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AME Project

Literature Review

Optimized Condensation for Energy Storage: Thermodynamics and Modeling

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Abstract

Condensation is a phenomenon which unfavorably occurs in a steam turbine, due to the formation of liquid droplets which lead to corrosion and drive the efficiency down. With a project goal of efficiently and accurately simulating a steam turbine flow, two nucleation models were thoroughly reviewed, and other aspects of these simulations were also carefully inspected. It was found that the diffuse interface theory of nucleation, proposed by Gránásy (1), can be appropriate for non-equilibrium homogeneous condensation simulations and therefore its implementation in a code will be pursued. Furthermore, the possibility of implementing the d^2 condensation scheme as a droplet growth model was examined and it was found that its utilization is possible. Lastly, it was discovered that heterogeneous condensation may be required to be modeled when comparing simulations results with experimental data.

Objectives

The project aims to model and simulate multiple physical phenomena in a steam turbine which are therefore firstly reviewed with the help of relevant literature. The objectives of this review are specified as follows:

1. Achieve a fundamental understanding of the nucleation process and review relevant models which describe this process and are implemented in steam turbine flows
2. Identify other critical elements and their corresponding models which attempt to further describe the condensation process in such or similar flows
3. Select the models which show promising results and potential

Regarding point 2), it is clear, that this line of work provides a significant amount of flexibility, and further assessing simulation parameters can be often necessary. Therefore, it should be noted regarding the project itself, that it is pertinent and worthwhile to pursue adding more sophistication to the CFD component if the scope and progression of the project allows it.

Contents

1. Introduction

In the process of releasing thermal energy, a fluid undergoes condensation, changing from a gaseous state to a liquid state. This phenomenon is observed in nature and used in technical processes such as distillation and refrigeration, however, it can also occur in unwanted locations such as during expansion of the fluid in a low pressure (LP) steam turbine stage (2). Although the vapor is expected to fully condensate in the condenser of the steam turbine cycle, there are a few reasons why condensation in the turbine itself can be highly unfavorable: corrosion can damage parts leading to more frequent maintenance and the efficiency and therefore power generation can be influenced (3).

Similar to other flows, computational fluid dynamics (CFD) can be extremely beneficial when trying to understand the nature of this occurrence and possibly mitigating it. In past years, due to improvement in CFD techniques, a relatively accurate compressible multiphase flows can be simulated. These include nucleation models of the droplets and different means of phase interaction. However, the computational cost of these simulations is frequently very high, making a practical application difficult to achieve (4). Therefore, in recent literature, one can easily find various methods of attempting to obtain accurate results at low computational costs.

In this literature review, nucleation models for condensation will be firstly and thoroughly reviewed, with the goal of identifying an accurate model which shows potential to be integrated in future simulations. Then, the review will shift to the computational side of compressible multiphase flows. These simulations introduce aspects other than the nucleation itself, such as the droplet growth or equilibrium properties. These models do not only differ in their implementation of the code itself, but also in the assumption of the nature of the condensation itself in the steam turbine. The results of these publications will be examined and a discussion about the findings will be held.

2. Nucleation theory

The origin of the classical nucleation theory was firstly laid by Gibbs in the second half of the 19th century but was put into mathematical form by Becker and Döring in 1935 (5). Literature however often references the article written by McDonald in 1962 (6), and this work will follow this trend.

For general insight, nucleation is considered homogeneous, when the process itself is completely isolated from all foreign bodies e.g. ions, surfaces or other contamination. In the case of "assisted" condensation from such foreign bodies, the process is referred to as heterogenous (6).

Although a few nucleation theories can be found in the literature (7), in this review, only two will be considered which are the most relevant for this project. Furthermore, it should be noted that these theories illustrate the homogeneous case.

