# Zusammenfassung

In der vorliegenden Arbeit werden inhomogene Druckverteilungen in Arbeitskammern von Schraubenspindelvakuumpumpen (SSVP) untersucht, die durch eine Überlagerung einer Schleppströmung und einer druckgetriebenen Strömung insbesondere bei niedrigen Kammerdrücken und hohen Drehzahlen auftreten. Infolge der Rotation wird in den Arbeitskammern ein Massenstrom in Richtung der bewegten Rotorzähne hervorgerufen, der im Profileingriff aufgestaut wird. Daraufhin stellt sich ein Druckgradient in entgegengesetzter Richtung ein, der diesen kompensiert. In der Arbeitskammer ist der statische Druck demzufolge ortsabhängig. Dieser Mechanismus führt zu einer deutlichen Vergrößerung der anliegenden Spaltmassenströme, da die Spalteintrittsdichte infolge der lokalen Druckerhöhung größer ist als bei einer homogenen Arbeitskammer. Beim Ansaugvorgang führt die inhomogene Druckverteilung dazu, dass weniger Masse in die Maschine angesogen werden kann und daraus folgend der Füllungsgrad reduziert ist.

Zur Berechnung der inhomogenen Druckverteilung wird die Arbeitskammer zunächst als Rechteckkanal abstrahiert, bei dem alle Wände (z.B. Rotorzahnflanken) eine Wandgeschwindigkeit entsprechend der kinematischen Beziehungen aufweisen. Anschließend wird eine eindimensionale Differenzialgleichung formuliert, die auf einer Überlagerung der Massenströme einer Druck- und einer Schleppströmung basieren. In Abhängigkeit der Gasverdünnung, der Geometrie und der Gas-Oberflächen-Interaktion ergibt sich ein Schließungsproblem, das separat mithilfe analytischer Lösungen und mit Ergebnissen der Direct-Simulation Monte Carlo (DSMC) Methode gelöst wird.

Das eindimensionale Modell wird in zweifacher Hinsicht validiert. Zum einen wird ein Vakuumprüfstand zur experimentellen Validierung errichtet, bei dem die Inhomogenität in einer Arbeitskammer über drei Druckmessstellen erfasst wird. Dabei zeigt sich eine gute Übereinstimmung zwischen Messungen und Modell. Zum anderen werden dreidimensionale numerische Strömungssimulationen (CFD) durchgeführt, die die Zulässigkeit einer Reduktion des Modells auf eine eindimensionale Strömung bestätigen. Mit instationären CFD-Simulationen wird außerdem die Kammerfüllung mit einem sich ausdehnenden Rechennetz untersucht. Durch eine Dimensionsanalyse wird gezeigt, dass die Inhomogenität in der Arbeitskammer sowohl für die Kammerfüllung als auch in gekapselten Arbeitskammern auf je einer Kurve zusammenfallen, sodass analytisch bestimmbare Funktionale abgeleitet und anschließend in die Kammermodelsimulationssoftware KaSim implementiert werden.

Abschließend wird eine Testmaschine simuliert und mit bereits vorhandenen Messergebnissen verglichen. Dabei können die Simulationsergebnisse von SSVPs mithilfe des inhomogenen Modells von Arbeitskammern deutlich verbessert werden. Dadurch, dass die Maschine in Betriebspunkten höherer Kammerinhomogenität deutlich ineffizienter ist, eignet sich die Auswertung der Funktionale in Abhängigkeit des geforderten Betriebspunktes zur Grobauslegung neuer Maschinen.

# Abstract

In the present work, inhomogeneous pressure distributions in working chambers of screw spindle vacuum pumps (SSVP) are investigated, which occur due to a superposition of a drag-driven and a pressure driven flow, especially at low chamber pressures and high rotational speeds. As a result of the rotation, a mass flow is caused in the working chambers in the direction of the moving rotor teeth, which is dammed up in the profile engagement. This causes a pressure gradient in the opposite direction, which compensates for this. The static pressure in the working chamber is therefore location-dependent. This mechanism leads to a significant increase in the applied gap mass flow rates, since the gap entry density is greater than in a homogeneous working chamber due to the local pressure increase. During the filling process, the inhomogeneous pressure distribution means that less mass can be sucked into the machine and the filling efficiency is reduced as a result.

To calculate the inhomogeneous pressure distribution, the working chamber is first abstracted as a rectangular channel in which all walls have a wall velocity corresponding to the kinematic relationships. Subsequently, a one-dimensional differential equation is formulated, which is based on a superposition of the mass flow rates of a pressure-driven flow and a drag-driven flow. Depending on the gas rarefaction, the geometry and the gas-surface interaction, a closure problem arises, which is solved separately using analytical solutions and results from the direct simulation Monte Carlo (DSMC) method.

