Effects of spontaneous condensation in steam-driven screw expanders

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Abstract. Condensation and its effects on turbo machinery operation are well understood and have been widely investigated. However, only little scientific work on condensation in positive displacement machines has been published. Although, depending on machine type, high expansion rates and, as a consequence, significant supersaturation can be achieved for working fluids with a negative saturation vapour curve. In this paper the effects of spontaneous steam condensation in screw expanders are discussed. Classical nucleation theory is used for the thermodynamic simulation of operational behaviour. The study shows at which point during the expansion phase spontaneous condensation can be expected, and typical nucleation rates are determined. Since the calculation of condensation requires a suitable fluid model providing consistent data for the metastable region, the advantages of Pollak's equation of state over the IAPWS property formulation are demonstrated. The impact of released latent heat during expansion on chamber states is depicted. Furthermore, a comparison of purely metastable expansion with equilibrium expansion is provided in order to show the full range discrepancies.

1. Introduction
Condensation phenomena occur not only in everyday reality such as in the formation of clouds, but in a wide range of technical applications of all kinds. In particular, the development of droplets in gaseous fluids has been investigated in supersonic nozzles with regard to wet steam operation in the low pressure stages of steam turbines. However, very little scientific work on condensation in positive displacement machines has been published. Since screw expanders are very robust, which permits operation with a considerable amount of liquid enclosed in working chambers, they are highly suitable for use with only slightly superheated vapours or even two-phase fluids. Thus, utilising screw expanders for power generation in Rankine cycles with low temperature heat sources is a promising concept. However, for performance prediction and correct design it is necessary to take condensation into account during simulation. Here, a first approach is presented for the application of classical nucleation theory to the thermodynamic simulation of screw expander operation.

2. Condensation phenomena
Condensation generally describes the phase change of a fluid from gas to liquid, whereby a significant release of latent heat occurs. This process is further differentiated in filmwise or dropwise condensation on cooled solid surfaces and spontaneous condensation, which is characterised by the formation of droplets in a gaseous phase. While surface condensation
involves heat transfer through the solid surface, which is eventually covered by a condensate film, latent heat from spontaneous condensation is directly transferred to the surrounding gas phase.

The simulation of spontaneous condensation, which is the main subject of discussion in this paper, requires three models: first a formulation is required for the properties of condensing fluid that allows for the calculation of supersaturated vapour states; next, a model is needed to calculate emerging condensate nuclei per volume; and finally a model is required to describe the growth of droplets, thus quantifying mass- and heat exchange between the droplets and the vapour phase.

What is today known as classical nucleation theory (CNT) is based on the work of Volmer and Weber, Farkas, Becker and Döring, Zeldovich as well as Frenkel [1, 2, 3, 4, 5]. A detailed overview of the development and improvement of classical nucleation theory is given by Bakhtar et al. [6]. It is the most commonly used model for condensation calculation. Experimental validation of CNT was carried out in cloud chambers [7, 8, 9] and also in divergent supersonic nozzles, which allow for faster expansion and thus correspond to grid flows in turbo machinery [10, 11, 12, 13].

Fundamental work was carried out by Gyarmathy who presented an analytical approach for the calculation of condensation phenomena in nozzles with constant relaxation speed which allowed for efficiency predictions of wet steam turbines [14]. In addition, he developed a calculation model for the growth of small droplets which is also used in this paper [15].

2.1. Spontaneous condensation

Spontaneous condensation is defined as the formation of a disperse condensed phase in a supersaturated (subcooled) gas phase [16]. This metastable state is maintained only for a limited period of time and is attained when the binodal curve of both liquid and gaseous phase is crossed e.g. by expanding saturated or slightly superheated steam in fluid machinery. Supersaturated states of vapour are described by saturation $S$ with $p_V$ being the pressure of vaporous components and $p_{V,\text{sat}}$ the saturation pressure of condensable components corresponding to vapour temperature $T_V$ [17].

$$ S = \frac{p_V}{p_{V,\text{sat}}(T_V)} \quad (1) $$

Supersaturation ($S > 1$) is the first of three consecutive steps of spontaneous condensation. The second process is nucleation where clusters, which are small assemblies of bound monomers, emerge. With increasing supersaturation formation probability of stable clusters grows, and a significant number of clusters form spontaneously, acting as droplet nuclei. The final step in spontaneous condensation is droplet growth, whereby further monomers attach to existing droplets and clusters while released latent heat successively reduces the subcooling of the gas phase.

