thermodynamic processes inside the machine. Naujoks first presented these processes by means of a chamber model for an adiabatic screw-type compressor /1/. Dreißig modified this model to allow the simulation of screw-type engines /2/. Gödde and Keller enhanced the simulation system by calculating the heat transfer between the working fluid and the mechanical components /3/, /4/. The thermal and mechanical simulation of the components allowed the calculation of the clearances under working conditions. The clearances have a considerable influence on the working characteristics of the screw-type machine. They even endanger its reliability /5/.

Commercial simulation systems prevail in the field of process simulation (e.g. logistics) and also in the calculation of problems that deal with only one physical discipline, such as the Finite-Element-Method or Computational Fluid Dynamics. Nevertheless the engineer who needs to simulate the thermodynamic behaviour of rotary compressors has to rely on special programs that are mostly self-developed. The advantage of a program that is specially designed for one machine is cancelled out by the problems that occur because of the small range of application:

- The limited expected usage of the program means that little effort is expended on designing a user interface with good operator convenience.
- The program is not as error-free as comparable commercial programs.
- To simulate another type of rotary compressor, a second program has to be developed. The user needs to learn the handling of the new program as well.

The software for thermodynamic simulation has not improved as fast as the computer hardware would allow.

1.1 Goal

The new program system is intended allow the simulation of the unsteady operation behaviour of every rotary displacement machine. It should be able to work with all kinds of gases, liquids and multi-phase composites.

A modular implementation will allow the integration of new fluids or additional thermodynamic effects without the need to adapt every part of the program system. The machine data will be provided by file input so as to acquire a good degree of versatility.

2 Basics

The common characteristic of all positive displacement machines is the existence of one or more working chambers, whose volume cycles during the working period. The state of the working fluids inside the chambers is approximately homogeneous. If the fluids consist of gases and liquids, the mixture can be inhomogeneous.

A closer look shows that there is also flow physics in the displacement machine, which has a disturbing effect on homogeneity in the chamber. To decide if the influence of the gas flow is negligible in relation to the homogeneous view of the displacement machine is up to the engineer.

2.1 State of the art

The chamber model described in /1/ views the working fluid from the machine inlet through the compression phase to the outlet. The changes in the fluid state are determined by the continuous change in the volume of the surrounding working chamber and the inflow or outflow of fluid and heat. The focus is implicitly on one representative chamber that is traced from beginning to the end. The operational behaviour of the total machine may be extrapolated from the representative chamber because of symmetries.

The advantage of this method lies in the simple view of the continual state curve of the fluid. But there can be problems in the definition of the representative chamber. In the case of most screw-type machines the gaps on the male and the female rotor that form a working chamber on the high pressure side are not connected on the low-pressure side, **Fig. 1**. They are connected with the preceding or the succeeding gaps. This suggests modelling each gap as a single chamber and connecting the male or female rotor chamber by the means of an interface area, see 3.3.

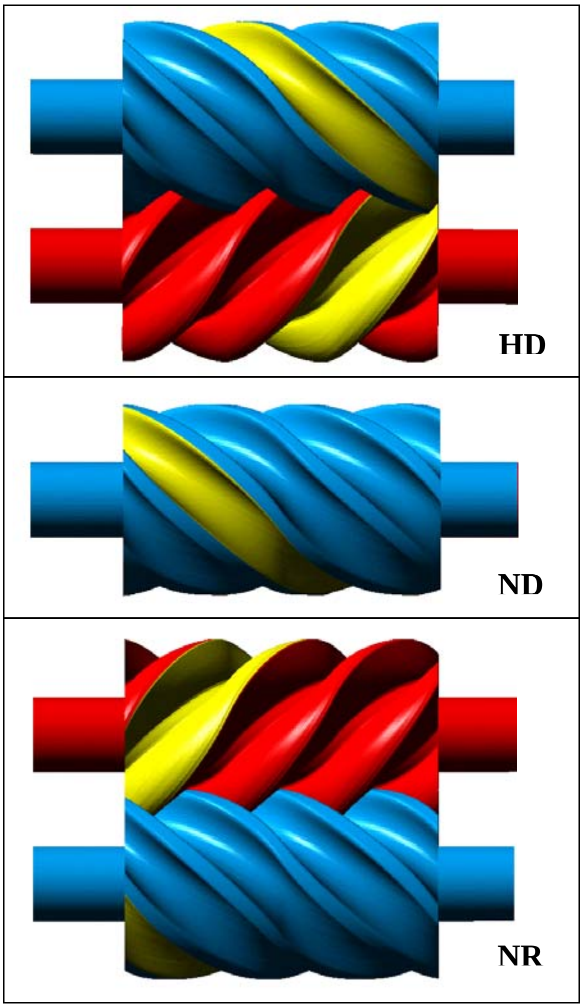

***Fig. 1:** Working chambers of a screw-type machine in three different views*

HD : Discharge side

NR : side view, female rotor

ND : suction side

2.2 A new chamber model - KaSim

This paper presents an alternative method for generating a chamber model. It is based on the analysis of something resembling frozen images of the total machine. For a number of given rotor positions all chambers are analysed regarding their geometric properties, such as volume, clearances or surface areas. These properties form the characteristic courses of the chambers during the period e.g. the volume curve or the course of the clearance area. Paragraph 4.1 exemplifies this on a Root's type compressor.

This method has the important advantage that it can be carried out by a computer program. It requires only simple rules to form a chamber model from the geometric model:

- the chamber volumes have to be separated unambiguously
- the interfaces between two chambers form the connections

Because every chamber and every connection of the total machine is analysed for every given rotor position, it is sufficient to limit the view to the rotor positions that are passed through in one working cycle. For most rotary displacement machines the necessary range of rotor positions equals the tooth pitch. To avoid confusion caused by the different tooth pitches of the male and female rotor, a unified phase angle will be used that is limited to the range of [0;1].