The one-dimensional model is validated in two ways. On the one hand, a vacuum test rig is set up for experimental validation, in which the inhomogeneity in a working chamber is measured via three pressure measurement points. This shows good agreement between measurements and model. On the other hand, three-dimensional computational fluid dynamics (CFD) simulations are carried out, which confirm the admissibility of a reduction of the model to a one-dimensional flow. Transient CFD simulations are also used to investigate the chamber filling process with an expanding computational mesh. By dimensional analysis, it is shown that the inhomogeneity in the working chamber coincides on one curve each for both chamber filling and encapsulated working chambers, so that analytically determinable functionals are derived and implemented in the chamber model simulation software KaSim.

Subsequently, a test machine is simulated and compared with existing measurement results. It is obtained that the simulation results of SSVPs can be significantly improved with the help of the inhomogeneous model of working chambers. Since the machine is significantly more inefficient at operating points with higher chamber inhomogeneity, the evaluation of the functionals depending on the required operating point is suitable for a rough design of new machines.

# **1** Introduction

Today, vacuum technology plays a central role both in research and in industrial applications. The word *vacuum* is derived from the Latin word *vacuus*, which means *empty*, *void* and describes a space in absence of matter. As it is not technically possible to create a perfect vacuum, the International Organisation for Standardisation (ISO) provides the following definition:

"Vacuum [is a] commonly used term to describe the state of a rarefied gas or the environment corresponding to such a state, associated with a pressure or a molecular density below the prevailing atmospheric level."<sup>1</sup>

The first proof that air is also matter was provided by Galilei in 1613, who weighed a glass bottle containing compressed air or air at atmospheric pressure and determined a density value. From this it could be concluded that if air can be regarded as matter with mass, it can also be removed from a container. The first proof of this was provided by Torricelli in 1644, who filled a glass tube sealed on one side with mercury and immersed it in a water bath with the sealed end facing upwards so that the open end was wetted with water. The mercury did not leak completely into the water bath, but a vacuum formed at the upper end of the glass tube. Pascal repeated the experiment in 1646 with other liquids and found that the maximum height of the liquid in the glass tube is inversely proportional to the respective density. Together with Descartes, he developed the idea of being able to determine the air pressure p at different heights. In 1650, Guericke invented a pump whose seals and valves were sealed with water, which he used to evacuate a spherical container. Because of this historical experiment, such machines are still called pumps today instead of compressors, which is usually associated with incompressible media.<sup>2</sup>

Although the first vacuum pump was invented very early on, the physical phenomena had not been understood well yet. In 1835 Clapeyron<sup>3</sup> presents a formula that is today called the ideal gas law which relates the pressure of a certain gas to its respective density and temperature. In 1856 Krönig<sup>4</sup> presents a relation of the pressure based on a kinetic theory, where the gas is described as a large number of submicroscopic particles (atoms and molecules) that have a mass and a velocity. This theory was refined by Clausius<sup>5</sup> in 1857 and connects the kinetic theory with the ideal gas law and he investigates the concept of a mean free path of molecules, which is the mean length a molecule travels until it collides with another molecule. This is inversely proportional to the pressure of a gas. In 1860 Maxwell<sup>6</sup> proposes a mathematical relationship for the velocity distribution of particles in an equilibrium state depending on their average kinetic energy and in 1871 Boltzmann<sup>7</sup> proved, that the particle model fulfils the laws of thermodynamics. In 1909 Knudsen<sup>8</sup> showed in experiments of pressure driven flows through pipes in a vacuum that the flow behaviour can be characterized by a dimensionless ratio which is today called the Knudsen number Kn. This defines the ratio of

flow regime	continuum	rarefied gas			
		slip flow	transitional flow	molecular flow	
Knudsen number	Kn < 0.01	$0.01 \le Kn \le 0.1$	$0.1 \le Kn \le 10$	Kn > 10	
gas rarefaction parameter	$\delta > 100$	$100 \geq \delta \geq 10$	$10 \geq \delta \geq 0.1$	$\delta < 0.1$	

