Numerical modeling of condensation and vaporization in turbulent flows

Background : the ECOBIOCLEAN project

The “CMR” ranking (carcinogenic, mutagenic and toxic for reproduction) of Formaldehyde (known as formalin) in industry (Cleanrooms, Pharmaceutical, Hospitals, Food ...) induced a complete overhaul procedures for bio-decontamination in these industries.

Substitution of formalin was made by adjuvanted or non adjuvanted peroxide hydrogen . This product change , passing form a gaseous to a liquid state , has led to better optimisation of the cleanroom environment in terms of ventilation , air conditioning , mastery of the materials used in all areas classified by using very inefficient broadcast equipment.

Each manufacturer has until now focused on its area of expertise without working with others in the cleanroom area. This results in answers to end customers at best unoptimized and at worse inefficient.

The project ECOBIOCLEAN aims to gather these actors to develop a comprehensive solution which guarantee both results and reproducibility over time.

For this purpose three manufacturers: a manufacturer of disinfection system , an air envelope manufacturer of cleanrooms, a conditioning system installer and two university labs have joined to complete this project.

This program will seek to determine:

- boundary conditions efficiencies of different tested biocides
- the most optimized in terms of consumption of biocide disinfection cycles and energy
- the optimum air flow rate for decontamination at any point
- easily decontaminated and consistent treatment by H2O2 materials
- the development of a fine unstable air handling control system
- the development of scenarios for energy optimization of air treatment direct expansion
- the development of a new method of counting
- the development of specific numerical code for phase changes during a decontamination cycle

Within this project, MECAFLU team of ICUBE laboratory is responsible for the numerical modeling of the parietal condensation and evaporation in turbulent flows and is looking for a Phd student to assist.

State of the art:

Condensation is a non-equilibrium exothermic thermodynamic process of phase transition from the gaseous state to the liquid state whose industrial applications have been studied for many years. There is a wide range of heat exchangers whose function is based on this phenomenon. The most common, present in almost every house, is the condenser in a refrigerator. Among industrial applications condensation is often involved in the energy sector. In conventional power plants (coal), the condensation of gases and spontaneous condensation of steam in the turbine condensers can be a source of serious problems. In nuclear power plants the condensation has important security implications which explains why most of the current research on modeling the parietal condensation is devoted to these applications.

Condensation in the presence of non-condensable gas is a very complex phenomenon. Identify the most important effects is quite difficult. However, one can identify three different cases because of their direct impact on the process of mass transfer and heat of condensation and their applicability to the study of risk in nuclear power plants: condensation, as a film of free water and forced, binary and ternary mixtures of convection, the interaction between the structure of the liquid film and the diffusion layer of mixture, and spontaneous condensation. All these effects can play an important role in the release of water vapor in the reactor. Karkoszka, 2007 describes in detail these three modes of condensation and associated bibliography.

These potential dangers explain the interest of research related to nuclear power for numerical modeling of condensation. The modeling follows two different approaches : the first one is directly related to the industry and is based on correlations derived from experimental observations (the most important is the heat transfer coefficient or Nusselt number). These relationships are generally functions of the Reynolds number, the Prandtl number and the mass fraction of non- condensable gas. The most common are those of Uchida, Tagami, Kataoka and Dehbi (Herranz et al. , 1998). The second approach is based on more fundamental studies that enhance the understanding of thermodynamics and the effects of diffusion in multi-component gas mixtures . There are two concepts in this approach: the diffusion layer model and its variants are based on an analogy between the transport equations of heat and mass fraction , the second concept is based on the resolution of a coupled system of equations (equations of transport and storage for liquid and gas phases). A detailed description of these approaches is provided by Karkoszka, 2007. Nabati, 2007 compared approaches based on Nusselt theory and that on the boundary layer diffusion.

We will look at this last concept that we will implement in this project through the CFD.

Many authors have already worked o, thos topic :

Jeon et al, 2009 studied the condensation to an isolated bubble in a cold flow method using the VOF (Volume of Fluid, which is to carry a passive scalar representing the interface between two immiscible phases). The simulations were compared to a similar experimental study (Kim et al, 2008) and the results showed that this methodology was able to account for the physical condensation of bubbles in the flow. Alizadehdakhel et al, 2010 also used the VOF method to the study condensation in a thermosyphon.

Sharma et al 2012 used a two-phase model and semi-empirical correlations in the CFD-ACE code to simulate the experience of parietal condensation COPAIN (Cheng et al, 2001). The same approach has been proposed by Liu et al 2004 and the results were compared to an experiment in a test chamber where they were interested in the spatial and temporal distribution of water vapor (introduced at the center of the test chamber) on the walls.

