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# Numerical modelling of the evaporative cooling effect on solid walls in steam sterilisers



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# ABSTRACT

Steam sterilisation is based on high heat transfer rates which occur during the condensation of steam on medical devices or the steriliser walls themselves. To ensure these high heat transfer rates, non-condensable gases (NCGs) such as air must be removed from the chamber. One method is to extract the NCGs by using vacuum pumps. Due to the reduction in pressure, the saturation temperature drops as well, causing water droplets to evaporate; thus, the walls and loads cool down. This mechanism was investigated using a three-phase CFD model. A highly time-efficient heat transfer model for the evaporation process was developed as a result of this investigation. Evaporative cooling effects on the steriliser walls could be achieved by using a mass source term which varied in terms of time and space. Our results indicate that the model can be used to predict the temperatures of the fluid as well as the solids in a numerically inexpensive manner. In addition, this model allows the user to predict whether surfaces can be completely dried, an aspect which is crucial for ensuring the quality of a sterilisation process. The model created allows researches to simulate the entire sterilisation cycle, addressing a previously existing knowledge gap. Furthermore, the presented methods are also suitable for use in other industrial applications where condensation and evaporation effects on solids need to be effectively and inexpensively determined.

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# 1. Introduction

One of the most well-known methods of sterilising medical equipment and thus making it reusable is steam sterilisation. This method is effective due to the high heat transfer raters which occur when steam condenses on medical equipment, such as dental drills and scalpels. This condensation causes the equipment to heat up quickly and, at the same time, helps to kill bacteria, as this is temperature-dependant [1]. An important advantage of using this method rather than, e.g. sterilisation by UV light, is that steam can reach even the smallest surfaces in internal cavities.

In order to ensure the highest possible sterility, all noncondensable gases (NCGs), normally represented as air, must be removed from the autoclave [2]. Various studies have already shown the immense decline in the heat transfer rates that occurs

\* Corresponding author. E-mail address: simon.pletzer@tugraz.at (S. Pletzer). during the condensation of steam in the presence of NCGs [3–7]. One common approach taken to remove the NCGs is to use a vacuum pump. During the so-called "pre-sterilisation phase" (Fig. 1), the pressure is alternately reduced (vacuum pump, see Fig. 1 mark "y") and increased by injecting steam into the chamber. By the end of these pulsations, all NCGs should have been removed, and the main "sterilisation phase" begins. As a result of these reductions in pressure, previously formed condensate starts to evaporate from hot surfaces, thus cooling them. While this is an undesirable effect in the "pre-sterilisation phase", as the strong cooling of the solids coincides with an increased energy or steam demand when the pressure subsequently increases, this effect is utilised in the last phase of the sterilisation process. In this so-called "drying phase" (Fig. 1) the pressure is reduced once more, forcing the condensate to evaporate from the hot surfaces of the medical equipment, thus both cooling and drying them. The principle of vacuum drying is also used in other fields, such as in the food [8] and nuclear industry [9]. A more detailed description of the entire sterilisation cycle can be found in [10-12].

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**Fig. 1.** Measured gas temperature (PT1000) and pressure inside the steam steriliser over the entire sterilisation cycle. Phase 1: Heating Phase (HEA); Phase 2: Pre-sterilisation Phase; Phase 3: Sterilisation Phase; Phase 4: Drying Phase. Markings: y - vacuum phases; I - simulated in a previous paper [12]; II - simulated in the present work.

It is of crucial importance to ensure dry loads at the end of the sterilisation process. A wet wrapping can not ensure a microbiologial barrier around the load, thus raising the possibility of recontamination [13]. Perkins, for example, found that wet textile packaging poses a significant hazard due to microbial migration [14]. Currently, it is assumed that other microbiological barriers are also ineffective when wet [15,16]. Van Doormalen et al. found out that 78% of 125 hospital sterilisation facilities recognised that wet loads occurred at frequencies ranging from monthly to every load [13]. Based on these data, there is a need to develop new and better autoclaves.

In the past years, more virtuell models of steam sterilisers have steadily emerged. Their advantages are clear: These models enable important factors to be identified in advance, reducing the need to build costly prototypes. Iacono et al. [17], for example, developed a neural network that can be used to predict the global course of fluid temperature and pressure within an industrial autoclave. Lau et al. [18] perfomed a 1D simulation of an empty steam steriliser which calculated the heat transfer under quasi steady state conditions. In a next step, these authors improved their model to predict the heat transfer to loads [19]. However, their approach has certain limitations regarding its ability to predict local phenomena. Feurhuber et al. [20-23] created a 3D model of a steam steriliser using computational fluid dynamics (CFD). Their main achievement was the development of a time-efficient heat transfer model based on condensation effects. In their model, however, the walls of the steriliser were never considered as solids, meaning that their temperatures were set based on measurements. While this approach has a justified use when considering existing sterilisers, it has limitations when developing new sterilisers or modifying the existing ones. Pletzer et al. [12] increased the level of detail by calculating the temperatures of the walls based on condensation effects. They investigated the "heating phase" (see Fig. 1 mark "I") of the sterilisation cycle. During this phase, steam is used to heat up the walls of the steriliser from the inside. Using steam has two main advantages: Firstly, no heating elements are required to heat up the chamber, and secondly, a large proportion of the NCGs have already been displaced from the chamber before the previously mentioned pre-sterilisation phase begins [12]. However, to the authors' best knowledge, no publication has addressed the modelling of the evaporative cooling effect in steam sterilisers, which mainly occurs during pressure reductions (see Fig. 1 mark "y" and "drying phase").

