DEGREE PROJECT IN PHYSICS,
SECOND CYCLE, 30 CREDITS

STOCKHOLM, SWEDEN 2017

CFD modeling of annular flow with a three-field approach

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TRITA-FYS 2017:56

ISSN 0280-316X

ISRN KTH/FYS/--17:56-SE

Abstract

Annular gas-liquid flow is one of the last flow regimes in boiling channels. It is characterized by a core flow of steam and liquid droplets and a thin liquid film wetting the wall of the channel. This type of flow can be encountered in many different industrial applications including boiling tubes, moisture separators, distillation towers and in particular nuclear Boiling Water Reactors.

The main concern about this flow regime is a phenomenon called dryout that happens when the liquid film completely evaporates leading to a fast increase of the wall temperature and possible structural damages.

Hence, it is of great importance for companies like Westinghouse Electric Sweden, which is involved in the production of fuel bundles for both PWRs and BWRs, to have a deep understanding of this phenomenon and to be able to properly take it into account in the fuel design and manufacturing processes.

The aim of this master thesis project is to develop a numerical simulation tool using the CFD commercial software ANSYS Fluent to predict the development of steam, film and droplets flow in annular flow.

A previous master student has started the development of a model for pipe geometries taking as a reference the work done by Li and Anglart at KTH-Royal Institute of Technology in Stockholm. This model follows a three-field approach meaning that the three different fields are modeled and the solution of each of them is coupled with the others.

This previous work was just a first attempt to a CFD - ANSYS Fluent model and one of its main problems was the long calculation time. Many changes and improvement have been implemented to the model in order to decrease the calculation time to a reasonable value. After the physics involved in annular flow and its implementation in CFD codes have been studied, some features of the model have been changed to obtain results closer to reality.

The final model has been validated with experimental data. The results approximate well the majority of the data points for different flow conditions and axial power distributions. However the model turns out to be particularly sensitive to certain parameters such as droplet diameter. This high sensitivity could lead to misleading results and it has to be further analyzed.

In this report, only pipe geometries have been analyzed, but keeping in mind the long term goal of fuel bundle geometries simulations, some changes have to be made. This has been taken into account and some recommendations are given for a possible follow-up of the project.

Acknowledgements

I would like first to thank my supervisors at Westinghouse Tobias Strömgren and Yann Le Moigne. When I started this thesis my experience with CFD was almost null and their advices and help have been fundamental. My gratitude goes also to Jean-Marie Le Corre who had a key role in deciding the path to follow in the development of the project. In addition I would like to thank the whole SES department in Westinghouse. It has been like a second home during these months passed in Västerås thanks to the welcoming and friendly environment. Besides they also gave me some useful feedbacks for the thesis project after the mid-term presentation.

I would like to thank Professor Henryk Anglart and researcher Haipeng Li from KTH who have been working on this topic for years. They shared with me some useful knowledge in a few meetings we had during the project development.

Particular thanks go to my whole family, my parents and my sister most of all. Even if we have been physically far from each other during the years of my studies they have always been next to me emotionally, supporting me and encouraging every choice I made.

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List of Abbreviations

BWR – Boiling Water Reactor
CHF – Critical Heat Flux
CFD – Computational Fluid Dynamics
DPM – Discrete Phase Model
EWf – Eulerian Wall Film
LPT – Lagrangian Particle Tracking
UDF – User Defined Function
1D – One Dimension
3D – Three Dimensions

List of Symbols

σ	surface tension, N/m
μ	dynamic viscosity, Pa·s
ρ	density, kg/m ³
τ	shear stress, N/m ²
C_d	drag coefficient, -
d	diameter, m
f	friction factor, -
g	gravitational acceleration m/s ²
G	mass flux, kg/m ² s
h	liquid film thickness, m
J	volumetric flux, m/s
k	mass transfer coefficient, -
$\dot{m}$	mass flow rate, kg/s
p	pressure, Pa
r	radius, m
S_m	mass source term, kg/m ² s or kg/m ³ s
S_{mom}	momentum source term, N/m ² or N/m ³
u	velocity, m/s

Subscripts

d	liquid droplets
dep	deposition
$evap$	evaporation
ent	entrainment
f	liquid film
v	vapor
w	wall

Chapter I. - Introduction

The boiling process in nuclear BWRs is characterized by different flow regimes. Water enters at the bottom of the nuclear core in an undersaturated liquid phase and leaves the upper part of the core in a saturated, high quality two-phase flow. In this process, different heat exchange mechanisms between water and fuel rods are involved. Parameters like wall temperature, heat flux and heat transfer coefficient have to be kept under control, otherwise severe structural damages can occur.