Besides this homogeneous mechanism taking place in pure vapour, droplet formation also occurs on wettable impurities, typically at lower supersaturation. This heterogeneous condensation affects the spontaneous condensation process, especially at a high particle number density of impurities [17]. The point of noticeable condensation onset is also referred to as the Wilson point in the literature.

In order to determine the course of spontaneous condensation, the first requirement is a calculation of the nucleation rate, which describes formation of stable clusters in terms of time and volume. Classical nucleation theory is based on an equilibrium model which allocates one cubic nuclei to each metastable fluid state [16, 1, 2, 3]. The first formulation of nucleation rate $J$ was later improved by adding factors for non-isothermality $\Theta$ and non-equilibrium $Z$ [17, 18]. The product of the condensation coefficient $\alpha_c$ and the first bracketed expression (collision probability) gives the number of colliding monomers with the critical cluster, given the particle density $n_V$, mean thermal velocity $\bar{c}_V$ and cluster surface area $O^*$. The exponential
expression denotes the formation probability of critical clusters with enthalpy of formation $\Delta G^*$ and Boltzmann constant $k$.

$$J = \Theta Z \alpha_c \left( \frac{n_V \bar{c}_V \bar{O}^*}{4} \right) n_V \exp \left( -\frac{\Delta G^*}{kT_V} \right) \quad (2)$$

Enthalpy of formation and ideal radius of critical clusters $r^*$ are highly dependent on supersaturation and surface tension of liquid phase $\sigma$. Here, an approach is used to calculate $\sigma$ without considering curvature radius of the droplets [19]. In the formulation $v_L$ is the specific volume of liquid and $R$ is the specific gas constant of condensing vapour.

$$r^* = \frac{2\sigma v_L}{R T_V \ln S} \quad (3)$$

As long as the vapour phase continues to exist in a supersaturated state, critical clusters grow swiftly by absorbing monomers, while releasing latent heat to the vapour phase. This exchange of mass and energy was described by Gyarmathy [15] for pure vapour and vapour gas mixtures where assumption were made in order to simplify the complex progress (e.g. homogeneous droplet state, no droplet interaction, no slip, phase equilibrium at droplet interface). The change in droplet radius over time $t$ for a pure vapour is hence described in the following. In this formulation $\Lambda_V$ is the mean free path, $\lambda_V$ is the thermal conductivity of the vapour phase, and $\Delta h_v$ is the specific latent heat. Temperature and supersaturation are determined for vapour outside the droplet near field. Gyarmathy’s formulation for droplet growth is based on complete heat exchange between droplet and vapour phase and considers both Knudsen and continuum range.

$$\frac{dr}{dt} = v_L \frac{1 - \frac{r^*}{r}}{r + 1.59 \Lambda_V} \frac{\lambda_V R T_V^2 \ln S}{(\Delta h_v)^2} \quad (4)$$

2.2. Implementation of classical nucleation theory for screw expander simulation

CNT is used to model droplet formation during steam expansion in screw expanders. An idealised expander cycle is analysed in order to show the full impact on operation, and to isolate condensation from typical loss effects such as leakage and throttling.

An ideal isobaric chamber filling is assumed, which reduces occurrence of condensation strictly to the expansion phase, which is assumed to be isentropic. Furthermore, isobaric discharging at a constant back pressure is postulated. The condensation model is implemented in self-developed simulation software. Since the calculation of nucleation rate and droplet growth depend highly on supersaturation, a suitable fluid model, which will be discussed later, is vital. Here, Pollak’s fundamental equation for water and steam is implemented [20]. It generates fluid state data with temperature and density input. Hence, root finding features are used for iterative calculation with differing input pairs. This provides highly accurate fluid data but requires high computation time.

An overview of the simulation process is given in figure 1. Based on the expander’s chamber volume history, the expansion phase is divided in calculation steps with a selected time step. During each time step pressure-volume work is calculated initially with current isentropic expansion coefficient. Updates of chamber pressure and temperature are calculated, based on changes in internal energy due to the pressure-volume work being performed. The updated chamber state is checked for supersaturation, and eventually the calculation routine for classical nucleation theory is deployed. Provided that the nucleation rate generates a sufficient number of nuclei, a new droplet set is initiated and needs to be considered during the remaining part of the simulation process. For a given expansion start near the saturation curve, the number of droplet sets is in the range of five percent of the calculation steps. After generation
of new nuclei, droplet growth of all existing droplet sets is calculated according to the current chamber state. Mass and heat exchange between the vapour and liquid phase are determined, based on the change in droplet radius over time. Chamber pressure, temperature and specific internal energy for the time step in question are finally calculated at a constant chamber volume. Indicated work $W_i = \int p \, dV$ and indicated power $P_i = n \cdot W_i$ are later determined by the integration of pressure history with respect to the chamber volume. This approach allows for implementation in more complex multi-chamber simulation, where initial changes of states are not only affected by performed pressure-volume work, but also by internal leakages, which result in higher simulation quality.