In general, the evaporation process that a single drop of liquid undergoes is already a highly complex physical process. In order to model this process, knowledge is required about the vapour diffusion in the gas phase, natural convection in the gas phase, convection in the liquid phase, evaporative cooling at the liquidgas interface, and even the heat conduction within the substrate [24]. Experimental and numerical studies on the evaporation of a single droplet as well as of thin films, can be found in the literature [24-29]. These studies involved investigations of transport phenomena on a micro-scale. Although those results are of enormous value for research, the methods used in these studies are not yet suitable for application on an industrial scale. Thousands of droplets would have to be finely resolved to perform an accurate simulation. Therefore, the aim of this work was to model the conjugated heat transfer due to evaporation in a numerically inexpensive manner at high temporal and spatial resolutions. For this purpose, the first vacuum phase of the sterilisation cycle (see Fig. 1 mark "II") was investigated by performing CFD simulations. These simulations were performed by using the Eulerian multiphase model. This approach is suitable for a variety of applications ranging from the simulation of steam turbines [30] to the simulation of water vapour transport in the porous structure of gypsum boards during a fire test [31]. The model for the calculation of the vacuum phase was validated by comparing the simulated and measured fluid and wall temperatures. The simulation was initialised by using the results of HEA (see Fig. 1 mark "I"), which were discussed in detail in a previous publication [12]. This model was also created to address an important knowledge gap, representing the final step in closing the loop and enabling the simulation of the entire steam sterilisation cycle (Fig. 1, t = 0 - 700 s). As a result, this model can be applied to gain new insights into the load positioning in the future, e.g. to prevent excessive load cooling during the pre-sterilisation phase or to improve load dryness at the end of the sterilisation cycle. The latter, as already mentioned, is an important factor for maintaining a microbial barrier around the



Fig. 2. (a) Numerical grid of the outer walls and symmetry plane; (b) Numerical grid of a cross section through the entire domain (fluid and solid parts), including locations of the six temperature sensors on the outer wall (T1-T6): T1 - left-hand side wall rear, T2 - door, T3 - bottom wall, T4 - back side wall, T5 - top wall, T6 - left-hand side wall middle, (c) water layer in which the mass source term is applied.

medical equipment [14–16]. Furthermore, the developed model can also be used in other industrial areas, where the heat transfer between solids and fluids due to condensation and evaporation plays an important role.

#### 2. Temperature and pressure measurement

The simulation was validated by making temperature measurements of the fluid phase and on the outer surfaces of the chamber. The fluid temperature inside the chamber was recorded by using a type J thermocouple and a PT1000 temperature sensor. The temperature on the outer wall of the chamber was measured at six different locations (see Fig. 2) by using type J thermocouples. In addition, the pressure of the gas phase was also measured. A more detailed description of the measurement system can be found in [12].

## 3. CFD model

The CFD simulations in this study were carried out by using the commercially available software ANSYS Fluent v20R2. User-defined functions (UDFs) were developed to model the saturation temperature as a function of the partial pressure, the heat transfer rates due to wall condensation and evaporation (see Section 3.3), and a mass source term near the walls (Section 3.4).

# 3.1. Problem description

As mentioned in Section 1, the present work placed a focus on the first vacuum phase (see Fig. 1, mark "II") in the sterilisation process. During this phase, the pressure is reduced from 1.2 bar to 0.4 bar by using a vacuum pump. Since the saturation temperature drops due to the lower pressure, the liquid water starts to evaporate from the hot walls. This phase change removes the previously added heat from the solids.

During HEA, the heat transfer due to the condensation effects was modelled by using a numerically inexpensive method that was first published by Feurhuber et al. [20]. Applying this method enables the enhancement of the heat transfer, applying so-called convective augmentation factor ( $CAF_{cond}$ ). The  $CAF_{cond}$  is defined from the ratio of the actual Nusselt number (due to condensation) to



Fig. 3. Liquid water distribution near the walls at the end of the HEA simulation (Fig. 1 mark "I").

that of an ideal flow (forced/natural convection), see Eg. (1) [32]. The value of this ratio can be determined by using empirical formulas. During HEA, the value of  $CAF_{cond}$  is approximately 250 [12]. The HEA modelling and results of applying this model, are presented in more detail in [12].

$$CAF_{cond} = \frac{Nu_{cond}}{Nu_{ideal}} \tag{1}$$

The advantage of applying this method, however, is that is becomes unnecessary to model the wall film, which would require a very fine grid resolution near the walls. Due to the simplified modelling process, the resulting condensate appears in the form of a "mist" near the walls. As an example, Fig. 3 illustrates the volume fraction of liquid water adjacent to a wall at the end of the HEA simulation. The volume fraction immediately indicates that no liquid wall film (volume fraction of liquid water close to 1) has formed. This result is not surprising since, as already mentioned, no wall film model was used; however, this leads to problems when simulating the vacuum phase.