2.1. Classical nucleation theory (CNT)

McDonald (6) illustrates the misconception of condensation being a spontaneous process which is initialized when a vapor enters the dome (crossing the saturated vapor line) observed in a typical water p-v diagram. To form condensate nuclei, the vapor requires a so called "activation energy" which enables the vapor to initialize the condensation process. To thoroughly demonstrate this, McDonald describes a theoretical process of compressing vapor isothermally. Here, the reader is referred to the work done by Liu and Cheng (8) which shows that the constant temperature assumption is not necessary and the process can also be described at a constant pressure with decreasing temperature. When reaching the dome, the compression continues on the isotherm which is now referred to as the "metastable extension" and the vapors is now considered supersaturated i.e., pressure beyond the saturation pressure without condensing. Kalikmanov (9) describes the metastable state as being at a local minimum, with the global minimum being the stable state (condensing). According to Gibbs, the tendency of a thermodynamic system is to assume a state of lowest free-energy (the global minimum), however, to get there from the metastable state, the system must overcome a barrier (6). The only way to decrease the free-energy further, the vapor must undergo dropwise condensation, nonetheless, as soon as embryonic droplets form, the surface-free-energy between the liquid and the vapor must be accounted for. Although the bulk-free-energy decreases when it transitions to the liquid phase i.e., the volume of the droplet forms, the free energy is increased by the creation of the interface. The total free-energy change of the system, ΔF, is formulated by McDonald (6).

$$\Delta F = 4\pi r^2\sigma - \frac{4}{3}\pi r^3 \rho RT ln(\frac{p}{p'}) \quad 1)$$

Here, r is the radius of the formed droplet, σ is the surface tension, ρ, R, T and p are the density, gas constant, temperature and pressure respectively and p' is the saturation pressure. Due to the quadratic term being larger than the cubic for a very small interval near zero, for very small droplet sizes, the surface term in equation 1) dominates and condensation will therefore not occur. The critical droplet size to which a droplet needs to reach to impel condensation can be determined by differentiating equation 1) with respect to the radius and the resulting equation is dependent on the level of supersaturation i.e., pressure ratio (6). It can be therefore concluded from McDonalds article, that the higher the supersaturation level is, the smaller the critical radius and therefore it is statistically more likely that homogeneous nucleation or rather droplets formation can occur (6).

2.2. Diffuse interface theory (DIT)

In contrast to the CNT which assumes a sharp interface, the DIT assumes that the interface between the phases is diffuse (10). The theory was first published in 1993 and was developed by Gránásy and collaborators (1) and was based on good predictions made by the Density Function Theory (DFT), which assumed the diffuse interface. As described by Kelton (10), Gránásy offered a variation to the DFT proposing a “ready to use” phenomenological thermodynamic approach.

The problem with the CNT originates from the capillarity approximation: the assumption that spherical particles possess volume and interface free energy is only valid if the thickness of the interface is negligible in comparison to the size of the nucleus (1). Gránásy continues and suggests that it is hardly the case for nuclei containing 30 to a few 100 molecules obtained in a lot of cases, and therefore, a correction to the CNT might be necessary. Furthermore, it is suggested that this conclusion is drawn from the failure of the CNT to predict vapor condensation in various systems (1).

The DIT assumes that the center of the droplet is characterized by the physical properties of the bulk and the thickness of the diffuse interface is size independent, an assumption that was later verified as reasonable by Gránásy in 1996 (11). The work, W, of a droplet formation can be then formulated (1)

$$W = \frac{4\pi}{3}(R_H^3 \Delta h_0 - R_S^3 T \Delta s_0) \quad 2)$$

where R_H and R_S are the midpoints of the enthalpy and entropy profiles across the interface and Δh_0 , Δs_0 are the local enthalpy and entropy densities of the droplet at $r = 0$, respectively. Hence, the area enclosed between Δh and $T\Delta s$ curves is proportional to the interfacial free-energy (10). Similar to the CNT, the critical radius of formation can be derived from this expression.

The theory was reviewed in 1998 by Gunton (7) in a journal article summarizing significant progress made in nucleation theory in recent years and was also reviewed by Kelton (10) in 2022 where the DIT was used for computer studies of glass nucleation. Although Kelton acquires good quantitively results with the CNT, he suggests that the theory might break down far away from equilibrium conditions, hence, the diffuse interface approach might be necessary (10).

3. CFD Models

In this chapter, various published work about two-phase steam turbine flows will be reviewed. The literature suggests, that the CNT is the favorable theory for modeling homogeneous condensation in steam turbines, but also in other machine components such as the converging-diverging nozzle as presented by Ma et al. (12) and Yang et al. (13). Other important aspects of these simulations will be firstly discussed before comparing their results.