2.3. Simulation parameters
The calculation model presented in this study requires several numerical parameters as well as machine parameters. The condensation coefficient in equation 2 for nucleation rate is $\alpha_c = 0.7$ for all presented data. In the formulation for droplet growth (equation 4) the selected droplet radius needs to be slightly larger than the critical value for initial growth rate of emerged critical clusters. Here $r^*$ is increased by 0.1%, which has no significant effect on simulation results. With respect to time-dependent droplet growth, the expansion phase is discretised with a defined time step $\Delta t$ and the droplet growth equation is linearised. A sensitivity analysis with regard to maximal supersaturation during expansion and indicated power $P_i$ implies $\Delta t = 1.0 \cdot 10^{-7}$ s being sufficiently small for the parameter range in question.

Relevant information on the machine geometry, which determines the volume curve and links tip speed with rotational speed, is shown in table 1.

3. Expander cycle with spontaneous condensation
The influence of spontaneous condensation on an ideal expander cycle is shown in figure 2. The following observations refer to expander tip speed $u_{male} = 80 \, m/s$, inlet pressure $p_{in} = 6.0 \cdot 10^5 \, Pa$, with no superheating and outlet pressure $p_{out} = 1.0 \cdot 10^5 \, Pa$. Ideally, chamber pressure equals inlet pressure during the filling phase. Isentropic expansion starts when the chamber volume reaches the start value defined by the built-in expansion volume ratio. At this point the high pressure control edge seals the chamber under examination. When maximum volume is reached the chamber passes the low pressure control edge, and ideally isochoric pressure compensation takes place. The outlet phase is assumed to be isobaric at outlet pressure level.
Since the expander is fed with saturated steam, the wet steam region is reached instantly when pressure drops at the start of expansion. If fluid states are calculated in thermodynamic equilibrium (which is the borderline case of infinitely slow expansion), optimal chamber pressure is reached and thus maximum pressure-volume work is obtained. If no phase transition is taken into account and the working fluid is dry supercooled steam, pressure develops at a lower level during expansion. The depicted metastable fluid states correspond to the borderline case of infinitely fast expansion, where all condensation phenomena are suppressed. It should however be noted that at the latest when the spinodal curve is reached, and metastability is no longer in force, condensation must occur.

The continuous line in figure 2 describes pressure history calculated with classical nucleation theory. At the start of expansion the steam is in metastable (dry) state, and due to low supersaturation, the nucleation rate is low, see figure 3. The nucleation rate raises rapidly with increasing supersaturation, until large numbers of emerging droplets release latent heat to the vapour phase, thus reducing supersaturation. The continuing expansion phase is characterised by low supersaturation, since heat and mass exchange between growing droplets and vapour take place without delay. The course of droplet growth during expansion is depicted in figure 4. The continuous grey line marks the critical radius of emerging nuclei, which is characterised by vertical asymptotes for \( S = 0 \). In general, the critical radius is small compared to droplet size at the end of expansion. As supersaturation decreases rapidly after reaching a global maximum,

![Figure 3: Supersaturation and nucleation rate during expansion.](image)

![Figure 4: Critical cluster radius and growth during expansion for exemplary droplet sets.](image)

| characteristic          | value                        |
|-------------------------|------------------------------|
| rotor profile           | SRM A                        |
| number of lobes         | 4 (male) / 6 (female)        |
| maximum chamber volume  | 26254 mm³                    |
| expansion volume ratio  | 4.0                          |
| rotor tip diameter      | 58.9 mm                      |
| axis to axis distance   | 46.2 mm                      |
the critical radius increases with ongoing expansion. This causes droplets that did not grow larger than the current critical radius to reduce in size (see formulation for droplet growth) and eventually reevaporate. Hence, the formation of stable droplets is limited to a relatively small window during the expansion phase. Continuous black lines show the course of droplet growth for representative sets. Weighting with the number of droplets per set $z_j$ makes it possible to calculate an average droplet size $\bar{r}$.

$$\bar{r} = \frac{\sum (r_j z_j)}{\sum z_j}$$

For the given example, the average droplet size is $\bar{r} = 1.7 \cdot 10^{-7}$ m, which indicates a shift of emphasis towards droplets emerging in range of maximum supersaturation.