**TAB.** 1.1 Definition of flow regimes according to the Knudsen number by Beskok<sup>10</sup>.

the mean free path of the molecules to a characteristic length of a geometry. Alternatively the gas rarefaction parameter  $\delta$  is often used in the literature which is inversely proportional to the Knudsen number. In case of tubes the diameter is chosen as characteristic length and therefore the Knudsen number shows the ratio of intermolecular collisions to collisions of molecules with the surrounding wall. This characterises the mechanism of momentum and energy transport, which is dominated by intermolecular collisions for small Knudsen numbers, so that the gas can be regarded as a continuum. With large Knudsen numbers, the momentum and energy transport is mainly described by collisions of the molecules with the walls, so that this is considered a molecular flow. Due to the different dynamic behaviour of gases depending on the Knudsen number, a classification according to the Knudsen number is made. An example is given in **Tab. 1.1**. Therefore, a continuum is defined for Kn < 0.01 where intermolecular collisions dominate. Typically such a flow can be calculated by means of a continuum model but a slip on the wall occurs proportional to the molecular free path, that can be neglected for Kn < 0.01. For Kn > 0.1 the flow must be described by means of the kinetic theory of gases and for Kn > 10 intermolecular collisions can often be neglected. Gases for which the mean free path is a non-negligible quantity are called rarefied. In contrast, one speaks of a dilute gas when the mean free path is much greater than the molecular diameter which is of the order of  $10^{-10}$  m.<sup>9</sup>

Nowadays, a variety of vacuum pumps with different mechanisms of action for different flow regimes are developed. The pressure range of technically produced vacuums now extends over more than 15 decades  $(10^{-10} \text{ Pa} - 10^5 \text{ Pa})$ , so that a classification into different vacuum ranges depending on the pressure has been established as shown in **Tab. 1.2** with rounded values for the number density (number of particles per unit volume) and the mean free path. The vacuum regimes are subdivided into low (rough) vacuum (> 100 Pa), medium (fine) vacuum (0.1 Pa - 100 Pa), high vacuum  $(10^{-6} \text{ Pa} - 0.1 \text{ Pa})$ , ultra-high vacuum  $(10^{-9} \text{ Pa} - 10^{-6} \text{ Pa})$  and extreme-high vacuum ( $< 10^{-9} \text{ Pa}$ ).<sup>1</sup> The generation of technical vacuums is an elementary component of many industrial and scientific applications. In particular, the generation of clean, oil-free vacuums plays an important role, for example in the semiconductor, pharmaceutical, chemical and food industries, but also in scientific applications such as mass spectroscopy. For these purposes, the development of dry-running vacuum pumps has been driven forward in the recent past, so that contamination by auxiliary fluids such as oil can be avoided.<sup>2</sup>

**TAB. 1.2** Pressure ranges of vacuum technology with corresponding values of the number density and mean free path for air at 300 K rounded on full decades<sup>1</sup>.

vacuum regime	rough	fine	high	ultra-high	extreme-high
pressure [Pa]	$10^5 - 10^2$	$10^2 - 10^{-1}$	$10^{-1} - 10^{-6}$	$10^{-6} - 10^{-9}$	$< 10^{-9}$
number density $[m^{-3}]$	$10^{25} - 10^{22}$	$10^{22} - 10^{19}$	$10^{19} - 10^{14}$	$10^{14} - 10^{11}$	$< 10^{11}$
mean free path [m]	$10^{-7} - 10^{-4}$	$10^{-4} - 10^{-1}$	$10^{-1} - 10^4$	$10^4 - 10^7$	$> 10^{7}$



FIG. 1.1 Classification of the screw vacuum pump according to its operation principle.<sup>2,12</sup>

## 1.1 Dry-Running Screw Spindle Vacuum Pumps

The focus of the present work is the thermodynamic simulation of dry-running screw spindle vacuum pumps (SSVP), which have become increasingly important in recent years because they are able to produce technically clean vacuums and at the same time have a good tolerance to dirt particles and small quantities of liquid. As few machine parts are required due to the design, the assembly and maintenance effort of these machines is comparatively low. Together with their high suction speeds (up to  $2500 \text{ m}^3/\text{h}$ ) these machines are particularly interesting for industrial purposes. They offer pressure ranges from 0.1 Pa to atmospheric pressure and are therefore settled in the low and fine vacuum. In many applications they are used as fore vacuum pumps in combination with roots pumps or other vacuum pumps for high suction speeds in the fine or high vacuum regime.<sup>2</sup> The most important quantity for rotary positive displacement vacuum pumps is the suction speed, which describes the volume flow on the low pressure side. The lowest pressure that can be reached in a recipient with a vacuum pump without external leakage is called ultimate pressure.<sup>11</sup>