Annular flow is the last of the boiling flow regimes happening in a nuclear fuel bundle and it is also the most dangerous one because dryout can occur. Hence, it is of great interest for companies involved in design and operation of nuclear reactors to model properly this phenomenon in order to make sure that safe conditions are kept during the whole lifetime of the nuclear fuel. So far, 1D sub-channel calculations are the most used model to calculate the critical heat flux (CHF) at which dryout may occur. However, these models cannot give any information on the local conditions of the liquid film and droplets. This information would be very useful to study dryout phenomena nearby flow obstacles such as fuel spacers. This is why a CFD 3D model is needed to have a better understanding of annular flow and safer design of fuel bundles.

Westinghouse Electric Sweden and KTH-Royal Institute of Technology have cooperated to develop such a model within the NORTHNET project. As a first approach, researchers Li and Anglart at KTH have started working at a 3D model for annular flow in pipes using the open source CFD software OpenFOAM. Then a previous Master Thesis student has worked in the Westinghouse offices in order to develop the same model created at KTH using the commercial software ANSYS Fluent instead of OpenFOAM.

These models treat annular flow with a three-field approach. For each one of the three fields involved (liquid film, liquid droplets and steam) a system of partial differential equations is solved, and the solution of each field affects the solution of the others.

There are three main mechanism with which the different fields interact with each other: evaporation of the film, entrainment of droplets from the film to the steam and deposition of droplets from the steam to the film. The proper modeling of these three mechanisms is the key to model annular flow.

It is in the scope of this Master Thesis project to study and further develop the already implemented model to be sure that evaporation, entrainment and deposition are modeled properly. To do so the model is validated with different experimental data points corresponding to different flow conditions. Besides, the application of the model to more complex geometries such as fuel bundles is assessed and recommendations are given for a possible follow-up of the project.

This report is organized in five chapters. First, the current introduction is given in order to have a general idea of what the thesis is about. Second, the theoretical background needed to understand what is done in the CFD model is explained. After that, in Chapter III the model is described, starting from an overview of the previous model and describing the changes made in order to improve it. Finally in the last two chapters, the results are presented and some conclusions and follow-up recommendations are given.

Chapter II. - Theoretical Background

Before talking about the numerical model, it is important to have a general understanding of the physical processes involved.

II.1. Boiling Regimes

Annular flow is one of the last flow regimes in vertical co-current boiling two-phase flow. The different regimes and the transitions between them have been widely studied and different names have been used by different authors. The most common ones and the ones used by Hewitt [1] are in order of appearance in the channel: see Figure 1.

Bubbly flow: gas phase distributed in bubbles within a liquid continuum.

Slug flow: when the gas bubbles increase in size to become almost of the same size as the channel diameter. In this regime, big gas bubbles are separated mainly by liquid with the presence of smaller bubbles.

Churn flow: continuing with the evaporation of the liquid phase, the vapor velocity increases to a level at which the bubbles structure become unstable and their shape is no longer conserved.

Annular flow: increasing even more the flow velocity, the vapor becomes the main phase travelling in the center of the channel, while liquid is concentrated in a thin film covering the channel walls and in small droplets that travel within the vapor core.

Figure 1 - Boiling flow regimes in a pipe

When all the film is evaporated and liquid is only under the form of droplets some authors speak about *Mist flow* [2]. In our case of interest, in BWRs boiling channels, mist flow should never be reached. In fact when the liquid film in the annular flow regime completely evaporates the heat transfer coefficient has a sharp decrease and the coolability of the nuclear fuel is compromised. At this point, the surface temperature of the fuel increases dramatically. This phenomenon, which is very important to avoid, is generally called dryout and the heat flux at which this condition is reached is called Critical Heat Flux. Prediction of CHF values are of vital importance for nuclear safety.

