Comparison of the Simulated and Measured Machine Characteristics of a Roots Vacuum Pump in Fine Vacuum

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Abstract

This paper presents the enhancement of the simulation software *KaSim*, integrating new models to increase modelling accuracy and to extend the application area to fine vacuum conditions.

The main objective of the software *KaSim* is the simulation of the thermodynamic behaviour of positive displacement vacuum pumps within the design and development process. The verification of the program has already been successful for rough vacuum conditions. In fine vacuum additional physical effects - not modelled so far - become predominant in the machine characteristics. On the one hand the influence of moving clearance boundaries on the characteristics of leakage flows is taken into account. Therefore the molecular clearance flow is simulated and analysed using a Monte-Carlo method. And on the other hand, further losses mainly caused by sorption and desorption are modelled via a heuristic approach derived from the experimental studies.

The operating behaviour of an industrial Roots vacuum pump is analysed varying several parameters (operating pressures, rotor speed, clearances). The comparison of simulated and measured machine characteristics for a vacuum booster in the fine vacuum region provides a validation of the enhanced program *KaSim*.

Notation

<u>Symbol</u>	Meaning	<u>Unit</u>
α	degree of rotation	0
δ	normed mass flow	-
А	clearance area	m²
b	clearance width	mm
I	clearance length	mm
C _{1,2}	empirical constants	-
ṁ	mass flow	kg/s

Symbol	Meaning	<u>Unit</u>
Kn	Knudsen number	-
P ₁₂	transmission probability	-
s	clearance height	mm
n	rotor speed (rpm)	min⁻¹
р	pressure	mbar
p∨	backing vacuum / outlet pressure	mbar
w	relative velocity of a moving boundary	m/s

1. Introduction

Higher standards in vacuum cleanliness and predominantly the objectives of cost reduction regarding maintenance and servicing (oil, oil changes and disposals) have led to the banning of cooling and sealing fluids inside the working chamber and led to a market trend with an increasing demand for dry-running vacuum pumps. In this context the focus of the industry is on the development and enhancement of positive displacement machines without lubrication fluids – also resulting in the design of screw-type vacuum pumps because of their advantages due to the working principle [1, 2].

The simulation of technical processes and the associated machines is nowadays an accepted means for the targeting analysis, evaluation and development of machines or methods. The main advantage of simulation over empirical research is the ability to examine new machines even before prototyping. Thus simulation is a tool supporting the engineer during the design process of a machine. Furthermore a theoretical examination may actually be easier than a corresponding experiment because every part of the simulation model is accessible at any time and physical factors determining the operating machine's characteristics can be analysed separately.

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Messages-			
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Operating Point	State	State	
Volume Flow [m ² /h] at Fluid 7.65 HD_	Fluid Capacity	ND 🗾 Fluid Cap	acity HD_Volume 💌
Model Frequency [Hz]	100 Pressure (mbar)	10.0 Pressure	[mbar] 1000 •
Mech.Power [kW]	4.00 Temperature (*C)	17.5 Temperat	ure [*C] 28.0
Mech.Power[KW]			

Fig.1: User interface of the program *KaSim* to simulate the thermodynamic processing in positive displacement machines With the main objective of simulating the operating behaviour of dry-running positive displacement vacuum pumps, the simulation software *KaSim* has been developed in recent years, **Fig. 1**. The simulation program calculates the thermodynamic behaviour of positive displacement machines generally – not only one particular machine type – based on a chamber model of the machine being investigated. The implementation of an experimentally based algorithm for the calculation of vacuum clearance flows enables the program *KaSim* to simulate the thermodynamic processing of positive displacement vacuum pumps.

The verification of the program has already been successful for rough vacuum conditions on a screw-type vacuum pump [3-5]. In fine vacuum the good degree of concordance between simulation and experiment obviously disappears. Here the degree of modelling inside the simulation is assumed to be insufficient so that additional physical effects - not modelled so far - become predominant in the machine characteristics.



Fig. 2:

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Roots vacuum pump investigated for the validation of the extended simulation software *KaSim*

- 1 Casing
- 2 Inlet port
- 3 Rotor
- 4 Gear wheels
- 5 Overflow valve

The aim of this study is to increase the accuracy of the simulation program and to enlarge the application range to fine vacuum conditions by modelling two further physical mechanisms presumed to be predominant in the machine characteristics of positive displacement vacuum pumps operating in this range of pressures. In the following the modelling of the influence of moving clearance boundaries on the characteristics of leakage flows as well as further losses mainly caused by sorption and desorption are described. A comparison of the simulated with measured machine characteristic of a Roots type vacuum pump operating in fine vacuum shows the validity of the extended model, **Fig 2**.