2.3 Linking of the chambers on the period transition

The fluid state in the piston of a reciprocating compressor at the end of one period equals the state at the beginning of the next period. This differs in the case of a rotary compressor. The fluid state in one chamber at the end of the period equals the fluid state of the following chamber at the beginning of the next period. Therefore every chamber that is still in existence at the end of the period must have a successor. If constant volumes like the inlet or the outlet also count as chambers, they will have themselves as successor, see 4.1.

2.4 Representation of the working fluid

The state of the working fluid inside the chamber changes through interaction with the surrounding environment. This can be caused by a fluid flow, a flow of mechanical energy or a heat flow, see **Fig. 2**.

The fluid state is modelled by the extensive thermodynamic variables of state:

- the mass m,
- the intrinsic energy U and
- the volume V

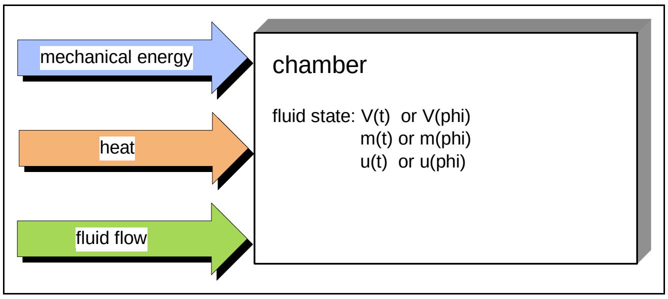

Fig. 2: Influences on the working fluid inside a chamber

The explicit calculation with extensive state variables in accounting for the mass and the energy flows inside the chamber model causes less numerical inaccuracy in comparison with intensive state variables.

The intensive state variables, temperature T and pressure p, will be calculated from the extensive state variables m, U, V at the moment of use. The method of calculation is determined by the representation of the fluid and will be explained in more detail in 3.1.

The calculation of fluid states distinguishes between gases, liquids and steam. Liquids are more or less incompressible and occupy part of the available volume depending on their mass and density. The gases share the rest of the volume. Every gas occupies the whole gas volume. The partial pressures of every gas aggregate to the total pressure in the chamber. The liquid pressure is equal to the total gas pressure.

The conservation of mass (eq. (1)) and energy (eq. (2)) in the form of the first principle of thermodynamic obtain for every single chamber:

$$m' = m + m_{zu} - m_{ab} \qquad \text{eq. (1)}$$

$$\begin{aligned} U' = U &+ (Q_{zu} - Q_{ab}) \\ &+ (W_{zu} - W_{ab}) \end{aligned} \qquad \text{eq. (2)}$$

2.5 Separation in capacities and connections

The program KaSim distinguishes between two basic element types of a chamber model:

- *capacities* and
- *connections*.

Capacities are able to store fluids, mechanical energy or heat. *Connections* allow the transport of fluid flow or energy flow between two or more capacities.

medium	storing capacity
fluid	chamber, constant volumes
heat	machine parts, fluids in chamber
mechanical energy	movable or deformable machine parts, fluids in chamber

Table 1: Examples of different capacities

Connections store neither energy nor fluids. Their actual state is always calculable from the boundary conditions. Both the mass balance and the energy balance are calculated only for the capacities. The aggregation of all capacities is also a closed system whose state variables are changeable by input or output flows of fluid or energy.

This paper summarises the energy forms heat und mechanical energy as well as fluids as media, as they are characterised by the possibility to store or transport them.

Some capacities are able to store different media, see **Table 1**, e.g. the rotors are able to store both mechanical energy and heat. A volume filled with gas is able to store additional fluids as well as mechanical energy or heat. Correspondingly some connections are also able to transport different media such as heat and mechanical energy, see **Table 2**.

medium	transporting connection
fluid	clearances, interfaces between chambers
heat	heat conduction, convection or heat radiation through surfaces of machine parts
mechanical energy	movable or deformable surfaces of machine parts

Table 2: Examples of different connections

2.6 Simulation sequence

The simulation emulates the transient machine operation by means of discrete time steps. It is possible to use fixed or variable time steps that adapt to the course of the simulation. The steady operation state can be calculated by choosing a sufficient duration of the simulation. It is also possible to analyse the convergence of the state variables in the model.

If the machine works at constant speed, the length of the time steps is proportional to the angle increment of the rotors. In the case of intense speed gradients it is necessary to calculate the actual angle increment for each time step. This allows the acceleration of the rotors, e.g. of a screw-type motor, to be simulated.

Fig. 3 shows the flow chart of thermodynamic simulation used in KaSim. It consists of two main loops, the calculation of the periods and within them the calculation of each time-step.

Every time-step begins with the determination of the phase to be examined, and results in the calculation of the rotor positions including the geometric boundary conditions of all chambers and connections. The calculations of fluid or energy flows exchanged through the differential connections and the compression / expansion of the chambers follow in sequence. Last of all state-changing processes is the calculation of fluid or energy flows through the integral connections, because they induce a balance between the capacities and therefore take all other state changes into account. At the end of each time-step the fluid states in the chambers at this stage are stored for later analysis.

At the end of the period it will be examined whether the model is already in steady state or still transient. The model has reached steady state when all state variables of all capacities of the whole period differ from the corresponding state variables of the preceding period by less than a given amount. In this case the simulation is finished.

If the simulation has not reached steady state or the end point within the simulation time, the contents of the chambers are transferred to their successors and the simulation continues with the next period.

3 Implementation of KaSim

The implementation of the simulation system KaSim is based on object-oriented paradigms. Modular algorithms and abstract data types improve the transparency of the complex system. The intensive use of derived classes allows a step-by-step specification from the abstract base classes to the concrete classes needed in the simulation. This policy requires a higher amount of generalized design, but it simplifies the assembling of the single modules and the maintenance and expansion of the program system. The objective is to ensure that future research results can be integrated into the simulation system as efficiently as possible.