3.1. Droplet growth

After the formation of droplets due to nucleation, the growth progression of the droplets through the simulation domain must be modeled, as it describes the development of the wetness fraction (14). As seen in several publications (15, 13, 16, 17), the droplet growth rate is often modeled after Moore et al. (18): Due to the size of the droplets being significantly smaller than the mean free path of the vapor molecules, the growth of the droplets should be governed by molecular and macroscopic transport processes (3). This is often referred to in the literature as the "Hertz-Knudsen" model. Tabata et al. (19) and other authors (see Table 1) utilize an extension to this model with additional coefficients. Wróblewski et al. (3) assumed that homogeneous and heterogenous nucleation is to be found in a 360MW steam turbine LP stage and therefore modeled both, however, because the heterogeneous nucleation is assumed to be triggered by flow impurities such as foreign nuclei, only the droplet growth was modeled for the heterogeneous case, starting from the impurities initial size . On the other hand, the homogeneous nucleation was modeled after the CNT, but the growth of the droplets was identically modeled as those from the heterogeneous case. The independency of the growth model from the nucleation model is beneficial, as it enables independent analysis of each model separately and therefore will simplify the implementation of alternative droplet nucleation/ growth models.

3.2. Equilibrium and non-equilibrium condensation

Condensation is assumed in equilibrium when the phase change occurs as the gas reaches the saturation line, therefore, for supersaturated vapor to be considered, non- equilibrium condensation must be modeled (19). The difference between equilibrium steam (EQS) and the non-equilibrium steam (NES) models is thoroughly presented by Liu et al. (16): the EQS model considers the domain to have single-phase flow which is then defined over the three conservation laws: mass, momentum and energy. As also described by Starzmann and Casey (14), the wetness degree is directly related to the pressure and enthalpy which is then acquired from an h-s diagram. In the

NES, both phases are treated separately (two sets of governing equations), with the vapor being a continuum and the liquid is dispersed within it. Therefore, the interaction between these phases is established by the corresponding source terms (16). Simulating both models can prove to be a powerful tool, as it enables the quantification of losses due to supercooling.

3.3. Results

The following table summarizes models used for condensation CFD modeling in a LP steam turbine stage. It should be noted that some characteristics of these simulations were and will not be discussed thoroughly in this work, as they are not within the scope of the project, however, depending on the project progression, results dependency on these parameters could be assessed.

Table 1: Reviewed work on turbine condensation simulations. Note, underlined models suggests that a modification to these has been made

Paper	Homogeneous/ Heterogeneous	Nucleation	Droplet growth	EQS/NES	Turbulence model	Frame of reference
Bagheri (2)	Hom	CNT	Knudsen	NES	unknown	Eulerian
Brinckman (20)	Hom	CNT	Knudsen	NES	$k-\epsilon$	Eulerian
Gerber (21)	Hom	CNT	unknown	NES	$SST\ k-\omega$	Eulerian
Liu (16)	Hom	CNT	Knudsen	Both	$k-\epsilon$	Eulerian
Patel (17)	Hom	CNT	Knudsen	NES	Many	Eulerian
Starzmann (14)	Hom	CNT	unknown	Both	$SST\ k-\omega$	Eulerian
Tabata (19)	Hom	CNT	Knudsen	Both	$SST\ k-\omega$	Eulerian
Wróblewski (3)	Both	CNT	Knudsen	NES	$SST\ k-\omega$	Eulerian

Wróblewski et al. (3) compared experimental results sampled from the LP stage of a 360MW turbine with the respective numerical setup. His implementation of the equation of state for describing real gas properties, modeled similarly to the virial equations, showed a good capability of capturing the fluids properties with the help of IAPWS-IF97 (The international Association for the Properties of Water and Steam) (3). This was done similarly in almost all other publications mentioned in Table 1, beside Brinckmann et al. (20) who investigated CO_2 as a medium and Bagheri et al. (2), who assumed that the medium behaves ideally. Wróblewski concluded that heterogeneous condensation might be the dominating driving force for droplets formation when impurities in the flow such as NaCl have sufficient concentration levels. He therefore assumed that this is the reason he did not experience any supercooling in the flow (3). Liu et al. (16) did not consider the heterogeneous case