2. Simulation

2.1 The Simulation Software KaSim

The simulation program *KaSim* calculates simultaneously the state of working fluids inside the working chambers, taking into account interactive mass and energy flows through chamber connections (clearances, inlet and outlet areas or other chamber connecting elements) for given angles of rotation and for the whole working cycle [6]. It can safely be assumed that the state of the working fluids inside the chambers is approximately homogenous. The machine under investigation is described by the so called chamber model as an input parameter for the simulation program. The chamber model contains basically specifications concerning the existing working chambers and the connections between them and the high and low pressure port, **Fig. 3**.



Fig. 3: Chamber model of the Roots vacuum pump under investigation – consisting of 7 chambers (fluid capacities), 2 ports (infinite fluid capacities), 11 clearances and 6 internal chamber connections

Notation: chambers F and G form late in the working cycle at α = 60° and 90°

2.2 Clearance Flows in Fine Vacuum

In previous studies the specific conditions of clearance flows in vacuum have been researched and an algorithm has been derived to quantify the clearance mass flow for continuum flow, Knudsen flow and molecular flow conditions [7, 8]. Therefore the experimental data base for vacuum clearance flows has been analysed based on static gap contours without moving clearance boundaries. The implementation of the calculation model for clearance rates enables *KaSim* to simulate the thermodynamic processing of positive displacement vacuum pumps.

The deviation obtained between the simulated and measured machine behaviour increasing with higher rotor speeds and lower pressures indicates an appreciable influence of the moving boundaries on the clearance flow rate. Here the mean free path is greater than the characteristic dimension (e.g. clearance height) and the rate of flow is determined by the collision of molecules with clearance boundaries rather than molecule-molecule collisions. For molecular flow alone the effect is well-known, causing the pumping mechanism inside turbomolecular vacuum pumps.



Fig. 4: Enhanced module for the calculation of clearance leakage flows in positive displacement vacuum pumps

To consider the influence of moving clearance boundaries on the flow rate for molecular flow regime, the transmission probabilities of clearances are calculated using a theoretical approach to simulate a molecular flow of molecules using a Monte Carlo method, **Fig. 4**.

In the calculation the flight path of single gas particles through the geometry is simulated, while particles hitting the wall are reflected directly according to the cosine law. The basic assumptions of the calculation of transmission probabilities under molecular flow conditions are [9, 10]:

- (1) the flow is assumed to be molecular, i.e. there are no collisions between gas molecules;
- (2) the flow is assumed to be steady;
- (3) the adsorption of molecules on the system surfaces is ignored;
- (4) molecules have equal probability of entering at any point at the entrance of the clearance and they arrive with a diffuse distribution;
- (5) particles colliding with the systems walls are reflected according to cosine law.

The computer program uses a random number generator to model the statistical distribution for the entry of molecules as well as their reflection from system boundaries. Regarding the flight paths of a very large number of particles, the transmission probability of any clearance geometry can be calculated with good statistical accuracy. Such computed transmission probabilities describe the likelihood that a molecule entering the clearance geometry passes through the clearance and leaves via the outlet area. Thus the clearance flow rate can be calculated for molecular flow conditions usually occurring with the fine vacuum, **Fig. 5**. A particle number of 10⁵ delivers quite a constant transmission probability, increasing with clearance height as expected. In the following, simulated particle numbers and gap widths are set to have no influence on the calculation result.



Fig. 5: Calculated transmission probability using Monte Carlo method as a function of simulated particle number (plane clearance geometry) varying the clearance heights but with constant gap length and width (fixed clearance boundaries)





Modelling and analysing the influence of moving boundaries on the varying clearance leakage flow rate, the Monte Carlo method includes a superposed velocity vector due to the transport mechanism of a molecule leaving a non-fixed gap boundary, **Fig. 6**.

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Gas molecules entering the inlet area of the geometry acquire forward momentum by collisions with the moving walls in the main flow direction and against it respectively, while moving in the opposite direction [11]. For gas molecules entering the geometry, the collision with moving walls in the direction of the outlet area induces a sort of incidental beaming effect, resulting in a greater transmission probability than without the moving walls.