The implementation of KaSim is done in C++. This program language supports the required means of object-orientation, is

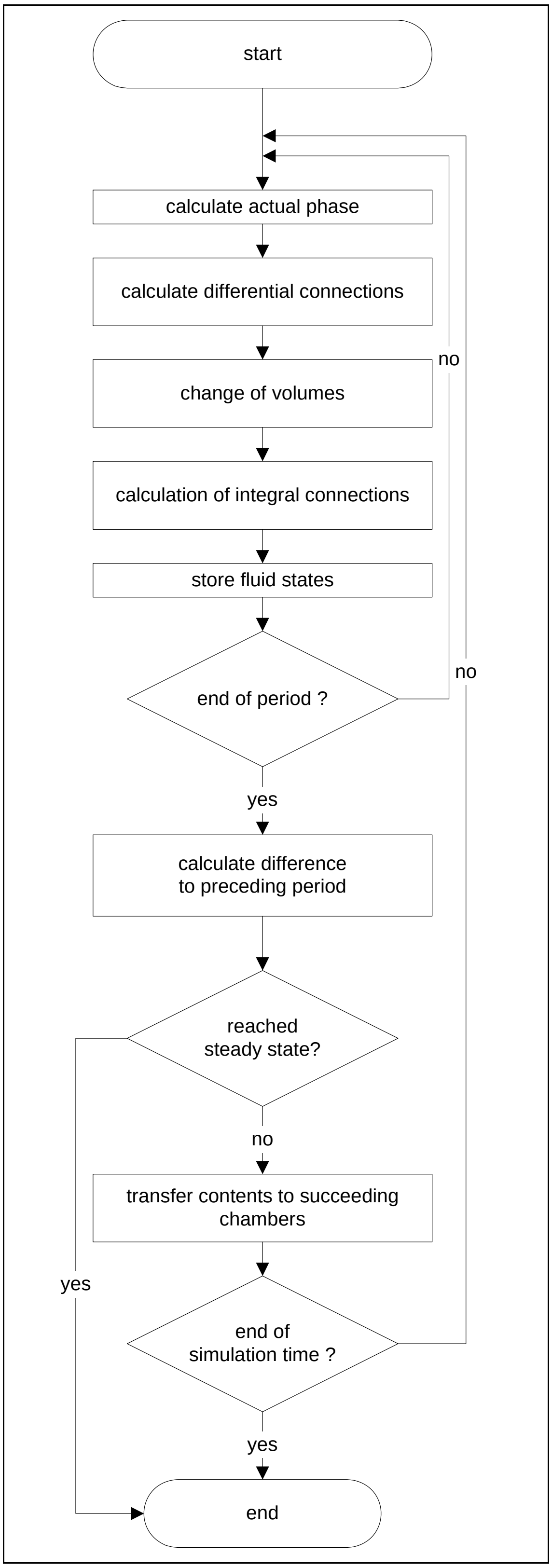

Fig. 3: ***Flow chart of the thermodynamic simulation***

available on most computer systems and produces fast executable programs.

3.1 Fluids

It is possible to use gases and liquids as well as composites and steam as working fluids. The calculation of the phase transition, in this case condensation and vaporisation, is planned but currently not implemented.

To assure the extensibility of the program regarding the working fluids, all properties of the fluids are defined inside the classes, including the equations for compression or heat influx. This is supported by the object-oriented design of the classes in hierarchical form, see **Fig. 4**.

The abstract base class CFluidType provides the basic functions for all fluids, although most of them are only empty function shells that have to be filled in the derived classes.

Every step in the heredity of the fluid classes involves a specialisation of the fluid, at first distinguishing between gases and liquids, later on dealing with, for example, actual gases with specific material properties (CAir).

The equations of state are part of fluid representation. For an example all fluids that derive from the base class CIdealGas automatically use the equation for ideal gas (eq. (3)) to calculate the pressure of the fluid.

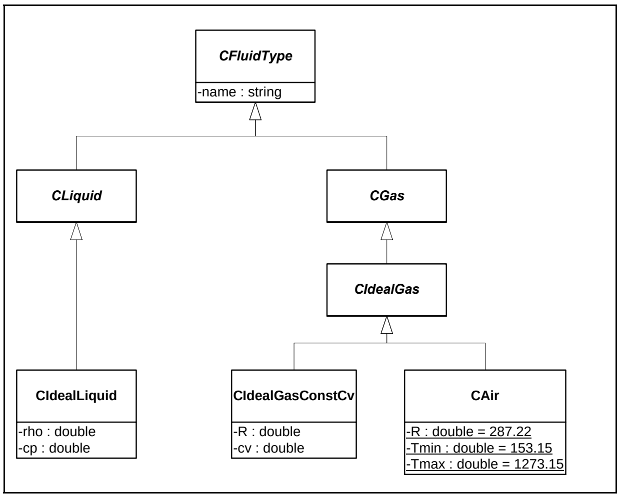

Fig. 4: Diagram of the fluid type classes

$$p = \frac{m \cdot R \cdot T(u,v)}{v} \qquad \text{eq. (3)}$$

The calculation of the temperature *T* of the gas from the state variables mass m, specific volume v and specific inner energy u, depends again on the gas in question. In the present implementation of air (CAir), the temperature is approximated by a polynomial function of the 5th grade from the specific internal energy. There is also a class for defining ideal gases with constant heat capacity c_v, where the temperature is proportional to the specific internal energy (CIdealGasConstCv).

The expansion of the fluid hierarchy is possible on every level of specification. Real gases could be catered for as an alternative to the ideal gases as a derived class of CGas.