## 1.1.1 Classification and Working Principle

The classification of vacuum pumps is typically performed according to the operation principle and design type as shown in **Fig. 1.1**. A first subdivision can be made according to the principle of gas transfer and gas-binding vacuum pumps. Gas-binding vacuum pumps make use of absorption, adsorption, condensation and diffusion mechanisms to store gas within the pumps. Gas-transfer vacuum pumps transfer the gas through the pump and can be subdivided in kinetic vacuum pumps and positive displacement vacuum pumps. While kinetic vacuum pumps exert momentum to the gas molecules in the direction of flow, positive displacement vacuum pumps enclose the gas in a working chamber, compress it by reducing its volume and expel it under higher pressure. This is done in



**FIG. 1.2** Typical rotor profiles for SSVPs: a) symmetrical single start cycloid profile b) symmetrical two start cycloid profile c) asymmetric single start quimby profile

a cyclic manner either by an oscillatory or by a rotary movement. Rotary positive displacement vacuum pumps can be either single shaft or twin shaft and the screw spindle vacuum pump is a subset of the twin shaft screw vacuum pumps. The last distinction is made because SSVPs have wrap angles much larger than 360° due to the large pressure ratios and therefore require a different profile shape than is usually used for screw compressors. However, Nadler<sup>13</sup> showed that standard compressor profiles can also be used for vacuum pumps when they are operated as blowers.<sup>2</sup>

A further classification can be made on the basis of the rotor profile. Like all screw machines, SSVPs can be described by their face section, which is then twisted in the axial direction. This can be symmetrical and asymmetrical. Similar to a gear wheel, a meshing condition of the two rotors is described by a curve that connects the inner circle with the outer circle and divides the face section into a full profile and grooves. The number of grooves within one face section equals the number of teeth and is also called number of starts. The working chamber is then formed in the grooves between the rotors and the housing. In a symmetrical arrangement, the teeth of the face section are mirror-symmetrical as shown in **Fig. 1.2**. This means that the formed working chambers can be clearly assigned to a rotor. The tooth flanks are usually generated in a similar way to gear wheels with involutes or cycloids, whereby the profile near the inner circle is closed by means of envelopes. Symmetrical profiles can be used in single start and two start configurations. Rotors with single start profiles offer larger grooves leading to a better ratio of fluid volume swept to the construction volume and better properties regarding gap sizes and leakage paths. Two start rotors, on the other hand, are almost free of imbalance, which makes them particularly interesting for high-speed pump applications.<sup>14,15</sup>

To be able to run dry, the two rotors must run without contact. For this purpose, gaps between the rotors and the housing are essential, but these have an unfavourable effect on the thermodynamic process. Most of these operational gaps can be adjusted via the clearance. However, all symmetrical profiles also have a blowhole, which occurs between the rounding of the tooth tip and the intersecting edge of the housing due to the profile. With asymmetrical profile arrangements it is possible to reduce or even completely close this blowhole on one side while it is enlarged on the other side. This can even lead to a complete connection between the working chambers of both rotors. This is done for the quimby profile, as inner circle and outer circle are connected with a trochoid on one side and with an archimedean spiral on the other side. Therefore, in the ideal profile the tip of the trochoid touches the intersection edge of the housing and thus the blowhole on one side is closed and the whole working chamber is formed on both rotors limited by the inner circle and the spiral. The quimby profile is restricted to a single start rotor as otherwise a complete bypass from the high pressure side to the low pressure side would be established for large wrap angles. As the wrap angle

for compressors above atmospheric pressure is typically smaller than  $360^{\circ}$ , almost all rotor types there exploit the asymmetric configuration<sup>16–23</sup>. For screw spindles, asymmetrical profiles can also mean increased manufacturing costs, as they often have an undercut<sup>15</sup>.<sup>24</sup>

Finally, a further classification can be made on the basis of internal compression. The simplest design is the isochoric machine, whereby the gas is only compressed by a backflow of gas through the gaps. At low intake pressures, this is the worst case in terms of energy. The use of isochoric rotors can be improved considerably in terms of energy by compressing against an end plate. In this way, the volume of the discharge chamber is first reduced before the gas is pushed out. This procedure is usually used in the area of compressors that have a low wrap angle. With a larger wrap angle, the disadvantage here is that a large part of the gas is then only transported without being compressed. On the one hand, this leads to a pure transport phase, similar to the isochoric machine, in which compression only occurs via gap backflows, which is energetically unfavourable. On the other hand, the majority of the compression only takes place locally in the high-pressure working chamber, which means that there occur extremely high gas temperatures due to the large compression ratios. Therefore, the machine cooling can be challenging. Furthermore, small outlet areas are required for the use of an end plate, which leads to larger fluid velocities that increase throttling effects and pulsations due to the cyclic process. Furthermore, the discharge of process-related liquid quantities is made more difficult, for example in the chemical industry.<sup>2</sup>