For backstreaming molecules entering through the

outlet area or colliding with moving walls, the velocity direction will be reversed toward the exit, resulting in a decreased transmission probability. When the velocity of moving walls is zero and the clearance geometry symmetrical, the probability of molecule transition for each direction becomes equal. As the velocity increases, the transmission probability in flow direction increases, while reverse transmission probability decreases rapidly, as shown in **Fig. 7** for a plane gap geometry.

For the plane gap geometry, a transmission probability of $P_{12} = P_{21} \approx 0.04$ is calculated with non-moving boundaries in both directions as expected for a symmetrical clearance situation. Increasing the relative velocity in the main flow direction causes a significant rise in the simulated transmission probability P_{12} and in the average collision rate of a molecule from 140 up to about 200. Here molecules are moving deeper into the clearance as a result of the transport mechanism. A further increase in the relative boundary velocity decreases the average collision rate while the transmission probability increases continuously with a decreasing gradient. For the technically interesting range of relative velocity from |w| = 20 to 100m/s, the transmission probability is more than doubled and increased more than tenfold respectively. The significantly changed clearance flow rate brought about by moving gap contours for molecular flow conditions suggests that this has a tremendous influence on the operating behaviour of positive displacement vacuum pumps in this flow regime.



Fig. 7: Calculated transmission probability P₁₂ and P₂₁ with the Monte Carlo method as a function of relative velocity |w| of moving clearance wall (plane gap geometry)

P (w=0)	transmission probability for non-moving boundaries
P ₁₂	transmission probability in the direction of the moving lower boundary
P ₂₁	transmission probability against the direction of the moving lower boundary
1	average collision probability - moving lower boundary in main flow direction
2	average collision probability - moving lower boundary against main flow direction

The calculation module for leakage mass flow inside *KaSim* distinguishes between different calculation methods according to the current flow regime. For viscous flow conditions the calculation is based on experimental results. Within the molecular flow regime the flow rate calculation is based on the Monte Carlo results regarding the influence of moving boundaries. In the transitional flow regime (Knudsen flow) an interpolation algorithm set up between the two calculation models is used to obtain a continuous model transition and avoid a jump in the modelling. Thus the interpolation algorithm is based on the Knudsen number and works in conjunction with the given interpolation function F for the calculation of the flow coefficient. Here within the transitional flow regime a minimum value for the conductance can be formed – the so-called Knudsen-minimum, **Fig. 8**.

$$\partial = \partial_{\exp}(1-F) + \partial_{MC-Sim} \cdot F$$
 (eq. 2) $F = \frac{Kn^{-1} - \ln(2)}{\ln(100) - \ln(2)}$ (eq. 3)



- Fig. 8: Interpolation algorithm to calculate clearance flows inside the Knudsen flow regime flow coefficient δ_0 as a function of inlet pressure (plane gap geometry)
 - δ_0 flow coefficient: ratio of leakage mass flow relative to theoretical maximum mass flow
 - A minimum flow coefficient in the transitional flow region (Knudsen-minimum)
 - 1 <u>molecular flow regime:</u> calculation of leakage flow based on Monte Carlo simulation results
 - 2 <u>Knudsen / transitional flow regime:</u> calculation of leakage flow by interpolation between Monte Carlo simulation results and experimental results [7]
 - 3 viscous flow regime: calculation of leakage flow based on experimental results [7]

2.3 Sorption and Desorption

Analysing the operating behaviour of positive displacement vacuum pumps – in particular Roots vacuum pumps in fine vacuum – the influence of physical effects such as sorption and desorption of gas molecules on solid machine surfaces (e.g. rotor) is used to explain the machine characteristics [12]. In general these phenomena are quite complex and very often depend on the given individual system of the fluids and surfaces (solid-fluid or fluid-fluid interaction).