3.2 Capacities

All elements of KaSim that are able to store energy or fluids are denoted *capacities* of the chamber model. These are distinguished by the type of medium that is stored:

mechanical energy	`CMechCapacity`
heat	`CHeatCapacity`
fluid	`CFluidCapacity`

Furthermore they divide into capacities whose intensive state variables change on the in- or outflow of energy or fluid, like all finite reservoirs, and capacities whose state variables remain constant, unaffected by inflow or outflow. The surrounding environment of a machine would be modelled as an infinite capacity. **Fig. 5** shows part of the hierarchy of the capacities.

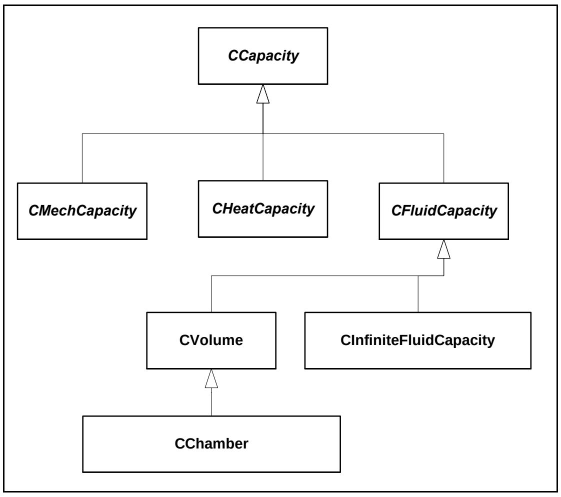

Fig. 5: Diagram of the capacity classes

It is very easy to integrate a new kind of capacity into the hierarchy by adopting the characteristics of a superior class. The class CVolume for instance represents a finite fluid reservoir with a fixed volume. The derived class CChamber adopts all properties from CVolume but possesses as a differing property a volume that depends on the phase angle.

The capacities that store heat (CHeatCapacity) allow the integration of heat transfer between the machine parts and the working fluid into the chamber model. The rotors may be modelled as a mechanical energy store (CMechCapacity). This makes the calculation of the mechanical load on the drive possible and acts as an interface to Finite-Element programs.

3.3 Connections

All elements in the chamber model that induce a fluid or energy flow are denoted *connections*. These can be clearances inside the machine that cause a clearance flow between two chambers, or a surface of a machine part that causes a heat flow between the working fluid and the mechanical component. The main focus of this paper lies in the fluid transporting connections, the clearances, the inlet and outlet, and the interfaces that connect chambers on the male and female rotors.

During one time step *Δt* of the simulation the interchanged fluid flows cause a change in the intensive state variables of the fluids inside the chamber. Depending on the size of the chamber, the length of the time-step and amount of the fluid flow the change of state turns out more or less severe. The course of the state variables of the capacities affects the calculation of the fluid flow itself. Two extreme cases can be used to simplify the calculation of the fluid flow, **Fig. 6**.

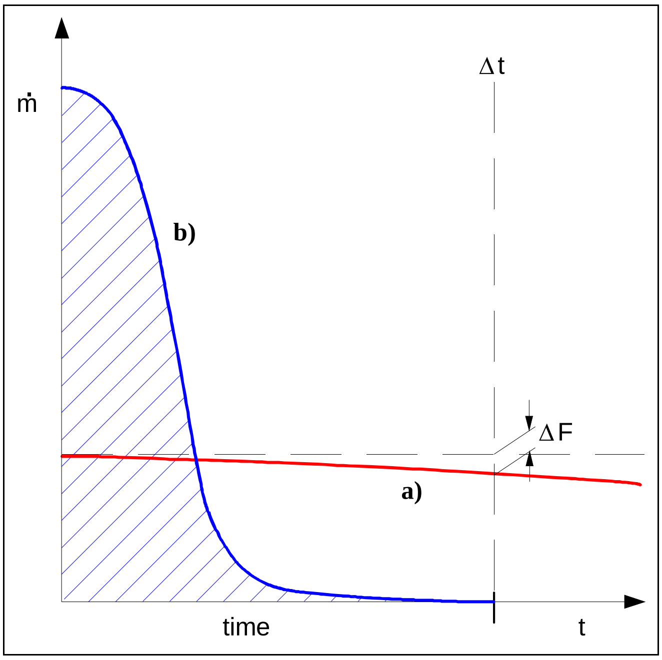

Fig. 6: ***mass flow $\dot{m}$ during a time step Δt for***
a) a differential clearance
b) an integral clearance

In the case of a very small change in the fluid state during the time step, Fig. 6 a), the fluid flow can be calculated approximately by assuming that the state variables of the connected chambers remain constant during the time step. The interchanged fluid mass is proportional to the length of the time step. We call this a **differential connection**. The deviation ΔF between the calculated mass flow during the time step and the mass flow calculated at the beginning of the next time step is an index for the inaccuracy of the calculation.

After a sufficient time two connected chambers reach a thermodynamic equilibrium, perhaps even within one time step. If the reservoir is small relative to the fluid flow, the interchanged fluid mass becomes independent of the length of the time step, Fig. 6 b). We call this an **integral connection**. The inlet and outlet of a screw-type machine show this behaviour. In the sequence of simulation the calculation of the integral connection is always at the end of the time step, in order to achieve a thermodynamic equilibrium.

If neither the state variables inside the chambers remain approximately constant nor a thermodynamic equilibrium is achieved within the time step, it is only possible to modify the length of the time step. As a rule the steps have to be shorter.

Currently six different differential connections are implemented in KaSim. Their structure is shown in **Fig. 7**. There are the isentropic clearance, the orifice and a clearance with frictional surfaces where the discharge coefficient depends on the form of the clearance and on the pressure. Additional all of the properties of the clearances may be phase dependent.