and compared CFD results acquired from EQS and NES. He established key differences in the results between the models such as the position of condensation and influence on outlet pressure. Liu et al. also compared results with experimental data, showing that the NES is more consistent when capturing the pressure profiles of the blades and the location of droplet formation on the suction side (16). Lastly, Tabata et al. (19) also acquired good agreement between the NES model and experimental data, concluding that that half of the total wetness losses are due to condensation and supercooling. Starzmann et al. (14) produced results which are consistent with those found by Tabata. As all four publications compare their result with experimental data, the contradiction between Wróblewski and the others, concerning the supercooling levels i.e., significance of non-equilibrium condensation, can be explained by a difference in the used medium: concentration of impurities must have been sufficiently higher in Wróblewski's experiment. However, due to Wróblewski only estimating the concentration level in his experiment's used medium (3), it is difficult to establish a clear correlation between medium impurity and the nature of the predicted condensation.

Patel et al. (17) introduced modifications to the $SST\ k-\omega$ turbulence model, concluding, that even for a steady simulation, the condensation phenomenon can be highly sensitive to the turbulence model. Because of stator -rotor interaction in the turbine flow, the flow exhibits properties such as flow transition, separation and mixing which involves turbulence, where momentum and heat exchange are accelerated, therefore, its correlation to nucleation rate and wet-steam flow properties is significant (17). This suggests that high caution is necessary when comparing results with those of Brinckman et al. (20) and Liu et al. (16), as both utilize the $k-\epsilon$ model.

4. Discussion

The code which will be written to simulate the condensation phenomenon in a turbine stage will be also formulated in the Eulerian- Eurlerian frame of reference. Beside the simplicity offered in this frame of reference, the computational demand will be significantly lower than the Eulerian-Langragian model, as no direct trajectories of the droplets are simulated (4), hence, technical use of such simulations remain possible.

The findings concerning the non-equilibrium homogeneous condensation found in the turbine suggests that the DIT nucleation model proposed by Gránásy et al. (1) can be appropriate for such simulations. This is supported by Kelton's (10) finding as discussed in chapter 2.2. Therefore, the integration of this model in the code will be pursued.

A droplet growth model was derived and integrated in a code prior to this literature review. The model is based on the d^2 evaporation model and a thorough derivation can be found by Turns (22). This evaporation model is often used to verify results produced in solvers simulating evaporation phenomenon and corresponds to the evaporation of a droplet under steady conditions in an infinite gas domain (23). It was found that a change in the boundary conditions and minor tuning of variables can lead to the opposite process i.e., condensation. The code follows the algorithm proposed by Abramzon et al. (24) and its integration in the steam condensation simulation will be sought.

Considering the contradictions found in chapter 3.3, heterogeneous condensation must be in some way tolerated within the simulations, as the comparison with experimental data might otherwise be misleading. Thus, non-equilibrium condensation will be firstly assumed to be the dominant phenomenon in a pure medium. Then, for the comparison with experimental data, a modification is expected to be necessary for this model to fit the observed data. This will be presumably done similarly to Wróblewski (3), by introducing additional impurities i.e., droplets, that will drive the supercooling down.

Lastly, other properties of the simulation such as turbulence modeling will be consistent with other works to enable proper comparison of results produced by the code.

5. Conclusions

Several aspects of the condensation phenomenon in a steam turbine CFD simulation have been examined. A fundamental understanding of the nucleation process was achieved. The literature suggests that the classical nucleation theory is the preferred method to model the homogeneous nucleation phenomenon. However, it was found that utilizing the diffuse interface theory model proposed by Gránásy et al. (1) is appropriate, as literature also suggest that non-equilibrium condensation plays a leading role in the losses calculated due to vapor wetness (19). Furthermore, it is concluded that the equilibrium characteristics of the condensation and the droplet growth model play a critical role when attempting to capture the nature of the flow in the turbine. Therefore, for the droplet growth, replacing the favorably used Hertz-Knudsen model with the reversed d^2 evaporation model will be pursued, as it offers a different and new path to achieve similar results. The non- equilibrium condensation model will be adapted from the literature, however, for experimental verification, modeling heterogeneous condensation might be necessary but will effect this equilibrium property.

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