II.2. Annular Flow

Figure 2 shows the main characteristics of annular flow. As previously explained, a steam core is travelling in the center of the pipe, occupying the majority of the volume. In the steam core, liquid droplets are travelling with a trajectory that can be strongly affected by the turbulent flow of the steam. This is particularly true for small droplets with a diameter of tenth of a millimeter. The remaining part of the liquid phase is travelling as a thin film wetting the pipe wall.

The interface between the liquid film and the steam core is never smooth but it has always ripples and large disturbance waves on its surface [3]. A particular feature of annular flow disturbance waves is the ratio between their amplitude to the mean film thickness. This ratio can be quite large, up to a value of five or more. Disturbance waves can be seen in almost every practical application. As a general rule it can be said that they are present in the flow when the liquid film Reynolds number Re_{lf} is greater than 200 [4].

In this case:

$$Re_{lf} = \frac{G_{lf}d}{\mu_l}, \quad (1)$$

where:

d = tube diameter [m];

μ_l = liquid dynamic viscosity [Pa·s];

G_{lf} = superficial liquid film mass flux [kg/m²s].

Figure 2 - Annular flow schematic

Since these waves are the major source of entrainment of droplets from the film, they have been studied a lot. It has been shown that the majority of the liquid film mass is carried by the waves. Besides it has been noticed that in small pipes ($d < 50\text{mm}$) waves have well-defined circumferential identity. This means that they are not localized in just small parts of the wall but they travel with approximately the same thickness and velocity in the whole cross-sectional region [3].

Looking at the results from experiments in which pictures of annular flow have been taken, it is possible to establish that the main process responsible for the entrainment of droplets is the creation of a filament of liquid which eventually shatters, leading to the creation of droplets. This mechanism is well shown in Figure 3. It is important to notice how the entrained droplets enter the steam core far from the film-steam interface.

Figure 3 - Main entrainment mechanism [3]

Once droplets enter the steam core, there are several processes they can undergo. First of all, they can interact between each other and either merge to form bigger droplets, this phenomenon takes the name of coalescence, or just bounce and change their trajectories. These phenomena are important when the liquid volume fraction is high and there is a large number of droplets in the steam core. However, in the development of this model, the low liquid volume fraction let us neglect droplet-droplet interactions. On the other hand, it can happen that due to high drag forces a large droplet can be split in two or more smaller droplets. Also this type of interaction is neglected in this project because of the low magnitude of the drag forces acting on the droplets.

Finally, entrained droplets can, after they have travelled through the pipe cross section, interact again with the liquid film and either being absorbed or bounce. Experiments have shown that the first interaction, which is named deposition, is the most likely.

Since evaporation, entrainment and deposition are the most important phenomena affecting the development of film and droplets flow, only these three are taken into account and modeled.

Chapter III. - ANSYS Fluent Model

As mentioned previously, a three-field approach has been chosen for the CFD model in ANSYS Fluent. Therefore, the solver handle a different set of partial differential equations for each one of the three different fields involved. The solutions of these equations are dependent from each other. This is why a coupled algorithm is used.

For both the continuum phases (the liquid film and the steam core) mass and momentum conservation equations are solved. Whereas, for the modeling of the discrete phase, the ANSYS Fluent function DPM - Discrete Phase Model is used.

The model follows an Eulerian-Lagrangian approach. It means that while the fluid phase is treated as a continuum by solving the Navier-Stokes equations in a global frame of reference, the dispersed phase is solved by tracking a large number of droplets in a local frame of reference. The dispersed and the continuum phases exchange momentum, mass and energy [5].

Besides, another set of equations is solved by ANSYS Fluent in order to model the turbulent phenomena in the flow. The Shear-Stress Transport (SST) k - ω Model is used for this purpose. In this model two transport equations are solved in order to obtain the turbulence kinetic energy k and the specific dissipation rate ω .

III.1. Three-field Approach

In this section the core of the model, consisting in the three-field approach is described, presenting the equations that are solved by ANSYS Fluent solver and describing each term that appears in them.

III.1.1. Steam Core

The term Steam Core refers to both the steam and the liquid droplets. It is the main flow solved by the model, whereas the film is solved as a boundary condition interacting with the Steam Core on the wall surface.