The **isentropic clearance** (CIsentropicClearance) is characterised by the non-dissipative flow between the connected fluid capacities. The basic property of this clearance is the cross-sectional area A, that may be phase-dependent (CIsentropicClearancePrd).

The **ideal orifice** (COrifice) is a model for an isenthalpic, dissipative flow, characterised by a pressure-independent flow coefficient α and the cross sectional area A. Both properties can be dependent on the phase (COrificePrd).

In cooperation with the *Arbeitsgemeinschaft industrieller Forschung AiF* the *Fachgebiet Fluidenergiemaschinen* carried out experimental research on the flow coefficients of clearances in vacuum. The clearances had different forms and were examined with varying pressure, clearance height and clearance width. The empirical data was integrated in KaSim in the form of a class of **real clearances** (CVacuumClearance). There is also an analogous clearance with phase-dependent geometric properties (CVacuumClearancePrd).

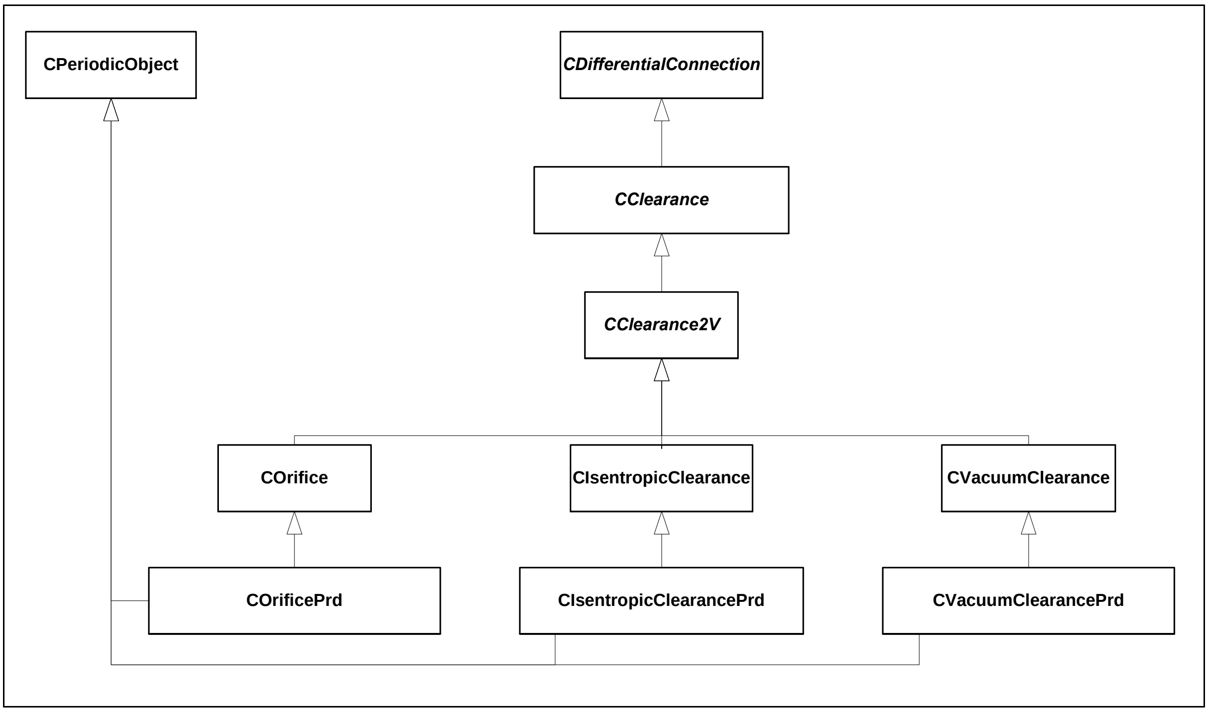

Fig. 7: Diagram of the differential, fluid transporting connections

To model the interfaces between two chambers with big area related to the volumes of the chambers, there is an integral connection (CPressBalClearance) that induces a pressure balance between the fluid capacities within one time step. This integral connection can be used to combine the gaps on the male and the female rotor, which have a large interface area in relation to the volume.

4 Sample results

The following section shows an example of modelling and analysing a Roots type compressor. We chose this machine for demonstration purposes.

4.1 Analysis of the chambers

Fig. 8 shows the course of all chamber volumes of the Roots type compressor during one period, that is the tooth pitch angle of 180°. Every chamber is assigned to one rotor to improve the clarity of the model. The splitting of the chambers at the crown circle of the male (right) rotor is more or less arbitrary. This does not produce an error in the model, because the state of the fluids is, according to the premise, homogenous. Therefore every chamber is arbitrarily dividable without causing an error in the chamber model.

At the rotor position of α_{HR} = 0°, six chambers (A-E), the outlet (HD) and the inlet (ND) can be located. During one period chambers A and B vanish in the area of the outlet (HD). As a substitute, chambers F and G rise into the area of the inlet (ND). After one period of 180° the rotor position is the same as at the starting position.