Modern SSVPs usually realise internal compression via a variable rotor  $lead^{14,15,25-27}$ . Since the chamber volume scales with the lead, continuous compression can be achieved in this way from closing the working chamber on the low-pressure side to opening the working chamber on the highpressure side. The compression heat is thus distributed over a larger area of the machine and can be dissipated more efficiently. This reduces temperature peaks on the high-pressure side. Additionally by reducing the lead the same number of chambers require a shorter rotor length which has a positive effect on rotor dynamics and the size of the machine. Furthermore, an end plate is no longer required, which eliminates the disadvantages mentioned  $above^2$ . The design of the ideal rotor pitch is part of various optimisation efforts.<sup>22,28,29</sup> The internal compression ratio is often designed for intake pressures around 300 mbar to reduce over-compression at high intake pressures, which can affect the maximum torque required. As there are often problems with pressure relief valves in dry-running machines, they are often dispensed with in order to reduce the maintenance effort considerably<sup>2</sup>. An idea to overcome this problem is to increase the gap heights on the suction side in order to increase gap flows for high intake pressures. As the sealing effect of gaps increases at a lower pressure due to changed fluid mechanical conditions, the overall power consumption of the machine can be improved this way<sup>14</sup>. There exist further ideas to realise internal compression for example due to change of rotor diameter along the axis leading to conical rotors with either parallel or non-parallel  $axes^{27,30}$ .

Figure 1.3 shows an example for a modern screw spindle vacuum pump with abstracted machine parts. The rotors have a symmetric single start profile with a decreasing lead from low-pressure side to high-pressure side. The working chambers are filled both axially and radially. When the rotor continues to rotate, the trailing rotor tooth closes the working chamber. When the rotor continues to rotate, the fluid is conveyed axially and compressed by the successive reduction of the chamber volume. At the end of the working process, the leading rotor tooth opens the working chamber at a low volume on the high pressure side, so that the fluid can be discharged. The housing is



FIG. 1.3 Sketch of an SSVP with working principle.<sup>31,32</sup>

water-cooled via cooling channels. However, there are also concepts for air cooling in which a fan is placed on the shaft and blows air over cooling fins. The main rotor is driven by an electric motor and synchronisation gears are used to drive the female rotor and enable contactless operation. Seals between the bearings and the working chamber prevent contamination of the process gas with oil. For particularly clean processes, seal gas can also be used, but this has a negative effect on the machine's performance. Usually, an internal oil circuit is also installed and driven by the shaft to supply the bearings and the gearbox with oil and to dissipate the heat generated. In addition to the bearing concept presented here, the rotors can also be cantilevered. This makes the rotor dynamics more difficult, but on the one hand the sealing of the low-pressure side is significantly simplified and on the other hand cleaning can be carried out without dismantling the bearings in processes including dirt particles<sup>15</sup>.