In CFX code (Kljenak et al , 2006), the flow is modeled as a single phase and condensation acts as a dissipation of energy and mass. in this approach, the liquid film and the influence of the layer of non-condensible gases are reduced to a simple sink term. The use of explicit process for evaluating the mass transfer and heat correlations, even if they represent a possible approach for large experimental facilities and reactors , ignore some of the useful information provided by detailed CFD models based on local conditions.

Another model is available in FLUENT (Forgione et al , 2005). With this approach , the correlations of heat and mass are replaced by the use of "fundamental" laws of physics but in this case a very fine grid computing is necessary.

For the two-phase flow with a gaseous mixture and spraying droplets, the GASFLOW code solves a model with two homogeneous phases (Jongtae et al, 2006) coupled to the heat transfer correlations.

NEPTUNE_CFD code (Mimouni et al , 2010 and Mimouni et al , 2011) is based on a two-fluid approach for simulating the mass transfer and heat transfer between the spray and the gas mixture. The condensation model is based on the fundamental laws of physics and solve a transport equation of the density of droplets. This approach takes into account both evaporation and condensation. Indeed Andreani et al, 2008 notes that from the point of phase change and the geometry of the enclosure, the liquid film could flow in dry areas where the liquid is evaporated. If the walls are hotter than the liquid film, the result is a higher rate of evaporation . This approach is the most comprehensive present as it can simultaneously take into account the mechanical drift between the droplet and gas, mass transfer and heat of the droplets in the heart of the flow phenomena and evaporation / condensation on the walls. Mimouni et al , 2011 also stressed the importance of turbulence modeling in the near-wall region for these flows .

The approach we propose to implement the code that NSIBM Mimouni et al based on a two-fluid model.

Approach :

The objective of this thesis is to develop and validate a numerical tool to optimize the flow and geometry of ventilation and the initial mass fraction of steam in order to obtain an optimal wetting of walls by the peroxide hydrogen in real configurations.

To do this we will rely on the NSIBM code developed at Icube (Durrenberger and Hoarau , 2013). This parallelized solver solves the incompressible Navier-Stokes equations on unstructured Cartesian grid and the geometry is taken into account via the Immersed Boundary Method with automatic mesh refinement. The implementation of turbulence models is being validated. This implementation of turbulence model is similar in fact a transfer of technology. Indeed modeling steady and unsteady turbulence requires the implementation and optimization of a model specifically tailored to the situation described.

The work required in this thesis is divided into four tasks :

1. After an extensive literature review, the proposed model of Mimoudi et al, 2011 will be implemented in the NSIBM solver and validated on experimental test case in the literature (PAL, TOSQAN (Ambrosini et al))

2. After this stage of implementation and validation of droplets of water vapor, the model will be applied to the case of the insulator developed by Areco. The experimental results obtained in this configuration (temperature profiles, film thicknesses of condensing vapor concentration ...) will allow us to refine the numerical model and adapt it to the condensation of many smaller droplets. This step is essential for the validation of the numerical tool in this project. Indeed , although the physics of condensation and thus the set of equations used is the same for water droplets and smaller droplets, the numerical model is based on several experimental correlations that we need to check here. The more extensive the experimental provided database will be, the more accurate the model will be. We will also conduct simulations to verify that the optimal parameters of temperature, flow rate and initial vapor concentrations obtained in the project are compatibles with optimal wetting of the insulator. This last step will give us dependency relationships that will be useful to optimize real configuration.

3. The code will be validated and used to model and optimize the actual configuration. This scaling does not affect the validation of the model, resulting in a larger and more complex geometry which will require a much more consistent mesh and therefore much larger simulation time. We will compute on the HPC center from the University of Strasbourg and the national centers.

4. In a second step we will use the level-set methodology to study in more detail and more fundamentally the physics of the condensation of a few drops on a wall. The interest in the level-set method is its ability to model

matching or tear droplets but this methodology has never been used to model and understand the phenomenon of condensation. This study will enhance the mass transfer correlations and heat used in most models .

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Candidate Profile :

Potential candidates must have an engineering degree or a Master's degree and two have experience in the fields of fluid mechanics and numerical simulation. A knowledge of Fortran programming and parallel computing will be highly appreciated. The salary will be about 1400-1500 € net per month for 36 months. The deadline for applications is 15 November 2013.

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