The steam is modeled as a single phase flow. Hence ANSYS Fluent is solving the mass and momentum conservation equations for such a flow. These equations are shown respectively in Eq. (2) and Eq. (4).

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v u_v) = S_{m,vap} \quad (2)$$

The left-hand side of the continuity equation, Eq. (2), contains the time derivative term and the divergence term which account for the change of mass in time and space. Here ρ_v and u_v represent respectively the steam density and velocity. On the right-hand side there is the source term $S_{m,vap}$ that accounts for the increase of mass due to evaporation of the liquid film.

Since this model is developed for annular flow in BWRs, a main assumption is that saturation conditions are present throughout the whole flow region and that all the heat flux on the walls is used to only evaporate the liquid film. These assumptions lead to a constant and uniform temperature in every point of the fluid and to the following equality for the evaporation mass source:

$$S_{m,vap}(z) = \frac{q''(z)}{H_{vap}}, \quad (3)$$

where:

$q''(z)$ is the power heat flux that can either be a constant value or have an axial distribution [W/m²];

and H_{vap} is the latent heat of vaporization at the specific operating pressure [J/kg].

Besides because of these assumptions the energy equation for the temperature calculations is not solved for any of the three fields.

The introduction of this source term in the equation is done using a User Defined Function (UDF). Such functions are scripts written in C language that are compiled and used by ANSYS Fluent. They are very useful when working with source terms or boundary conditions that cannot be implemented directly using ANSYS built-in functions.

The second equation solved for the single phase steam flow is the momentum conservation equation shown below.

$$\frac{\partial(\rho_v u_v)}{\partial t} + \nabla \cdot (\rho_v u_v u_v) = -\nabla p_v + \rho_v g + \nabla \cdot \tau_v^{eff} + S_{mom,vap} + S_{mom,d} \quad (4)$$

The left-hand side describes acceleration through the time derivative term and the divergence term. Whereas, the right-hand side terms are all the forces acting on the fluid. From left to right there are pressure forces, gravity forces, stress forces. The last two terms are momentum sources due to evaporation, $S_{mom,vap}$, and to the flow of droplets inside the steam, $S_{mom,d}$.

The evaporation momentum source term is simply calculated multiplying the evaporation mass source term calculated with Eq. (3) by the velocity at which evaporated steam is entering the flow. Since the evaporated steam comes from the liquid film, this velocity will be equal to the film velocity at the film-steam interface.

The calculation of the droplets momentum source term is more complex. This term is taking into account the flow of droplets inside the steam. Hence, it comes from the solution of the ANSYS Fluent built-in function Discrete Phase Model introduced at the beginning of this chapter. This function enables the user to use the Lagrangian Particle Tracking (LPT). This tool groups different droplets with similar flow parameters like velocity and spatial position in parcels. Each one of these parcels is then tracked until it impacts with the liquid film or escapes the flow from the outlet surface. When this

happens the mass contained in the parcel is removed from the total discrete phase mass and in the first case is added to the mass of the liquid film.

In order to calculate the momentum source term $S_{mom,d}$ it is important to know the mass and velocity of the droplets. A simplification done in this model is to consider that all the droplets are perfect spheres with the same diameter. Using this assumption it is easy to know the mass of each droplet, obtained as the product of the sphere volume to the liquid water density. The velocity is instead calculated by solving the equation of motion for each parcel.

$$\frac{du_d}{dt} = \frac{1}{\tau_d} (u_d - u_v) + g \left(1 - \frac{\rho_v}{\rho_d} \right) \quad (5)$$

Here, τ_d is the droplet relaxation time and can be expressed as:

$$\tau_d = \frac{\rho_d d_d^2}{18\mu_v C_d Re} \cdot \quad (6)$$

Eq. (5) shows the equation of motion solved by the DPM in ANSYS Fluent. Only gravity and drag forces are considered because they are the ones that mostly affect the droplets flow. For steady state flows the time derivative is equal to zero and the equation reduces to a simple form in which the droplet velocity is equal to the steam one plus a negative term given by drag and gravity forces.

$$u_d = u_v - \tau_d g \left(1 - \frac{\rho_v}{\rho_d} \right) \quad (7)$$

III.1.2. Liquid Film

Whereas the steam core represents the main fluid solved in the model, the liquid film is treated as a boundary condition on the surface of the pipe wall. In ANSYS Fluent it is possible to use the built-in function Eulerian Wall Films (EWF) that can predict the creation and flow of thin liquid films. The EWF main assumption is that the thickness of the film compared to the radius of curvature of the surface is small enough so that properties do not vary across the thickness and the film flow can be considered parallel to the wall, with an assumed quadratic shape of velocity.