## 1.1.2 Simulation of Screw Vacuum Pumps

Since prototyping is very time-consuming and expensive, predicting machine behaviour is of utmost importance. For this purpose, there are various approaches at different levels of complexity. The simplest level is based on analytical approaches, which usually make many simplifications and therefore serve to estimate orders of magnitude in order to carry out a rough design<sup>33</sup>. Ohbayashi et al.<sup>34</sup> investigated an analytical approach to estimate the suction speed for isochoric machines based on an isothermal approach by means of predefined dimensionless flow rates. Rohe<sup>35</sup> developed an analytical function for estimating the ultimate pressure of an SSVP using a series connection approach of pump stages. Nevertheless, for more complex models this needs to be solved by means of numerics. The model of a series of pump stages can be extended to calculate the suction speed in steady-state and is mainly used for screw spindles when conveying incompressible media, but has also been applied on SSVPs<sup>28</sup>. This can be seen as a simplified version of the chamber model simulation, which can generally be used to calculate positive displacement machines by abstracting them through one or more fluid volumes and different connections. Such a simulation tool named KaSim<sup>13,36</sup> based on mass and energy balance has been developed at the Chair of Fluidics at TU Dortmund University. A sketch of a chamber model for an SSVP with a symmetric two start cycloid profile is shown in Fig. 1.4. The different chambers are fluid volumes that are enclosed between the rotors and the housing and connected by gaps. The clearance between the rotor and the housing forms the housing gap and connects to adjacent chambers on the same rotor. The clearance between both rotors can be divided in the radial gap and the inter-lobe gap according to their shape. The radial clearance is placed between the inner diameter of one rotor and the the outer diameter of the other rotor and also connects chambers on the same rotors. The inter-lobe clearance is formed by the minimum distance between the lobes of both rotors. It connects both chambers on the same rotor and chambers of both rotors. The blow hole is the only gap that is given by the profile and not by a clearance and connects adjacent chambers of different rotors. Each chamber has a time dependent volume carrying mass and energy in axial direction. The fluid state inside the chamber is typically assumed to be homogeneous and is changed by mass and energy flows due to the gaps and heat can also be exchanged with the rotors and the housing due to temperature differences of fluid and solid. The characteristic properties of an operating point can be calculated by means of a time-stepping method via a work cycle. Therefore, the fluid state in each time step is changed by the change of volume and by inflowing and outflowing mass and energy flow rates due to the connections. On the low and high pressure side the chamber gets filled or discharged due to connections to the suction or discharge port respectively. The chamber model method is established in the simulation of rotary positive displacement machines<sup>36–40</sup> and is also applied for SSVPs<sup>24,28,35,41,42</sup>. Nevertheless, comparisons to measurements show remaining deviations of the operation performance at low intake pressures that need to be improved<sup>28,41</sup>. The quality of the method depends above all on the modelling depth of the gap flows  $^{22,35,43,44}$ . Particularly in the case of rarefied gap flows, many investigations have been carried out to determine the respective mass flow rates as a function of given boundary conditions<sup>12,35,41,45–50</sup>. Furthermore, modelling of heat transfers<sup>35,42</sup> can be important. While outlet throttling impacts the machine when an end plate is  $used^{2,51}$ ,  $Stratmann^{41}$  found out that this can be neglected without an end plate. He further investigated inlet throttling for large intake pressures in SSVPs, where a back flow from leading chambers can lead to a pressure rise in the suction chamber before it is closed. He was not able to investigate the chamber filling process for low intake pressures where gas rarefaction effects dominate.

A more detailed simulation approach is provided by multi-dimensional transient fluid dynamics simulations. These simulations are typically based on a continuum assumption, which is quickly violated in vacuum pumps due to the narrow gaps and the associated large Knudsen numbers at low pressure ranges. For moderate Knudsen numbers in the slip regime (**Tab. 1.1**), the continuum model can still be used if the boundary conditions at the walls are adjusted<sup>52,53</sup>. For more rarefied gases, a coupling with solvers based on the kinetic theory of gases would be needed. A coupling of such methods is under investigation<sup>54,55</sup>, nevertheless, this is not yet state of the art in commercial solvers and extremely time-consuming. Huck<sup>12,48</sup> calculated mass flow rates of single gaps using the stochastic Direct Simulation Monte Carlo (DSMC) method which sometimes took several days on a computing cluster. For compressors in the continuum regime such coupling is not needed and although the mesh generation is challenging for rotary positive displacement machines<sup>56–58</sup> these



FIG. 1.4 Sketch of an SSVP with two start cycloid profile and the corresponding gaps.

simulations have been successfully carried out since several years <sup>59–64</sup>. But even in the continuum regime the high wrap of SSVPs would be problematic due to the large amount of chambers and clearances that need to be meshed.

In the free molecular regime Nadler<sup>65</sup> simulated a roots pump that operates in fine and high vacuum by means of a test particle method where single molecules are simulated without intermolecular collisions where no mesh is needed. This method is not sufficient for SSVPs that also reach atmospheric pressure.

# 1.2 Investigation of Gas Flows

In addition to simulating the entire machine, it can also be useful to restrict oneself to partial aspects and investigate these specifically. Therefore, in this section investigations about internal flows for different driving forces are presented.

# 1.2.1 Poiseuille Flow

A main driving force for flows is a pressure difference causing a fluid to flow from high pressure to low pressure. Hagen and Poiseuille<sup>66</sup> derived an analytical solution for the resulting mass flow rate for such a flow through a pipe in the laminar continuum regime. Therefore, a pressure-driven flow through a channel or pipe is widely called Poiseuille flow. Maxwell<sup>67</sup> derived a solution for slightly rarefied gases predicting a velocity slip at the wall. Measurements in the whole range of the gas rarefaction have been done by Knudsen<sup>8</sup>. These results are reproduced by simulations based on the kinetic gas theory by Loyalka<sup>68</sup> and later by Sharipov<sup>69</sup>. Numerical and experimental investigations for a rarefied Poiseuille flow through short pipes have been carried out by Lilly et al.<sup>70</sup>

The pressure-driven flow between parallel plates in the continuum regime is found in almost any textbook for fluid dynamics, see for example Refs. [66, 71, 72]. For rarefied gas flows this is investigated by Cercignani et al.<sup>73,74</sup>, Loyalka et al.<sup>75–77</sup> and Sharipov<sup>78</sup> with different methods based on the kinetic gas theory. Analytical solutions for the mass flow rate in the slip regime are provided by

Arkilic<sup>79</sup>, Sharipov<sup>78</sup> and Graur et al.<sup>80</sup> and experimental investigations are carried out by Ewart et al.<sup>81,82</sup>.