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# 3.2. Multiphase flow modelling

The multiphase flow inside the steam steriliser was modelled using a three-phase Eulerian model in which steam was defined as the primary phase, and liquid water and air were defined as the secondary phases. The material properties of all phases were set with references to the Fluent database. The turbulence was considered by applying the realisable  $k - \varepsilon$  turbulence model, which was first published by Shih et al. [33]. By using the Eulerian multiphase model, the continuity equations for mass (Eq. (2)), momentum (Eq. (3)) and energy (Eq. (5)) are solved for each phase. Eq. (2) illustrates the mass continuity equation for the  $q^{th}$  phase:

$$\frac{1}{\rho_{rq}} \left( \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) \right) = \sum_{p=1}^n (\dot{m}_{pq} - \dot{m}_{qp}) + S_q$$
(2)

where  $\rho_{rq}$  represent the volume averaged density,  $\alpha_q$  is the volume fraction, and  $\vec{v}_q$  is the velocity of the  $q^{th}$  phase. The mass transfer due to condensation and evaporation are considered by  $\dot{m}_{pq}$  respectively,  $\dot{m}_{qp}$ . The last term  $S_q$  represents the mass source term of the  $q^{th}$  phase. By default, its value is zero, but this was set by using a UDF in order to simulate the evaporative cooling effects. More detailed information is provided in Section 3.4.

The conservation of momentum is solved for each phase according to Eq. (3):

$$\frac{\partial}{\partial t} (\alpha_q \rho_q \vec{v}_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla \mathbf{p} + \nabla \cdot \tau_q + \alpha_q \rho_q \vec{g} + \sum_{p=1}^n (K_{pq}(\vec{v}_p - \vec{v}_q) + \dot{m}_{pq} \vec{v}_{pq} - \dot{m}_{qp} \vec{v}_{qp})$$
(3)

$$K_{pq} = \frac{\rho_p f}{6\tau_p} d_p A_i \tag{4}$$

where  $\tau_q$  is the  $q^{th}$  phase stress-strain tensor, and  $\vec{v}_{pq}$  is the interphase velocity. The interphase momentum exchange coefficient  $K_{pq}$  is calculated according to Eg. (4). The drag function f was determined using the Schiller-Naumann approach and the interfacial area density  $A_i$  using the "symmetric" model [32].

The conservation of energy in Eulerian multiphase applications, can be written for each phase as:

$$\frac{\partial}{\partial t}(\alpha_q \rho_q h_q) + \nabla \cdot (\alpha_q \rho_q \vec{u}_q h_q) = \alpha_q \frac{dp_q}{dt} + \overline{\tau}_q : \nabla \vec{u}_q - \nabla \cdot \vec{q}_q + \sum_{p=1}^n (Q_{pq} + \dot{m}_{pq} h_{pq} - \dot{m}_{qp} h_{qp})$$
(5)

where  $h_q$  is the specific enthalpy of the  $q^{th}$  phase,  $\vec{q}_q$  is the heat flux,  $Q_{pq}$  is the intensity of heat exchange between the  $p^{th}$  and  $q^{th}$  phases, and  $h_{pq}$  is the interphase enthalpy. More detailed descriptions of Eqs. (2)–(5) can be found in the literature [32].

A double-precision pressure-based solver was used to calculate all governing equations. The "Quadratic Upstream Interpolation for Convective Kinematics" (QUICK) scheme was used to discretise all quantities. The time step size  $\Delta t$  was set to 0.02 s, and the number of iterations per time step was set to 40. Halving the time step size resulted in no notable deviations in temperature, pressure and volume fraction curves. Additional information about the modelling, e.g. the phase diameters, can be found in [12].

#### 3.3. Heat transfer modelling

As already mentioned in Section 3.1, the heat transfer due to condensation during HEA was modelled by using the  $CAF_{cond}$ . Several studies [12,20–23] have successfully demonstrated the enormous advantages of applying this approach. This approach enables the user to calculate the heat transfer due to condensation on an

arbitrarily shaped surface with a relatively coarse mesh resolution near the wall with a high level of numerical efficiency. Other studies by Zschaeck et al. [34], Mimouni et al. [35], Qiu et al. [36], Yoon et al. [37], Phan et al. [38], and Li [39], which also determined the heat transfer due to condensation, had certain limitations regarding the surface shapes or requirements related to the mesh resolution. However, this model has the effect, as already described in Section 3.1, that no homogeneous water film is formed near the walls in the numerical simulation. Consequently, the solver underestimates the heat transfer during evaporation, since it cannot represent all processes that occur on a microscale (e.g. internal flow in the water film due to convection). Therefore, we extended the heat transfer model from Feurhuber et al. [22] for the case of evaporation. Empirical formulas were used to calculate the Nusselt number resulting from evaporation (Eq. (7)) and natural convection (Eq. (12)) on a horizontal rectangular plate.

$$CAF_{eva} = \frac{Nu_{eva}}{Nu_{ideal}} \tag{6}$$

Firstly, the boiling characteristics were determined by investigating the temperature difference  $\Delta T$  between the wall and the fluid. Measurement data indicated a natural convective boiling behaviour, since  $\Delta T$  was less than 2 K during the vacuum phases. Stephan et al. [40] proposed using an empirical correlation to determine the Nusselt number for natural convection boiling *Nu*<sub>eva</sub>. These authors conducted a regression analysis of almost 5000 experimental data points and obtained the following correlation for water:

$$Nu_{eva} = 0.246 \cdot 10^7 X_1^{0.673} X_2^{-1.58} X_3^{1.26} X_4^{5.22} \tag{7}$$

$$X_1 = \frac{qd}{\lambda_l T_{sat}} \tag{8}$$

$$X_2 = \frac{rd^2}{a_i^2} \tag{9}$$

$$X_3 = \frac{c_{p\_l} T_{sat} d^2}{a_l^2}$$
(10)

$$X_4 = \frac{\rho_l - \rho_g}{\rho_l} \tag{11}$$

where  $\dot{q}$  is the heat flux density, d is the equilibrium break-offdiameter,  $\lambda$  is the thermal conductivity,  $T_{sat}$  is the saturation temperature, r is the enthalpy of evaporation, a is the thermal diffusity,  $c_p$  is the heat capacity, and  $\rho$  is the density.