In order to calculate the creation and development of the film, mass and momentum conservation equations are solved.

$$\frac{\partial(\rho_f h)}{\partial t} + \nabla_s \cdot (\rho_f h u_f) = S_{m,dep} - S_{m,ent} - S_{m,vap} \quad (8)$$

The continuity equation shown in Eq. (8) looks like the one solved for the vapor phase in Eq. (2), except for the fact that the density in the time and divergence terms is multiplied by the film thickness h . The evaporation mass source term in the right-hand side, $S_{m,vap}$, is exactly the same one that appears in Eq. (2) and Eq. (3) but now with a negative sign. Besides, for the liquid film, two other source terms have to be taken into account. These two terms refer to the mass exchange between the liquid film and the liquid droplets due to deposition and entrainment.

The deposition term $S_{m,dep}$, is calculated with the DPM as described in the previous section of this report.

The entrainment term $S_{m,ent}$, is calculated using an empirical correlation that is implemented in the model with a UDF used as a negative mass source term for the Eulerian Film Wall. The same mass lost by the film is injected in the core as droplets using a DPM injection.

Different correlations exist to predict entrainment of droplets in annular upwards flow in pipes. Secondi, Adamsson and Le Corre have assessed which of this correlation is the most suitable to be used for dryout prediction in BWR fuel bundles [6]. The model developed by Okawa is shown to have overall the best performance and so it is the one chosen in this project.

Okawa developed empirical correlations based on experimental data for both deposition and entrainment phenomena. The entrainment correlation is created starting from mechanistic considerations. It is assumed that the dominant mechanism of droplet entrainment is the shearing-off of roll wave crests. As a consequence the entrainment mass source term is considered to be proportional to the interfacial shear force and inversely proportional to the surface tension force, as shown in Eq. (9) [7].

$$S_{m,ent} = k_e \rho_f \frac{f_i \rho_v J_v^2 h}{\sigma} \left(\frac{\rho_f}{\rho_v} \right)^n \quad \text{for } Re_f > Re_{fc} \quad (9)$$

Here, k_e is the entrainment mass transfer coefficient, f_i is the interfacial friction factor, h is the film thickness, J is the volumetric flux and σ the surface tension. The suggested values for k_e and the exponent n are 4.79e-04 m/s and 0.111, respectively.

As mentioned in section II.2 the creation of waves and consequently of entrained droplets begins when the liquid film Reynolds number is greater than a critical number Re_{fc} , the value of 320 is adopted by Okawa.

It is important to point out that this correlation is developed for 1D sub-channel codes. Therefore Okawa gives also an expression to calculate the film thickness. However, in the CFD model, the thickness is calculated in the EFW model by Eq. (8) and Eq. (13). Hence, the film thickness is calculated using Okawa's expression only to set the inlet boundary condition. The equation for the film thickness is:

$$h = \frac{1}{4} \sqrt{\frac{f_w \rho_f J_f}{f_i \rho_v J_v}} D, \quad (10)$$

where the interfacial friction factor f_i and the wall friction factor f_w are calculated as follow

$$f_i = 0.005 \left(1 + 300 \frac{h}{D} \right) \quad (11)$$

$$f_w = \max \left(\frac{16}{Re_f}, 0.005 \right). \quad (12)$$

Also in the momentum conservation equation, Eq. (13), the first four terms are the same as described for the steam core in Eq. (4) multiplied for the film thickness h .

$$\begin{aligned} \frac{\partial(\rho_f h u_f)}{\partial t} + \nabla_s \cdot (\rho_f h u_f u_f) = & -h \nabla_s p_f + \rho_f h g + \frac{3}{2} \tau_{lv} - \frac{3\mu_l}{h} u_f + \\ & S_{mom,dep} - S_{mom,ent} - S_{mom,vap} \end{aligned} \quad (13)$$

In the right-hand side there are also two terms describing the shear forces in the film-steam interface $\left(\frac{3}{2} \tau_{lv}\right)$ and in the film-wall interface $\left(\frac{3\mu_l}{h} u_f\right)$. Besides, there are three momentum source terms due to deposition, entrainment and evaporation. These terms are simply calculated multiplying the respective mass source terms by the velocity of droplets, steam and liquid film respectively.