Analytical solutions in the continuum regime for other cross sections can be found in Ref. [72]. Varoutis et al.<sup>83</sup> provide numerical and experimental investigations for rarefied gases through channels with circular, square, triangular and trapezoidal cross sections. Numerical and analytical approaches for channels with circular and elliptic cross sections are also investigated by Zhvick and Friedlander<sup>84</sup>. For the slip regime different analytical solutions for a flow through a rectangular channel are derived by Méolans et al.<sup>85</sup> and Titarev and Shakhov<sup>86</sup>. The latter also derived an analytical solution for the free molecular regime. In the transitional regime solutions are provided by Sharipov<sup>87,88</sup> as tabulated data.

For converging or diverging channels an analytical solution for the continuum regime is provided by Jeffrey and Hamel<sup>66</sup>. Measurements for rarefied gas flows are made by Graur and Ho<sup>89</sup> and Hemadri et al.<sup>90</sup>.

An upper limit for adiabatic frictionless mass flow rates is provided by Saint Venant and Wantzel<sup>91</sup>. This can be used for estimations in compressible flows, where the maximum flow velocity in a constant or converging channel is limited by the speed of sound.

# 1.2.2 Couette Flow

Another driving force causing a fluid flow is shear stress. Due to a movement of a wall, fluid is dragged in direction of the wall movement. This phenomenon occurs in any machine and is often investigated in the context of a flow between coaxial cylinders where the inner cylinder is rotating. Experimentally this is widely studied to investigate gas properties related to fluid friction.<sup>92–94</sup> Also a flow between parallel plates with relative tangential movement can be considered. In the continuum regime, this fundamental flow is found in any fluid mechanics text book<sup>66</sup> and is called Couette flow named by the physicist who originally formulated the problem. For rarefied gases both the flow between parallel plates and coaxial cylinders is widely investigated in the literature<sup>78,95–100</sup>.

An analytical solution for a Couette flow in a rectangular channel in the continuum regime is derived by Rowell and Finlayson<sup>101</sup> to describe the flow in a screw viscosity pump.

## 1.2.3 Thermal Creep Flow

Reynolds<sup>102</sup> investigated that a temperature gradient causes a fluid flow from cool to warm and named this flow thermal transpiration. Furthermore, he noticed that a temperature gradient can cause a pressure gradient with a zero net mass flow rate for finite inlet and outlet reservoirs in steady state. Therefore, the two driving forces cancel each other out. In his velocity slip condition on the walls, Maxwell<sup>67</sup> could also explain this phenomenon by non-equilibrium conditions of slightly rarefied gases and derived a solution based on a velocity slip that leads to a superposition of both Poiseuille and thermal transpiration mass flow rate. Nowadays this is a rather named thermal creep flow and is numerically investigated by Sharipov<sup>103</sup> in a flow through a pipe. A superposition of a Poiseuille and thermal creep flow between parallel plates is investigated by Sharipov and Siewert<sup>104–106</sup>. Numerical solution for a flow through a rectangular channel in the whole range of the gas rarefaction for such flows is also provided by Sharipov as tabulated data<sup>88</sup>.

#### 1.2.4 Mixed Flows

Fukui und Kaneko<sup>107–109</sup> derived based on the kinetic theory of gases, that the total mass flow rate in a channel caused by mixed driving forces (Poiseuille, Couette and thermal creep) can be calculated by superposition of the mass flow rates caused by the individual forces. They exploited this to calculate the behaviour of rarefied gas flows in slider bearings. Alexander et al.<sup>110</sup> use a similar approach and compare their results with numerical simulations of the DSMC method. Li and Hsieh<sup>111</sup> present an analytical solution for the flow in a single screw extruder pump where the flow is calculated by a laminar Couette-Poiseuille flow for high viscous fluids. Sharipov et al.<sup>112</sup> use a similar approach in the context of rarefied gases to simulate the operation behaviour of a Holweck pump. Similarly Huck<sup>12,47,48</sup> calculates the mass flow rates in the gaps of vacuum pumps. A comparison to experimental results shows that the model fits perfectly for rarefied gases, but fails in the continuum limit as the predicted fluid velocity exceeds the limit of the speed of sound. He additionally performs simulations based on the kinetic gas theory for the gap flows where he notices that there is no clear distinction between the flow in the gaps and the connected reservoirs in rarefied gases when there are moving walls applied.