In contrast, the Nusselt number for convection  $Nu_{ideal}$  was calculated according to Eq. (12). Ra stands for the Rayleigh number and Pr for the Prandtl number.

$$Nu_{ideal} = 0.766 \cdot \left( Ra \cdot \left( 1 + 0.536 \cdot Pr^{-11} / 20 \right)^{-20} / 11 \right)^{1/5}$$
(12)

Depending on the temperature difference  $(\Delta T)$  between the wall and the fluid, i.e. the driving force for natural convection,  $CAF_{eva}$  falls within a range of 7 ( $\Delta T=10$  K) to 18 ( $\Delta T=1$  K) during the vacuum phase. Since the temperature difference between the walls and the fluid was less than 2 K, when the walls were mainly cooled due the evaporative cooling effect,  $CAF_{eva}$  was set to a constant value of 18. By extending the heat transfer model from Feurhuber et al. [22], three cases can now be distinguished, depending on whether the wall temperature is above or below the saturation temperature.

$$Nu = \begin{cases} Nu_{ideal} \cdot CAF_{eva} & T_{wall} \ge T_{sat} \\ Nu_{ideal} \cdot \frac{CAF_{cond}}{2} & T_{wall} < T_{sat} \text{ and } \phi_{steam} < 0.9 \\ Nu_{ideal} \cdot CAF_{cond} & T_{wall} < T_{sat} \text{ and } \phi_{steam} \ge 0.9 \end{cases}$$
(13)

#### Table 1

Comparison of the wall temperatures at the end of the vacuum phase (t = 135 s).

	T1	T2	T3	T4	T5	T6
measurement CFD - $S_w \& CAF_{eva}$ CFD - no models	94.7 91.4 99.9	93.2 88.5 94.6	82.0 84.6 95.1	82.5 84.7 95.9	78.3 80.7 98.9	86.8 86.9 98.6

In the first case in Eq. (13), the wall temperature  $T_{wall}$  is higher than or equal to the saturation temperature of the water  $T_{sat}$ . As a result, evaporation occurs, and the ideal Nusselt number, as calculated by the CFD code, is multiplied by  $CAF_{eva}$ . The two other cases represent the existing model created by Feurhuber et al. [22]. Both address the case for condensation, depending on the volume fraction of steam  $\phi_{steam}$ . If the volume fraction of steam falls below a value of 0.9,  $CAF_{cond}$  is halved. This distinction is made because an increased occurrence of NCGs significantly reduces the heat transfer due to condensation effects [22].

The extended heat transfer model as well as the saturation temperature were implemented into the CFD code using a UDF. The saturation temperature  $T_{sat}$  is thereby specified as a function of the partial steam pressure, and more detailed information about this is provided in [12]. The phase change of the water was modelled with the Lee model [41]. Thereby, the fluid condenses when its temperature  $T_p$  is below the saturation temperature  $T_{sat}$  (see Eq.(14)) and evaporates when its temperature  $T_q$  is higher than  $T_{sat}$  (see Eq. (15)). The important values for the evaporation ( $r_{qp} = 10,000 \text{ s}^{-1}$ ) and condensation frequency ( $r_{pq} = 2000 \text{ s}^{-1}$ ) were chosen, to reflect the measured data as closely as possible. The heat transfer between the phases was modelled by taking the Ranz-Marshall approach [42,43].

$$\dot{m}_{pq} = r_{pq}\phi_p\rho_p \frac{T_{sat} - T_p}{T_{sat}}$$
(14)

$$\dot{m}_{qp} = r_{qp}\phi_q\rho_q \frac{T_q - T_{sat}}{T_{sat}}$$
(15)

#### 3.4. Modelling the evaporative cooling effect

As already described in Section 3.1, simulating the vacuum phase turned out to be a difficult task. The condensate that had previously formed in the HEA simulation (Fig. 1 mark "I"), did not evaporate from the walls; therefore, they cooled only by convection. The difference in the wall temperatures between the measurements and simulation reached up to 20 K by the end of the vacuum phase (Table 1). The lack of the evaporative cooling effect is attributed to the formation of condensate "mist" (Fig. 3), which has formed due to the used heat transfer model for condensation. As already described in Section 3.1, the advantage of using this model is that extremely efficient calculations of the condensation on the walls can be made. This efficiency results from the circumstance that no wall film model is needed; hence, no homogeneous condensate film formes on the walls (Figs. 3 and 4). This means, on the one hand, that few evaporation effects occur, because the contact between the wall and liquid water is absent (see Fig. 4), and on the other hand, that the wall adhesion effects are underestimated due to the lack of information about the droplet shape, whereby the condensate is easily transported away from the walls when the vacuum is generated. In order to calculate the vacuum phase as efficiently as possible, a mass source term of liquid water  $(S_w)$  is applied in the first cell layer near to the walls (see Fig. 2). However, this source term is considered to be constant neither in time nor in space which is linked to uneven distribution of the condensate by the end of the simulation of HEA (see Fig. 5 a).