III.2. Overview of Previously Developed Model

Since this master thesis project is a continuation of the work done by a previous master student, it is important to start giving an overview of the model she developed [8]. A short description of the previous mesh, boundary conditions and computational set-up is given in order to understand the changes that have been made to improve the model.

III.2.1. Mesh Set-up and Boundary Conditions

To understand how the model works it is important to present the mesh and the boundary conditions used. The equations shown in section III.1.1 and III.1.2 need boundary conditions in order to be solved. The way these boundary conditions are given in the CFD model is strongly related to the mesh configuration. First, all the needed boundary conditions are listed, and then a description of the mesh shown in Figure 4 is given.

Figure 4 - Mesh representation

The boundary conditions needed in the solver are:

- Pressure Outlet,
- Inlet steam velocity,
- Liquid film inlet velocity and thickness,
- Droplets Injection (inlet velocity, mass flow rate and droplet diameter).

A structured hexahedral mesh, with around two hundred thousand elements is used. This type of mesh is better than an unstructured mesh because it gives better convergence and higher resolution. However, usually unstructured meshes are more used because it is difficult to use structured ones to model complex geometries. Luckily, the geometry analyzed in this project is a simple one and a structured hexahedral mesh is used. Some recommendations on what to change in the model in order to be able to use it with unstructured meshes are given in the last chapter of this report.

In Figure 4 both a cross section and the axial section of the mesh are shown. In the cross section it is possible to see that the mesh is refined in order to have more elements in the near-wall zone where the flow quantities like pressure and velocity have large gradients and where more accuracy is needed for the calculations on the film flow. In each cross section there are one thousand three hundred elements.

What is more interesting for this discussion is the axial view of the mesh. In fact you can see that the mesh is divided in the axial direction in three parts: injection wall, stabilization wall and annular wall. The length of the annular wall is the same as the length of the pipe used in the experiments chosen to validate the model. The length of the injection and stabilization walls together is the same as the annular one. These two parts are used in the model just to set the inlet boundary conditions for the liquid film and the steam.

In the Eulerian Film Walls model it is not possible to set directly inlet condition of the film thickness and velocity. It is instead possible to set a mass flux through a surface in order to inject the liquid film that then develops on the wall surface. It is also possible to set a momentum rate value. By solving the mass and momentum balance equations for the injected film it is possible to calculate the values of the mass flux and momentum rate in order to obtain the inlet values of the film thickness and velocity at the exit of the injection wall.

After the film liquid is injected, a second wall called stabilization wall, is used to let the film develop in a smooth way.

Steam is given a uniform inlet velocity at the inlet of the injection wall. Then in the injection and stabilization wall the steam flow develops a turbulent profile of velocity with the peak in the center of the pipe and no slip condition at the interface with the film on the wall.

The actual annular flow is starting after the stabilization wall and it develops in the third part of the mesh called annular wall. Droplets are injected with the same axial velocity as the steam and zero radial velocity at the inlet-annular internal surface via a DPM injection.

III.2.2. Computational Set-up

Since the inlet boundary conditions for the film and droplets involve an inlet mass flux and a consequent development through the pipe length, a transient solver is needed. The transient calculation is only needed for the development of the flow until a quasi-steady state solution is obtained. The final results are obtained looking at the instantaneous result at the end of the transient.

The amount of time needed for the transient calculation is partially driven by the boundary condition development. In order to have a smooth development of all the three different fields, evaporation and droplets injection are started after 1 s from the start of the transient, while entrainment is started after 1.5 s from the start. Additional 0.5 s are needed for the fully development of the global flow in the annular region. This brings to a total simulated time of two seconds.

A time step of 0.1 ms is chosen and in order to reach convergence, the model does fifty iterations per time step. New droplets are injected via the DPM injections (one at the inlet-annular and one for entrainment at the annular wall) every time step. A coupled pressure-based solver is used.