Therefore, in addition to the effect of leakage flows through clearances, the influences of other losses are modelled en bloc, eq.4. A heuristic approach derived from the experiment is tested to describe the phenomena regarding a bypass given a dependency on the rotor speed f and outlet pressure p_V and also with a experimental factors, eq. 5, similar to [13].

$$\dot{V}_{eff} = \dot{V}_{th} - \dot{V}_{clearance} - \dot{V}_{return} \quad (eq. 4) \qquad \dot{V}_{return} = \dot{V}_{return}^* \cdot \frac{1}{1 + \frac{(p_V)^{C_1}}{p_{return}^*} + C_2} \quad (eq. 5)$$

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3. Experiment

To validate the enhanced simulation software and to analyse the quality of the modelling, an experimental investigation of a test machine operating in fine and adjacent rough vacuum is performed while varying a wide range of parameters (inlet and outlet pressure, rotor speed, clearance heights).

3.1 Test Machine

A widely-used dry-running Roots-type pump is examined on a test rig. Due to the simple machine design and operating principle without internal compression as well as quite clear clearance geometries, this machine type has been chosen as suitable for verifying modelling in the simulation.

The test machine utilises two figure-eight-shaped rotors which, synchronized by external gears, counterrotate in a housing without touching each other or the housing. Therefore necessary clearances limiting the working chamber are formed – the housing, intermesh and front clearances – causing undesirable internal leakage flows. To minimize other leakage flows through radial sealing outside the gear and bearing chambers, and also to minimize pump down time, the test machine operates with a magnetic coupling and gear chamber evacuation, **Fig. 9**.



Fig. 9: Test rig, schematic conception and measurement instrumentation to analyse the operating behaviour of the test machine (Roots vacuum booster WKP250, made by Pfeiffer Vacuum) in fine and adjacent rough vacuum

3.2 Experimental Set-up

The operating behaviour of the Roots vacuum pump is analysed in the range of 10⁻³ to 50mbar, varying the inlet and backing (fore) pressure as well as the rotor speed from 2700 to 6000rpm. The test machine is always operated with a backing pump. Here a screw-type vacuum pump with variable rotor speed is used – setting the discharge pressure of the test machine. Another backing pump working with the Roots mechanism is intended to achieve lower pressures in the fine vacuum region. To describe the main parameters of the machine characteristics, operating pressures and the flow rate are measured. To investigate the volumetric efficiency ambient air is sucked in while the regulating valves are used to adjust the inlet pressure of the test machine. When measuring the ultimate achievable compression ratio, the regulating valves are closed completely. Focussing on the leakage flow through clearances and their modelling within the simulation, the experimental investigation includes a variation in clearance heights. Therefore in the first instance two couples of figure-eight-shaped rotors are mounted with the same profile but different in dimensions. So a variation in housing and intermesh clearance is realized, **Fig. 10**.



Fig. 10: Investigation of different clearance heights – distribution of clearance height A and relative variation of clearances¹

¹ As the thermal loading of the test machine is quite low – maximum casing temperature is about 80 degrees for a maximum discharge pressure of 50mbar - constant clearance heights are assumed in the investigation.

4. Results and Discussion

4.1 Pumping Performance

Simulation results concerning the suction speed of the analysed Roots vacuum pump in fine vacuum characterise operating behaviour as expected, **Fig. 11**.

With constant outlet pressure and decreasing inlet pressure, the suction speed decreases continuously until the ultimate pressure is reached for a suction speed of zero. This is due to an increased pressure ratio at machine gaps, resulting in higher leakage mass flows and lower volumetric efficiencies. As a result of the transition from Knudsen to molecular flow characteristics inside the machine clearances, the operating pressure range increases with decreasing outlet pressures for the given data. Increasing the rotor speed results in higher suction speed and widens the application area, whereas the ultimate pressures achieved are lower.



A comparison of simulated and measured suction speed – given for a rotation speed of 3000rpm in Fig. 11 – shows quite good agreement. The influence of enlarged clearance heights causing lower suction speeds is reproduced by the simulation, as indicated in the experiment. For the given data the operating behaviour seems to be determined by leakage mass flows as this is the predominant physical effect indicated by the simulation.

1.2

n = 3000rpm 1 profile A profile B 0.8 0.6 0.4 profile C 0.2 0 0.01 0.1 10 100 1 outlet pressure pv [mbar]-1.2 $n = 6000 \text{min}^{-1}$ profile B 1 profile A 0.6 profile C 0.4 0.2 0 0.01 0.1 1 10 100 outlet pressure pv [mbar]

Fig.12: Measured ultimate compression ratio as function of the outlet pressure for different clearance heights

> rotor speed n = 3000rpm top: down: rotor speed n = 6000 rpm

Notation:	data is given relative to
	K _{0,max} (3000rpm) = 1

Clearance heights:

profile A: standard clearance heights +45% housing gap profile B: profile C: +45% housing gap +63% intermesh gap

4.2 Ultimate Compression Ratio K₀

The quite frequently used characteristic value to describe the operating behaviour and quality of vacuum pumps is the ultimate attainable compression ratio K₀ as a function of the outlet (backing pressure).² Based on the investigation of the influence of clearance heights on the ultimate compression ratio attainable, Fig. 12 shows the experimental data for two different rotor speeds 3000rpm and 6000rpm.