4. Influence of expander operation on spontaneous condensation

Figure 5 shows a comparison of indicated power for a process with spontaneous condensation and a process in thermodynamic equilibrium for inlet pressure $p_{\text{in}} = 6 \cdot 10^5$ Pa and back pressure $p_{\text{out}} = 1 \cdot 10^5$ Pa. Expander tip speed is varied from $u = 20$ to $120 \text{ m s}^{-1}$. Superheating is displayed from 0 K to 30 K. With increased superheating spontaneous condensation takes place later during expansion phase since the saturation curve is crossed at a later point in time and at lower pressure. However, a greater influence on pressure history by means of spontaneous condensation is determined for superheated steam. The calculated nucleation rates decrease with increasing superheating, and thus higher supersaturation is reached. Higher supersaturation and consequently lower pressure-volume work is also observed at higher expander speed. This results from smaller time frames for heat and mass exchange between droplets and the vapour phase. In general it needs to be noted that spontaneous condensation only has minor effects on ideal pressure history and thus expander power.

CNT provides valuable information on droplet size and distribution, see figure 6. It can be shown that the effect of superheating on droplet size at the end of the expansion phase is negligible. Droplet size is mainly affected by expander speed, and average droplet radius also decreases with faster expansion. Within this study, droplet size is in the range of 0.1 to $0.5 \cdot 10^{-6}$ m, which, according to Gyarmathy’s studies, indicates relatively uniform droplet distribution and deceleration times in the range of $10^{-6}$ s, which leads to practically no slip between droplets and vapour [14]. This furthermore allows for the correct choice of two-phase
flow models for gap and port flows for future detailed simulative investigations of steam-driven screw expanders.

Despite having only a minor impact on chamber pressure, detailed modelling of condensation process illustrates the correct development of temperature during expansion. Maximum supersaturation for variations of expander speed and inlet pressure is depicted in figure 7 for saturated steam. A major impact factor on supersaturation during expander operation is the negative slope of the saturation curve, which decreases for water at low pressures. Expanders operating with low pressure steam are more likely to be affected by condensation effects than expanders operating at high pressure levels. Moreover, only consideration of intermittent supersaturated vapour states allows for correct modelling and analysis of heat transfers during expander operation. Figure 8 shows the temperature history during expansion for variations in inlet superheating. The temperature calculated in thermodynamic equilibrium is depicted for saturated steam only for reasons of clarity. It is noted that assuming change of state in thermodynamic equilibrium for complete expander process might lead to defective temperature course.

5. Property formulations for metastable fluid states

Calculation of time-dependent spontaneous condensation process requires a suitable fluid model to provide accurate data for the metastable region. Non-ideal fluid data is normally calculated with fundamental equations, which are adapted to extensive experimental data. However, it seems there are no experimental data on subcooled steam, as common measurement principles affect metastable fluid states (e.g. surface condensation on temperature sensors). As a consequence, property formulations for superheated steam need to be extrapolated in the metastable region. Figure 9 shows isobars calculated with various fluid models [20, 21]. Metastable isobars show continuous progression, whereas isobars in the thermodynamic equilibrium feature the familiar discontinuity when passing the saturation curve. It is noted that extrapolation of the IAPWS equation for the pressure in question is limited to a maximum supersaturation of $S_{\text{max}} = 2.8$. The depicted low gradients of metastable isobars calculated with IAPWS equation are characteristic for all pressure ranges. Since the measurement of higher supersaturation than maximum values calculated with IAPWS formulation is documented in the literature (e.g. in [11]), extensive extrapolation is not recommended. However, excellent
accuracy is achieved for steam data in thermodynamic equilibrium.

A slightly less complex approach for a canonical equation of state was presented by Pollak and is used for this investigation [20]. As depicted in figure 9 it shows reasonable behaviour when applied to supersaturated states and coincides with alternative formulations like Young’s simplified equation while offering higher accuracy and wider range [22]. Advantages over real gas equations (e.g. Van-der-Waals, Redlich-Kwong) are the provision of accurate data for both liquid and vapour phase, and the ability to determine all required data by derivates of just one equation for specific free energy.

6. Outlook
Classical nucleation theory provides an initial model for the prediction of spontaneous condensation in screw expander chambers. The calculation of subcooled steam states permits future modelling of heat transfer to expander machine parts at non-equilibrium temperature levels. Future work will focus on this external heat exchange and eventually combine mist formation and surface condensation on machine parts. It is noted that latent heat transferred to machine parts is lost and cannot raise the temperature of expanding vapour. Furthermore, a calculation of droplet size and formation time in expander chambers with CNT lays the foundation for detailed droplet simulation in order to map their trajectory, and where appropriate identify collisions with expander surfaces.