III.2.3. General Results and Conclusions

The model has been validated with one experimental data set taken from experiments done at KTH in Stockholm. The calculations have been run with a parallel solver, using 144 processors and with a calculation time of approximatively seven days.

Results using a droplet diameter of 0.7 mm are in agreement with the one obtained by the researchers at KTH who use the OpenFOAM model and also got quite good agreement with the experimental data except for an underprediction of the film mass flow rate in the first part of the pipe. The model has also been tested using a droplet diameter of 0.1mm but this time with results far from both the OpenFOAM model and the experimental results.

It has been concluded that the model needs to be further developed and improved, especially regarding the film injection which requires too much computational cost and effort.

III.3. New Development of the Model

The results obtained in the previous master thesis project point out that CFD modeling of annular flow requires many boundary conditions and flow parameters to be set and that their values strongly influence the final results. Therefore, in order to further develop the model and make it more accurate, sensitivity studies have to be done.

However, this type of study requires a large number of simulations. As it is pointed out in the conclusion of the previous master thesis report [8], the model requires high computational cost and effort. Hence, in order to proceed with the sensitivity studies the computational set-up of the model has to be changed in order to get faster calculations.

III.3.1. Changes to Computational Set-up

The first goal of this project is to reduce the calculation time without affecting the final results. In order to do so, the following major changes are done to the computational set-up:

- Removal of the stabilization wall.
- Total simulated time reduced from 2 s to 0.5 s.
- Decrease of the frequency of droplets injection in the DPM.
- Introduction of a convergence criterion.

First of all, the stabilization wall is removed. Calculations are run with and without the stabilization wall and it is seen that the two models give the same results using a droplet diameter of 0.7 mm. This change decreases the number of elements in the mesh and as a consequence the calculation time of each iteration is reduced.

It is thought that the reason why the stabilization wall was used is to get better results when using a droplet diameter of 0.1 mm. However, in the current project a case with only droplets of 0.1 mm diameter is not considered and the stabilization wall has been removed from the mesh. A detailed discussion about droplets diameter and a better explanation for this choice is given in section IV.3 of this report.

The second change made in order to get faster calculation is to decrease the total simulated time from 2 s to 0.5 s. To do so, all the interactions between the phases are started at $t=0$ s, instead of introducing each interaction in the model at different moments. The value of 0.5 s is a minimum value needed in the transient solution in order to let the three flow fields develop and reach a quasi-steady state, so this value cannot be further reduced.

Starting entrainment and deposition at $t=0$ s does not influence the model results. However, a different consideration has to be made for evaporation. At $t=0$ s no liquid film is present on the annular wall and no evaporation should occur in this region. Hence, it is unphysical to introduce the vapor in the dry part of the pipe already at the beginning of the transient. However, there is no interest in what is happening during the transient since the only interest is in the final result after 0.5 s. At this point in time the whole annular wall is covered with film and evaporation occurs everywhere in the wall surface. Hence evaporation is also introduced in the model at $t=0$ s.

It is important though to point out that this can be done only in pre-dryout modeling. In fact if dryout occurs then there will be no film in some part of the mesh and evaporation should be removed in those points. This problem will be discussed in the last chapter of this report where some recommendations will be given for a follow-up of the project.

This second change reduces the calculation time by a factor of four and the final result is not affected. Besides it was noticed that modeling evaporation since the beginning, even if physically incorrect, helps the model to reach a better convergence with a lower value of the residuals.

Another change, done in the computational set-up, concerns the injection of droplets in the DPM. In the Discrete Phase Model in Fluent it is possible to choose the frequency of the injections [9]. In the previous model new droplets were injected at every time step. If instead of doing so, new droplets are injected every five time steps, the total number of droplets will remain the same but since the droplets are grouped in parcels and the number of parcels depends on the number of elements in the surface of the injection, the total number of parcel will be reduced by a factor of 5. Since the LPT is tracking parcels and not droplets, having less parcels to track reduce drastically the computational effort. This number cannot be reduced too much otherwise the solution will lose accuracy.