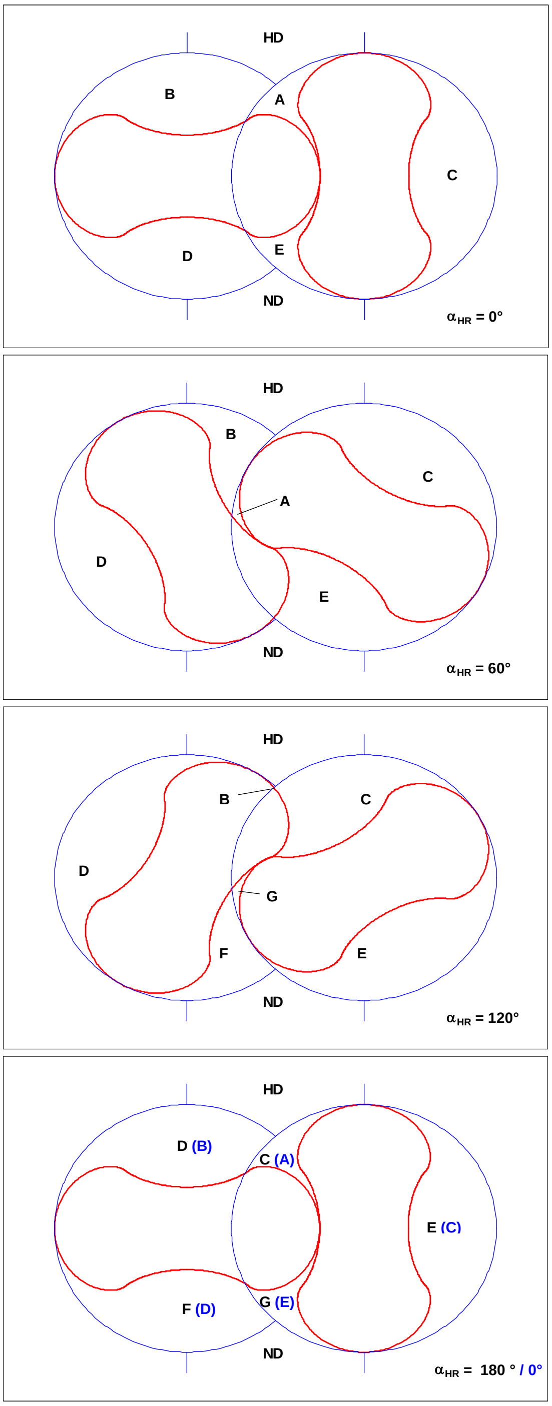

Fig. 8: Course of the chambers of a Roots type compressor for one period

Fig. 9 shows the course of the chamber volumes as functions of the unified phase angle. A phase of φ = 1 correlates with a rotor angle of α_{HR} = 180°. It is easy to see that the single chambers represent only a part of the volume course of the whole compression process. Chambers that show a volume of v = 0 are nonexistent at the corresponding rotor angle, e.g. chamber G for φ < 0.5 or chamber A for φ > 0.5.

A comparison of the chamber notations at the end of the period (α_{HR} = 180°) with the starting position (α_{HR} = 0°) allows the definition of succeeding chambers. The working fluid contained in chamber D at the end of the period will be the same as in chamber B at the beginning of the next period. Likewise chamber A starts with the fluid contents of chamber C at the end of the preceding period. The successors of the chambers E, F and G are determined in the same way. Chambers A and B do not have a successor because they vanish during the period. Likewise chambers F and G do not have a predecessor, because they arise within the period. The inlet and the outlet use themselves as successors.

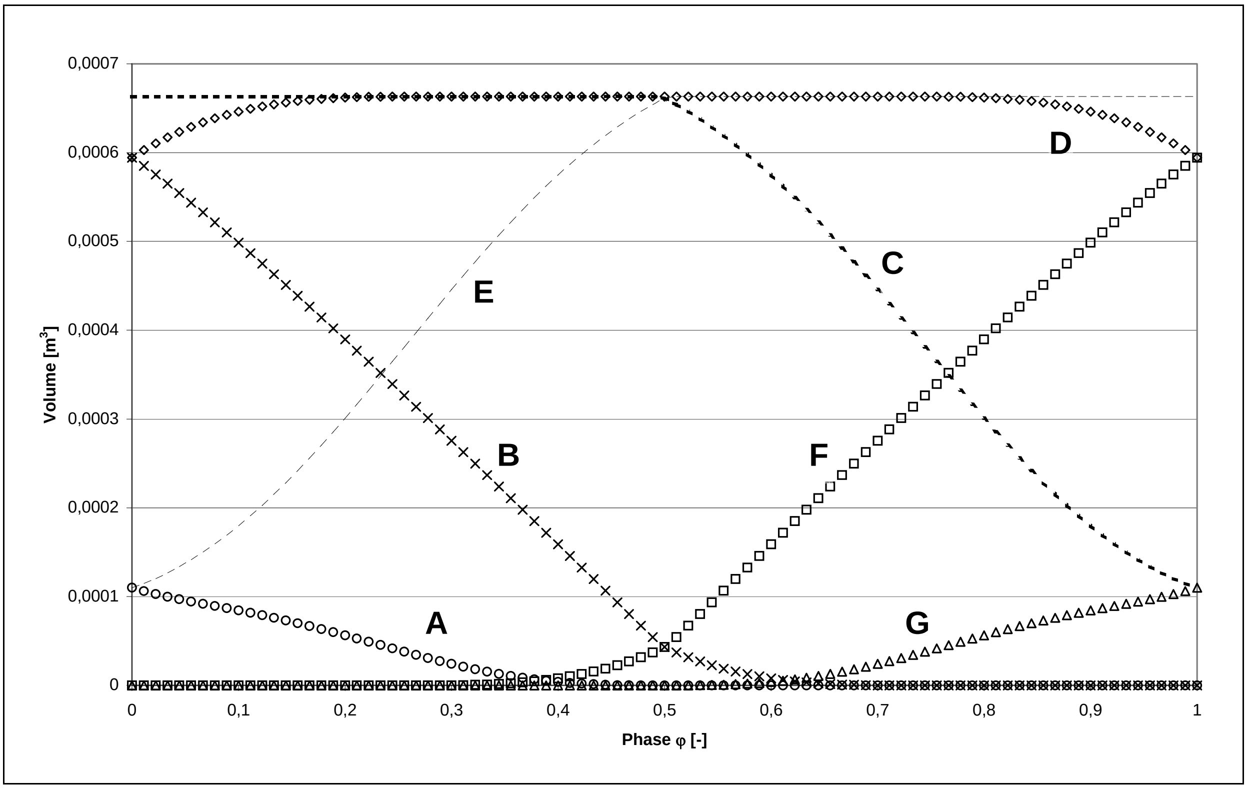

Fig. 9: Course of the chamber volumes A to G of a Roots type compressor

4.2 Analysis of the connections

As an example, some of the connections in the machine are depicted in **Fig. 10** and **Table 3**. A further analysis of all rotor positions will give a total of 18 different connections in the chamber model. What kind of fluid connection will be used in the modelling depends on the geometric parameters of the clearances or interfaces and on the supposed shape of flow.