Decreasing the outlet pressure from 50mbar to about 1mbar causes a continuous rise in the compression ratio. Here higher rotor speeds leads to higher compression ratios. A further decrease in the outlet pressure below 1mbar results in decreasing compression ratios. Under theses pressure conditions dependence on the rotor speed is less significant, and other tendencies reverse.

For constant rotor speeds the maximum compression ratio decreases significantly with increased clearance heights, while the maximum moves to lower outlet pressures due to the changed transition pressures of the intermediate to molecular clearance flow. The influence of clearance heights is significantly inferior in fine vacuum compared with lower rough vacuum, as a result of the reduced molecular conductance of clearances.



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² Typical values for $K_{0,max}$ are in the range of 40 to 60.



Fig. 13:

Comparison of simulated and measured compression curve with constant rotor speed 3000rpm

- A <u>Kn < 0.5:</u> molecular flow regime
- C <u>Kn > 0.01:</u> viscous flow regime
- s exemplary clearance height / characteristic length

Notation:

data is given relative to ultimate compression ratio $K_{0,max,exp}$ (3000rpm) = 1 (profile A)

Given Knudsen numbers Kn are based on a constant gas temperature of T = 293K

Fig. 14:

Comparison of simulated and measured compression curve with constant rotor speed 6000rpm

- A <u>Kn < 0.5:</u> molecular flow regime
- B 0.01 < Kn < 0.5: Knudsen flow regime
- C <u>Kn > 0.01:</u> viscous flow regime
- s clearance height / characteristic length

Fig. 13 and **Fig. 14** compares the ultimate attainable comparison ratio in simulation and experiment. Also the expected transition pressures of different flow regimes are signified above the diagrams for technical used clearance heights.

The characteristic dependencies on the operating pressure, rotor speed and clearance height are mapped by the simulation. With outlet pressures above 3mbar the simulated compression ratios are predicted higher than measured. Deviancies increase with lower operating pressures from 50 to 3mbar and with higher rotor speeds. The maximum attainable compression decreases with increased clearance heights in experiment and simulation comparably, while the backing pressures do not coincide exactly. The movement of the maximum compression ratios to lower outlet pressures with increased clearances in the experiment is not reproduced in the simulation. Overall in this pressure range the influence of leakage flows through clearances is supposed to be predominant.

The substantially decreasing attainable compression ratios with lowered outlet pressures beneath 1mbar are modelled in accordance with the experiment. Here in the molecular flow regime the influence of other physical effects are getting predominant signified in the simulation. For the chosen approach an increase in the rotor speed regularly causes a higher attainable compression ratio. This does not cover the inversed dependency on the rotor speed observed for 6000rpm in the experiment.

5. Conclusions

The enhancement of the simulation software *KaSim* to describe the thermodynamic processing of positive displacement vacuum pumps presented here, increases the modelling depth and accuracy - so the application area is extended to fine vacuum conditions.

The molecular clearance flow is simulated and analysed using a Monte-Carlo method to include the influence of moving clearance boundaries on the leakage mass flow – a process which has not been modelled so far. Here a calculation program has been developed to analyse the transmission probabilities of any clearance geometry in detail. Results of the Monte-Carlo simulation indicate a significant impact on the calculated conductance of clearances with moving gap geometries even for relatively quite low velocities. The modelling of further losses mainly caused by sorption and desorption is described, using a heuristic approach derived from the experiment. A back flow is assumed, increasing with decreasing operating pressures.

Outlook:

Further investigations are intended to analyse the used empirical function to model sorption and desorption. Here the physical meaning have to be checked as well as the assignability and simplification of the empirical parameters for other Roots vacuum pumps.

Targeting additional validation and verification of the simulation system, further investigations will focus on the simulation and verification of screw-type vacuum pumps especially for operation in fine vacuum.

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