For compressible channel flows with constant cross-section, analytical solutions exist for adiabatic frictional flows (Fanno flow) and for diabatic frictionless flows (Rayleigh flow). Shapiro<sup>113,114</sup> develops a one-dimensional differential equation with which a channel flow can be determined numerically for compressible frictional and diabatic flows with a change in cross-section. Müller<sup>46</sup> uses this differential equation and extends this model for rarefied pressure-driven gas flows by using Sharipov's flow coefficients for the friction closure problem in plane channels. Jünemann<sup>49</sup> extends this model so that a diabatic Couette-Poiseulle flow with variable cross-section in the entire range of gas rarefaction can be calculated, as occurs, for example, in the radial gap of SSVPs. He also takes into account flow separations<sup>50</sup> on the basis of an analogy to the Jeffrey Hamel flow.

### 1.3 Gas-Surface Interactions

The works presented in the previous section are related to a full heat and momentum exchange of the gas molecules with the wall. Maxwell<sup>67</sup> was the first who predicted a velocity slip between gas and wall for rarefied gases, that is increased if molecules that collide with the wall keep part of their tangential velocity leading to a reduced shear stress. This phenomenon is widely modelled with the so-called tangential momentum accommodation coefficient (TMAC) which is a dimensionless number depending on the pair of the gas and surface material<sup>115,116</sup>. Similarly a reduced heat flux can be obtained by non-complete heat exchange which is modelled with the so-called energy accommodation coefficient (EAC)<sup>115,117</sup>. Different models exist with slightly different definitions of these coefficients as described in detail in Sec. 3.5.5. The idea is that the coefficients for the gassurface interactions can be obtained by measurements. Therefore, Arkilic et al.<sup>79,118,119</sup> developed a measurement technique to extract the TMAC in a plane Poiseuille flow for rarefied gases by comparison to analytical solutions. A similar approach is used by Graur et al.<sup>120</sup>. Missoni et al.<sup>121</sup> compare simulation results to measurements of a thermal creep flow to extract the TMAC and EAC. Gabis et al.<sup>93</sup>, Loyalka<sup>122</sup> and Bentz et al.<sup>94</sup> use a spinning rotor gauge experiment to extract the TMAC. Acharya et al.<sup>116,123–125</sup> developed a procedure via disc spin-down time to extract the TMAC for different gas-surface material combinations and provide an overview about many works and results about this topic in Ref. [116].

Based on given parameters for the gas-surface interactions Sharipov provides dimensionless flow rates in tabulated form for Poiseuille flow and thermal creep flow through parallel plates<sup>126</sup> and through long tubes<sup>127</sup> for different combinations of gas surface-interactions with the result that the Poiseuille flow is mainly affected by the TMAC and hardly by the EAC. Furthermore, he derived slip coefficients for the continuum model by comparison to the kinetic gas theory<sup>128</sup>. Cercignani et al. use a variational approach based on the kinetic gas theory to provide reduced flow rates as tabulated data of a rarefied Poiseuille flow<sup>129</sup> and Couette flow<sup>95</sup> between parallel plates that have different TMACs.

In addition to the effect that the shear stress can be reduced by incomplete accommodation, surface roughness can even cause molecules to be scattered back in the opposite direction, leading to an increased shear stress. The effect of surface roughness is investigated experimentally by Lilly et al.<sup>130</sup>. Analytic surface roughness models are presented by Aksenova and Khalidov<sup>131–133</sup>. Zhang et al.<sup>134</sup> investigate the effect of surface roughness in a plane Poiseuille flow for rarefied gases and Yan et al.<sup>135</sup> simulate this behaviour for pipe flows while Su et al.<sup>136</sup> simulate the effect of surface roughness. Further numerical investigations are performed by Sazhin<sup>137–139</sup> where the surface roughness is abstracted geometrically with a surface structure in periodic patterns. In summary surface roughness leads to a comparably higher friction and thus to lower flow rates through the channel.

As already mentioned for slider bearings, rarefied gas flows do not only exist in vacuum application, but also in micro and nano electro-mechanical systems (MEMS/NEMS)<sup>140</sup>. An overview of different applications and phenomena is given by Narendran et al.<sup>141</sup> and Taassob et al.<sup>142</sup>. A critical review about the different measurement techniques for microfluidics is given by Morini et al.<sup>143</sup>.