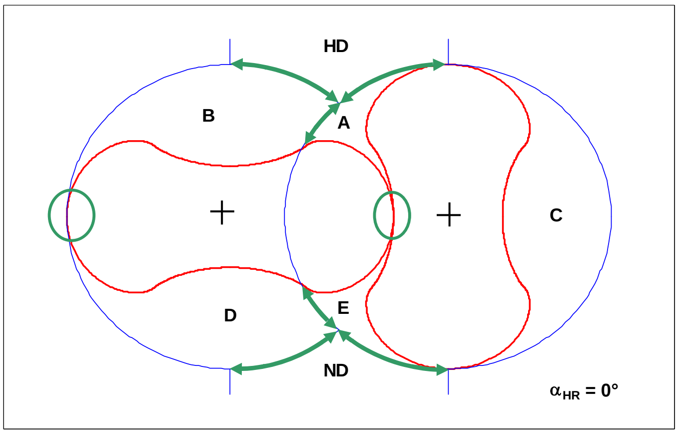

Fig. 10: ***Connection between the chambers at one rotor angle (α_{HR} = 0°)***

connection	capacity 1	capacity 2
outlet 1	HD	chamber A
outlet 2	HD	chamber B
inlet 1	ND	chamber D
inlet 2	ND	chamber E
chamber interface 1	chamber A	chamber B
chamber interface 2	chamber D	chamber E
casing gap 1	chamber B	chamber D
intermesh clearance 1	chamber A	chamber E

Table 3: ***Type of connections in the examined chamber model***

The complete chamber model of the Roots type compressor under examination, including all chambers and all fluid transporting connections, is shown in **Fig. 11**. A chamber model of a machine with more chambers or a more complex geometry is likely to become confusing for the user. The further development of KaSim will therefore include a method for the automatic generation of chamber models from a geometric model.

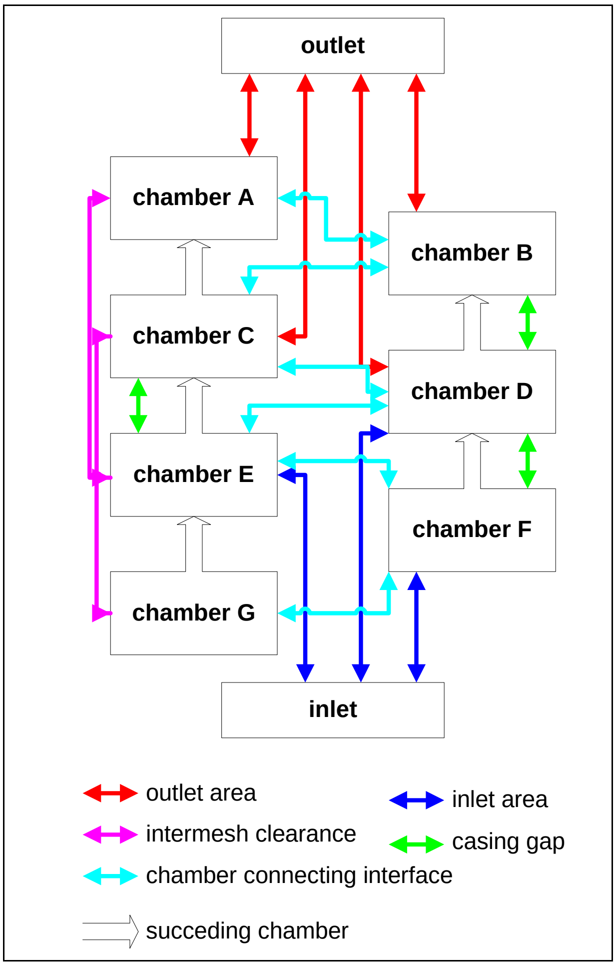

Fig. 11: ***Chamber model of the examined Root's type compressor***

4.3 Course of fluid states

The chamber model simulation of the operational behaviour at given operating conditions results in the course of fluid state in all chambers during the period. To optain a view of the fluid state course of the complete compression process, it is necessary to link the state curves of the single chambers according to the way the fluid is transported through the machine. Often more than one way is possible.

Fig. 12 displays the state curves of the working fluid during transport from the inlet through the chambers G, E, C and A to the outlet. The pressure in the outlet is p_{out} = 1000 [mbar], the inlet pressure is p_{in} = 500 [mbar]. The speed of the rotors is n = 1500 min^{-1}. The fluid temperature in the inlet and in the outlet are constant at 18°C.

When chamber G **(2)** opens up, the fluid flows into the new volume and the temperature rises by 70° due to the enclosed enthalpy. Subsequently the temperature goes down because of a continuing inflow of cold gas from the inlet. Simultaneously hot gas from the high pressure side enters the chamber through the casing gap and the intermesh clearance. This results in a partial rise in temperature at **(3)** and **(4)**. On the opening of the chamber to the outlet **(4→5)**, and the simultaneous separation from the inlet, the pressure rises instantaneously from 0.5 [bar] to 1.0 [bar] and a corresponding rise in the temperature of 40° occurs. During the exhaust of the fluid into the outlet **(5→6)** receding clearance flows to the low pressure side cause a small decrease in temperature.