In addition, CNT is applicable to compressible vapour flows in screw expanders. For example, considerable supersaturation might occur during inlet phase, especially at the beginning and end of filling process, due to small port cross sections and relatively high pressure ratios at the opening. The same effect might take place in gap flows when working chambers with high pressure differences are connected. It is a debatable point whether or not the supersaturation period in these accelerated flow is long enough to induce spontaneous condensation, since the steam is decelerated again in the chamber.

The performance of screw expanders is significantly influenced by internal leakages. High flow velocities in the gaps lead to high heat fluxes. If the surface temperature is below the vapour temperature film- or dropwise condensation might occur. Future work should focus on leakage flow in order to analyse vapour states and identify potential condensation phenomena on expander surfaces.
7. Conclusion
Spontaneous condensation during the expansion phase of screw expander was modelled with classical nucleation theory providing a first simulation tool for droplet formation in screw expanders. Despite showing only a minor effect on indicated power, the study provides valuable information on temperature development during expansion and subcooling during the period after the saturation curve is crossed. Furthermore, droplet size is determined, which allows for the detailed simulation of interaction between the vapour and liquid phases. Typical droplet size for screw expander in question is between 0.1 and 0.4·10^{-6} m. One major influence on droplet size is expander speed. Maximum supersaturation is in the range of 1.8 to 3.0. The level of supersaturation during expansion is mainly affected by pressure boundary conditions.

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## List of symbols

| Symbol | Unit                  | Property                        | Subscript | Property                  |
|--------|-----------------------|---------------------------------|-----------|--------------------------|
| \( \bar{c} \) | m s\(^{-1} \)      | mean thermal velocity           |           |                          |
| \( J \)  | m\(^{-3} \) s\(^{-1} \) | nucleation rate                 |           | \( CNT \) classical nucleation theory |
| \( k \)  | J K\(^{-1} \)       | Boltzmann constant              |           | \( i \) indicated        |
| \( \dot{m}_{VL} \) | kg s\(^{-1} \)     | condensation mass flow          |           | \( in \) inlet           |
| \( n \)  | m\(^{-3} \)         | particle density                 |           | \( j \) control variable |
| \( n \)  | s\(^{-1} \)         | expander speed                  |           | \( L \) liquid           |
| \( O \)  | m\(^{2} \)          | surface                         |           | \( max \) maximum        |
| \( p \)  | Pa                   | pressure                         |           | \( out \) outlet         |
| \( P \)  | W                    | power                            |           | \( sat \) saturation     |
| \( \dot{Q}_{LV} \) | W                   | latent heat flow                |           | \( TE \) thermodynamic equilibrium |
| \( r \)  | m                    | radius                           |           | \( V \) vapour           |
| \( R \)  | J kg\(^{-1} \) K\(^{-1} \) | specific gas constant          | \( CNT \) | \( * \) critical cluster |
| \( s \)  | J kg\(^{-1} \) K\(^{-1} \) | specific entropy                |           |                          |
| \( S \)  | –                    | supersaturation                  |           |                          |
| \( t \)  | s                    | time                             |           |                          |
| \( T \)  | K                    | temperature                      |           |                          |
| \( u \)  | m s\(^{-1} \)       | tip speed                        |           |                          |
| \( U \)  | J                    | internal energy                  |           |                          |
| \( v \)  | m\(^{3} \) kg\(^{-1} \) | specific volume                 |           |                          |
| \( V \)  | m\(^{3} \)          | volume                           |           |                          |
| \( W \)  | J                    | work                             |           |                          |
| \( z \)  | –                    | number of                        |           |                          |
| \( Z \)  | –                    | non-equilibrium factor           |           |                          |
| \( \alpha_c \) | –                    | condensation coefficient         |           |                          |
| \( \Delta G \) | J                   | enthalpy of formation            | \( CNT \) |                          |
| \( \Delta h_v \) | J kg\(^{-1} \)       | specific latent heat             |           |                          |
| \( \Delta t \) | s                   | time step                        |           |                          |
| \( \lambda \) | W m\(^{-1} \) K\(^{-1} \) | thermal conductivity            |           |                          |
| \( \Lambda \) | m                    | mean free path                   |           |                          |
| \( \Pi \) | –                    | pressure ratio                   |           |                          |
| \( \sigma \) | N m\(^{-1} \)       | surface tension                  |           |                          |
| \( \Theta \) | –                    | non-isothermal factor            |           |                          |