The mass content of liquid water in each cell of the water layer  $(m_{Cell_l})$  is used as the basis for determining whether the mass source term is applied or not. This content can be calculated from the volume fraction of liquid water  $\phi_l$  and the volume  $V_{cell}$  of the respective cell (see Eq.(16)).

$$m_{Cell_l} = \phi_l \cdot V_{cell} \cdot \rho_l \tag{16}$$

In a second step, this mass needs to be adjusted, since the condensate formed by the end of HEA is located in several cell layers near the wall, as shown in Fig. 3. Firstly, the mass distribution of the liquid water in the first cell layer near the wall  $\psi_{water-layer}$  is calculated by dividing the mass of the liquid per cell  $m_{Cell_1}$  by the total mass of liquid water in the water layer  $m_{tot-layer_1}$  (see Eq.(17)). The location of these two masses are shown in Fig. 4.

$$\psi_{water-layer} = \frac{m_{Cell_l}}{m_{tot-layer_l}} \tag{17}$$

Secondly, this distribution is then multiplied by the total mass of liquid water present in the whole fluid domain  $m_{tot_1}$ . This adjusted mass of liquid water  $m_{UDM}$  is finally stored in a so-called User Defined Memory (UDM), illustrated graphically in Fig. 5 b. By using a UDM, the previously mentioned problem of wall adhesion can be avoided, as its values are not influenced by the flow field. As a result, drop adhesion as it exists in reality can be simulated with high efficiency. In general, due to the low velocities of the gases (i. e. less than 0.02 m/s) during the vacuum generation process, negligible droplet movement can be assumed. Another advantage of using the mass as a decision variable is the grid independency. If the height of the first cell layer varies, the volume fraction can be an unreliable variable for determining the actual condensate distribution (see Eq. (16)). This also explains the noticeable differences in Fig. 5 a and b. For example, areas with a comparably low volume fraction have a higher mass than vice versa.

$$m_{UDM} = \psi_{water-layer} \cdot m_{tot_l} \tag{18}$$

The described procedure is performed before running the actual simulation of the vacuum phase. During the simulation, the stored mass of the liquid water in the UDM  $m_{UDM}$  changes as a result of evaporation and condensation. In each time step, the CFD code calculates the mass transfer rates resulting from the Lee model (see Eqs. (14) and (15)) and passes the associated change in mass of each cell (see Eqs. (19) and (20)) to the UDM (Eq. (21)). In the case of condensation, this means that the liquid water mass increases in the UDM and decreases in the case of evaporation. As soon as a value of zero is reached (i.e. all liquid water has evaporated), the mass source term is deactivated. By applying this method, wet spots can be identified at the end of the vacuum phase and especially the drying phase. Thus, simulations can be used to determine in advance whether loads can be dried or not.

$$\Delta m_l = \dot{m}_{pq} V_{cell} \Delta t \tag{19}$$

$$\Delta m_{\nu} = \dot{m}_{qp} V_{cell} \Delta t \tag{20}$$

$$m_{UDM_{l+1}} = m_{UDM} + \Delta m_l - \Delta m_\nu \tag{21}$$

#### 3.5. Computational grid

A poly-hexcore mesh consisting of 475,383 elements with a maximum skewness of 0.79 and a maximum aspect ratio of 21.81 was generated. As shown in Fig. 2, the geometrical symmetry was used to simulate only one-half of the chamber. In order to be able to simulate the evaporative cooling effects, the walls were modelled as solids. As already mentioned, considering the walls as solids in steam sterilisers is a difficult task, because it requires the



**Fig. 4.** Multi-phase approach for water vapour and water liquid near the walls. Graphical representation of the mass of liquid water per cell in the water layer  $m_{cell_i}$ , the total mass of liquid water in the water layer  $m_{tot-layer_i}$  and the total mass of liquid water in the whole fluid domain  $m_{tot_i}$ .



**Fig. 5.** (a) Volume fraction of liquid water at the start of the vacuum phase which was obtained from the simulation of HEA [12], (b) Distribution of the adjusted mass of liquid water  $m_{UDM}$  (in milligrams), which is stored into the UDM at the beginning of the simulation.



**Fig. 6.** Grid dependence study for the first 25 s of the vacuum phase for the results of the average gas temperature and the solid temperature at the location of T5.

user to model complex physical processes such as wall condensation or, as in this case, evaporation cooling. In general, this is the first paper to present a method for modelling the latter phenomenon on an industrial scale using CFD.

The thermally inert behaviour of the thermocouple was considered by modelling a simplified copper cylinder (Fig. 2). A grid independence study was conducted using a grid with 806, 512 cells. Due to the increased number of cells and the associated increased computation time, the first 25 s (t = 80-105 s - compare Fig. 1) of the vacuum phase were examined. Fig. 6 demonstrates that there has been hardly any change in the course of the average gas temperature (*Tgas*) as a result of the grid refinement. Similar small deviation can be observed in the wall temperature of measuring point T5. The remaining five measuring points (T1-T4 & T6) showed an equally good agreement. Furthermore, it should be noted that the coarse mesh has already been used for the simulation of HEA as well. The results of the grid independence study allow the conclusion that both phases (HEA and vacuum phase) can be simulated with the same grid. Therefore, the coarse grid was used to calculate the remaining part of the vacuum phase.