In the model of the Roots type compressor an infinite volume was used to represent the outlet. Therefore no change in temperature of the fluid is noticeable in the outlet, though it might be expected. The first step towards optimising the model would be to insert a sequence of finite volumes between the rotating chambers and the infinite volume that models the destination reservoir. The modification will allow a rise in temperature in the finite outlet volumes to be observed.

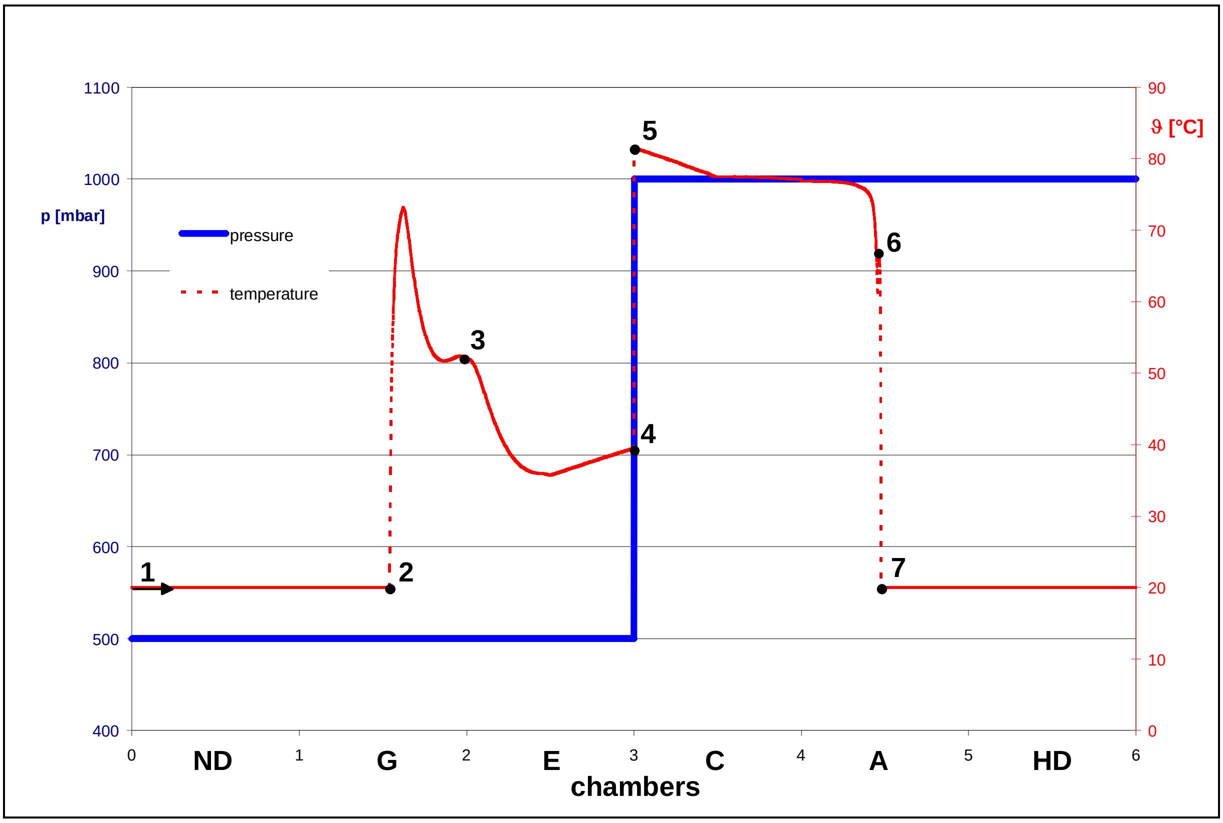

Fig. 12: ***State curve of the working fluid during the compression in the succeeding chambers***

1→2 : Inlet ***2 : Development of chamber G***

3 : preceding chamber opens to discharge end

4→5 : detachment from inlet, connection to discharge end

5→6 : Exhaust ***6,7 : Vanishing of the chamber***

5 Perspective

The presented system for modelling and simulating rotary displacement machines will aid the researcher and the engineer in the task of evaluating contemporary or future machines. It will also help in understanding the thermodynamic behaviour of this type of machine.

The modular architecture of the system allows the integration of future research results. Consequently it is possible to improve the modelling accuracy in the different application fields of rotary displacement machines step by step. Simultaneously the wide range of application provides sufficient justification for a further development and verification of the simulation system. This will be part of the future work at the university.

6 References

/1/ **Naujoks, R.** Zustandsänderungen in trockenlaufenden Schraubenmaschinen - Ein Vergleich von Rechnung und Experiment. Dissertation, Universität Dortmund, 1982

/2/ **Dreißig, B.** Ein Beitrag zur Auslegung von trockenlaufenden Schraubenmotoren. Dissertation, Universität Dortmund, 1989

/3/ **Gödde, R.** Simulation des instationären Betriebs von Schraubenkompressoren. Fortschrittsberichte VDI Reihe 1 Nr. 231, VDI-Verlag, Düsseldorf, 1993

/4/ **Keller, G.** Simulationsgestützte Entwicklung des Motors einer Heißgasschraubenmaschine. Dissertation, Universität Dortmund, 1997

/5/ **Rofall, K.** Ein Beitrag zur Verifikation eines Simulationssystems für trockenlaufende Schraubenkompressoren. Fortschrittsberichte VDI Reihe 1 Nr. 299, VDI-Verlag, 1998

/6/ **Kauder, K., Wenderott, D.** Der Spaltformwiderstand von Strömungen im Vakuum. In: Schraubenmaschinen Nr. 9, S.93 - 104, ISSN 0945-1870, 2001