### 3.6. Boundary conditions

During the simulation of the vacuum phase, only the outlet is opened. The reduction in pressure, caused by a vacuum pump, was considered by using a time-dependant pressure profile which was obtained from the measurements. The heat transfer to the solid walls was calculated on the basis of the model described in Section 3.3. During the measurements, the whole chamber was isolated with mineral wool; therefore, the outer walls were assumed to be adiabatic in the simulation. The mass source term of Section 3.4 was defined with a value of  $S_w = 5 \frac{kg}{m^3 s}$  as long as the values in the UDM were greater than zero, as soon as this limit was reached the source term was deactivated. An initial estimation for this value was made from the average cooling of the chamber during the measurement. From the associated heat loss, a value for the mass source term can be calculated via the evaporation enthalpy, the volume of the first cell layer in which the source term emerges (see Fig. 2) and the duration of the vacuum phase. In addition, simulations with a mass source term of 2.5  $\frac{kg}{m^3s}$  and 10  $\frac{kg}{m^3s}$  were performed as well. While the cooling was underestimated with the lower value of 2.5  $\frac{kg}{m^3s}$ , the simulation with an increased source term of 10  $\frac{kg}{m^3s}$  showed few differences in terms of wall temperature as compared to the one with 5  $\frac{kg}{m^3s}$ . This can be explained by the circumstance that, beyond a certain value, the mass source term cannot be completely evaporated. In Summary, all boundary conditions are shown schematically in Fig. 7.



Fig. 7. (a) Geometry and boundary conditions for exterior walls, interior walls, outlet, and symmetry plane, (b) boundary conditions for the interior walls and the mass source term of liquid water  $S_w$ .



Fig. 8. Measured and simulated fluid temperatures and pressures in the steam steriliser during the first vacuum phase.

## 4. Results

#### 4.1. Fluid temperature and pressure

Fig. 8 compares the measured (thermocouple (TC) and PT1000) and the simulated fluid temperatures in the steriliser. Two temperature curves from the simulation were used for the validation. The first is the mass-weighted average temperature of the whole fluid domain (CFD - Tgas avg - red dashed line) and the second is the mass-weighted average temperature of the 1-mm solid cylinder (CFD - Tsensor - red solid line) which is placed in the rear part of the fluid domain (Fig. 2). No source term was used around this simplified sensor; however, both simulated temperature curves fit the measurement curve closely. The maximum deviation of the simplified sensor is only 1.5 K as compared to the thermocouple (TC). The simulated average gas temperature is always slightly lower than the measured values, which can be explained perfectly by considering the thermal inertia of the temperature sensors. This close agreement is also an indication that the volume fractions of air and steam were determined correctly, since the saturation temperature is a function of these quantities.

In addition, the average gas temperature without using the models to induce an evaporative cooling effect (*CFD* - *Tgas\_avg* without - red dotted line) is shown in Fig. 8. This means that no mass source term  $S_w$  (see Section 3.4) or the *CAF*<sub>eva</sub> (see Section 3.3) was used in this calculation. In the first 35 s (t = 80-115 s), few differences can be observed between the global course of the fluid temperatures with or without the models. In Fig. 9 b,

however, it can be seen that the gas beginns to heat up at t = 115 s due to the hot walls. This heating process accelerates from this point on, due to the decreasing amount of water droplets in the gas. At the end of the simulation (t = 135 s), the simulated temperature without the models is 13 K above the measured temperature. This leads us to the conclusion that modelling the evaporative cooling effect is also essential for correctly determining the fluid temperature.

Lastly, the consistency of the pressure curves was achieved by applying the previously mentioned time-dependant boundary condition at the outlet.

#### 4.2. Temperature of the walls

The focus of this work, however, was placed on correctly determining the wall temperatures. As mentioned in Section 2, six thermocouples were attached to the outer wall of the pressure chamber (Fig. 2). The first two measurement points which will be discussed are located on the rear left side wall (T1) and on the door (T2). The simulation, including the modelling of the evaporative cooling effect, overpredicts the cooling at both locations. The deviation as compared to the measurement (i.e. 3.3 K and 4.7 K, respectively) occurs at the end of the vacuum phase (t = 135 s)(Fig. 10). Due to the hydraulic circuit, a steam inflow was audible in the first seconds of the vacuum phase. It is, therefore, highly likely that additional condensate was flushed away, thus reducing the cooling effect. This process has the greatest influence on the measurement points of T1 and T2, as these two have displayed the least cooling out of all six measuring points (Table 1). For this reason, the simulation with the standard models shows the best agreement at these two locations. However, the situation is completely different for the remaining four measuring points of T3-T6. These exhibit a deviation ranging between 13 K und 20 K at end of the simulation (t = 135 s). Fig. 11 b immediately demonstrates that hardly any cooling has occurred on the walls. The main result was only a more homogeneous temperature distribution. One reason for the minimal cooling effect can be seen in Fig. 12. The initial distribution of the condensate did not remain for 2 s on the walls. This circumstance can be attributed to the heat transfer model used for condensation, as already described in Section 3.4. In this way, the effects of wall condensation can be calculated efficiently, meaning that there was no need to model the wall film, but that the model greatly underestimate, for example, the wall adhesion effects. Simulations using wall adhesion models with increased contact angles did not significantly improve the results. A different approach was taken by setting the velocity of the liquid water phase in the boundary layer to zero. Liquid water could only escape from this region by transforming into its gaseous state. Again, no evaporative cooling effect was observed, and the main

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**Fig. 9.** fluid temperature at three cross sections at four different time steps: at t = 80 s - start, at t = 95 s, at t = 115 s and at t = 135 s - end of the simulation, (a) simulation with the proposed models ( $S_w \otimes CAF_{eva}$ ) for the evaporative cooling effect, and (b) without.

problem remained the same: The condensate interacted very little or not at all with the walls. Consequently, no evaporation occurred, and the walls cooled only as a result of convection.

For these reasons and in order to maintain numerical efficiency, the method described in Section 3.4, was developed. Fig. 10 reveals the excellent agreement of the measuring point T3 to T6 over the whole period. The maximum deviation of these four measuring points is 2.6 K at the end of the simulation (Table 1). The course

of T6 is particularly highlighted, as the simulation could be used to determine the point in time (t = 115 s) at which the condensate had completely evaporated and thus the strong cooling effect had ended. Based on the presented results, it is possible to conclude that the initial condensate distribution (Fig. 12 a) was determined correctly during the HEA simulation. This circumstance can be attributed to the flow field. In HEA, areas formed in which the condensate is collected, i.e. so-called 'dead water' areas. As a result,



Fig. 10. Comparison between the measured and simulated wall temperatures at all six locations. Simulation with the mass source term and the enhanced heat transfer due to evaporation ( $S_w \otimes CAF$ ) and without these models (no models).

gravitational forces represented a subordinate role. In comparison, maximum velocities of 0.02 m/s were observed in the vacuum phase, breaking up these dead water areas, and the condensate fell towards the bottom due to gravity. This led to an increased occurrence of condensate on the base, which can be seen in Fig. 12 b. Finally, the outstanding efficency of the presented models must be mentioned. The application of the  $CAF_{eva}$  (Section 3.3) and the mass source term  $S_w$  (Section 3.4) did not result in any appreciable increase in computing time. With a Threadripper  $3960 \times 24$ -core, the simulation time was 81 h. The advantage of using this model in terms of time saved as compared to using a wall film model cannot be quantified without further studies. However, it is possible to assume that the application of such models would require much more computation time due to the required boundary layer resolution and the additional transport equations that need to be

solved. Therefore, the described methods can be applied to achieve excellent results on an industrial scale.

#### 4.3. Wet spots

Lastly, the wet spots inside the chamber were investigated. Fig. 13 illustrates the change in the adjusted mass of liquid water  $m_{UDM}$  (Section 3.4) throughout the period of the vacuum phase. As already described, these mass values changed due to the mass transfer rates determined by applying the Lee model. Fig. 13 d identifies the locations where the condensate could not evaporate completely, and most of this condensate remains on the lower edge of the door and on the back side wall.

It is extremely useful to be able to examine the dryness of surfaces, and especially with loaded chambers during the

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**Fig. 11.** Temperature distribution on the interior walls at four different time steps: at t = 80 s - start, at t = 95 s, at t = 115 s and at t = 135 s - end of the simulation, (a) simulation with the proposed models ( $S_w \otimes CAF_{eva}$ ) for the evaporative cooling effect, and (b) without.

drying phase. This final stage of the sterilisation process (Fig. 1) can be a major challenge when developing new sterilisers. As already mentioned in Section 1, a completely dry package is required around the medical equipment to maintain a microbial barrier. Being able to estimate how effective the drying process will be in advance by performing numerical simulations provides an enormous benefit. This section highlights the benefits offered by using the proposed methods. A reliable

measurement of the actual condensate content and the distribution of this content after the first vacuum phase could not be achieved, in part due to the negative pressure and the resulting difficulty in reaching the interior. Nevertheless, the entire sterilisation cycle, including the drying phase, will be simulated in a future study. At the end of this final phase, ambient pressure is present in the chamber, allowing an accurate validation of the drying process.



**Fig. 12.** Volume fraction of the liquid water (a) at t = 80 s - start of the simulation and (b) at t = 82 s.



**Fig. 13.** Adjusted mass of condensate  $m_{UDM}$  (in milligrams) in the first cell layer next to the wall (Section 3.4) (a) at t = 80 s - start of the simulation, (b) at t = 95 s, (c) at t = 115 s and (d) at t = 135 s - end of the simulation.

# 5. Conclusion

In this study, a numerically inexpensive CFD model of a steam steriliser was developed to simulate the evaporative cooling effects which occur, and especially during the vacuum and drying phases. To validate the simulation, the fluid temperature inside the steam steriliser and wall temperatures at six different locations on the outside of the steriliser were measured. The temporal course of the fluid temperature and that of all six wall temperatures fits well with the measured values. The numerically inexpensive heat transfer model for condensation from Feurhuber et al. [22], was then augmented for the case of evaporation. To achieve a noticeable evaporative cooling effect, a mass source term of liquid water was defined in the first cell layer near the walls. This can be attributed to the simplified condensation model and the associated non-modelling of the wall film. The results demonstrate that the developed CFD model can be used to calculate the fluid and wall temperatures in both time and space with high degrees of accuracy. Futhermore, the use of the developed models only slightly increased the computing time. Using the presented models, it became possible to simulate the entire sterilisation cycle, including the drying phase. On the one hand, this enables reasearchers to even more precisely determine the temperature curves for loads in steam sterilisers, and on the other hand, to determine the quality of the drying process itself. As a result, causes of poor drying can be located and corrected, enabling the quality of steam sterilisers to be further improved. Finally, the proposed models for considering the condensation and evaporation effects on solids are not limited to steam sterilisers and can easily be used in other industrial applications.

A	[m <sup>-1</sup> ] interfacial area density
<i>a</i> .	$[m^2 s^{-1}]$ thermal diffusity of the
u	liquid phase
	iiquid phase
$c_{p_l}$	[] kg <sup>-1</sup> K <sup>-1</sup> ] specific heat capacity of
	the liquid phase
CAF	[-] convective augmentation factor for
er in cona	[] convective augmentation factor for
	condensation
CAFeva	[-] convective augmentation factor for
	evaporation
d	[m] equilibrium break-off-diameter
d	[m] diameter of the a <sup>th</sup> phase
c c	[1] diameter of the q phase
J	[-] drag function
hq	[] kg <sup>-1</sup> ] specific enthalpy of the q <sup>th</sup>
	phase
$h_{pa}, h_{ap}$	[] kg <sup>-1</sup> ] interphase enthalpy
K <sub>na</sub>	$[kg m^{-3} s^{-1}]$ interphase momentum
rpq	avchange coefficient
	(hall many of limit out on a sell in
m <sub>Celli</sub>	[kg] mass of liquid water per cell in
	the water layer
	[kg] total mass of liquid water in the
m <sub>tot</sub> lavar	water laver
m	[kg] total mass of liquid water in the
e e o e l	whole fluid domain
m <sub>UDM</sub>	[kg] adjusted mass of liquid water in
	the water layer which is stored into to
	UDM
m <sub>ma</sub>	[kg m <sup>-3</sup> s <sup>-1</sup> ] mass transfer rate
in pq,	hotwoon the phases
111qp	between the phases
Nu <sub>cond</sub>	[-] Nusselt number for condensation
Nu <sub>ideal</sub>	<ul> <li>[-] Nusselt number for convection</li> </ul>
Nueva	[-] Nusselt number for evaporation
r	$[I k \sigma^{-1}]$ specific enthalpy of
	avaporation
p	[Pa] absolute pressure
Pr	[-] Prandtl number
$Q_{pq}$	[J m <sup>-3</sup> s <sup>-1</sup> ] intensity of heat exchange
-71	between the phases
đ	$[W m^{-2}]$ heat flux of the $a^{th}$ phase
4q	[W III ] Heat hux of the q phase
Ra	[-] Rayleign number
Sq	[kg m <sup>-3</sup> s <sup>-1</sup> ] mass source term of the
	q <sup>th</sup> phase
Sw	[kg m <sup>-3</sup> s <sup>-1</sup> ] mass source term of
	liquid water
т	[K] saturation tomporature
Isat	
t	[s] time
V <sub>cell</sub>	[m <sup>3</sup> ] cell volume
$\vec{v}_{q}$	[m s <sup>-1</sup> ] velocity of the q <sup>th</sup> phase
$\vec{v}_{nq}$	$[m \ s^{-1}]$ interphase velocity
Greek	i i i i i i i i i i i i i i i i i i i
CUM	
Sy111-	
DOIS	
$\alpha_q$	[-] volume fraction of the q <sup>th</sup> phase
λ,	[W m <sup>-1</sup> K <sup>-1</sup> ] thermal conductivity of
	the liquid phase
0~	$[k\sigma m^{-3}]$ density of the gasous phase
PB .	[kg m <sup>-3</sup> ] density of the liquid phase
$\rho_l$	[kg iii -] density of the liquid phase
$\rho_{rq}$	[kg m <sup>-3</sup> ] volume averaged density
$ ho_q$	[kg m <sup>-3</sup> ] density of the q <sup>th</sup> phase
$\tau_{p}$	[s] particulate relaxation time
τ <sub>α</sub>	[Pa] stress-strain tensor of the a <sup>th</sup>
~4	nhace
<i>φ</i> steam	[-] volume fraction steam
$\phi_l$	<ul><li>[-] volume fraction liquid water</li></ul>
	[-] mass distribiution of liquid water
Vultar lavar	in the first cell layer next to the wall
r water-layer	
Abbrowistions	
Abbreviations	
CFD	Computational fluid dynamics
HEA	Heating phase
NCGs	Non-condensable gases
OLIICK	Quadratic Unstream Interpolation for
Zoren	Convective Vinematics
TO	
TC	Thermocouple
UDF	User defined function
UDM	User defined memory

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# **Declaration of Competing Interest**

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Simon Pletzer reports financial support was provided by W&H Sterilisation S.r.l.

#### **CRediT authorship contribution statement**

Simon Pletzer: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – original draft, Visualization. Marco Miranda: Investigation, Writing – review & editing. Marzia Lucchesi: Investigation, Project administration. Marino Magno: Supervision, Project administration. Christoph Hochenauer: Conceptualization, Methodology, Writing – review & editing, Supervision, Project administration, Resources, Funding acquisition.

### Data availability

The authors do not have permission to share data.

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