Finally, the last thing that is changed in the computational set-up in order to have faster calculation is the introduction of an absolute convergence criterion for the residuals. In the transient solution the solver is doing 50 iterations per time step in order to reach convergence. However these many iterations are needed only at the beginning of the transient. After a certain point, convergence is reached after few iterations at every time step. Using a convergence criterion, the solver stops the calculation and skips to the next time step once convergence is reached, avoiding unnecessary iterations and therefore reducing the calculation time.

Besides these major changes, a few minor changes are done to the computational set-up. The numerical scheme for particle tracking in the DPM is changed from analytical to implicit and the discretization method for time in the EFW model is changed from explicit to implicit. In fact the implicit formulation has broader stability characteristics and reaches convergence much faster than the explicit one [5][9].

These changes made to the computational set-up of the model result in a decrease of the computational time from roughly seven days to a few hours. An assessment of the usage of processors in the parallel solution is also done and it is concluded that using 144 processors does not bring any increase of rapidity, so the number of processors used for each simulation is decreased to 8. In this way the same results can be obtained with less computational time and effort and also costs.

Once this first goal is achieved the focus can be moved to the sensitivity study of the model to improve the accuracy of the results. As previously explained, the main interactions governing the annular flow are evaporation, entrainment and deposition. The first one is treated as a mass source given via an UDF to the solver. Hence the main focus of the studies is on the modeling of entrainment and deposition which are more complex than evaporation and involve many different parameters.

III.3.2. Entrainment Modeling

As explained in details in section III.1.2, entrainment is modeled using Okawa's empirical correlation. The usage of correlations depending on global flow parameters like this one is a poor choice in a CFD model, since it cannot be used to have local results in each point of the mesh depending on local variables. However, in ANSYS Fluent currently there are no functions able to model this phenomenon properly and the usage of a correlation seems to be the only way.

Okawa's correlation is the most appropriate when modeling annular flow in pipes, but in order to model more complex geometries it has to be changed with a correlation depending on local flow parameters. A bibliographic study of possible correlation usable for this purpose is done and the results are shown in the last chapter of this report as follow-up recommendations.

Even if the correlation used and its implementation in the model via an UDF are not changed, going through the C language script of the UDF it has been noticed that the value of the steam velocity used in eq. (9) and (10) in the previous model is the one in the interface between steam and liquid film. However, Okawa's correlation uses a bulk velocity value. Considering a turbulent profile for the steam axial velocity, the near wall velocity magnitude is small compared to the bulk one. As a consequence the entrainment mass source is underestimated using such a value.

The UDF is hence changed accordingly.

III.3.3. Deposition Modeling – Inlet Boundary Conditions

The choice of modeling deposition by the DPM Lagrangian Particle Tracking is considered the most appropriate choice among the available functionalities in ANSYS Fluent and it has been kept in the present work. When modeling deposition with the LPT, the way the droplets are injected in the model plays a primary role. Hence, sensitivity studies on the droplets inlet boundary conditions are done to see how they affect the results and to get conditions as close as possible to the real ones.

In section III.2.1 of this report it has been explained that in the previous model, droplets are injected with the same axial velocity as the steam and zero radial velocity. As a consequence the droplets are starting their trajectories travelling straight across the pipe length. In a second time, the droplets flow is affected by the flow of the steam and so their axial velocity is decreased due to drag and gravity forces and their radial velocity changes due to vorticity created by turbulence.

Using these inlet conditions, the LPT is not tracking any droplets depositing in the liquid film in the first part of the pipe. As a consequence the deposition is highly underpredicted and so is the film mass flow rate. This gives an explanation of the underprediction noticed by the previous master student in the conclusions of her report.

This problem will be referred from now on as entrance effect. Such an effect is normally seen in every CFD problem where complex inlet boundary conditions have to be set. In this particular case it is caused by different factors, of which the one that most affects the deposition modeling is the droplet inlet velocity.

To overcome this problem the injection type has been changed in the DPM injection settings. Instead of using a surface type injection with zero radial velocity and uniform axial velocity a file type injection is chosen. This type of injection let the user determine for each injected parcel the position, velocity, diameter, temperature and mass flow rate. A detailed explanation of how injection file works is given in Appendix B.

In order to get the values of each of the parameters to set in the injection file an inlet development model is needed. The general idea is to use a secondary model called “inlet development model” and to use its outlet flow conditions as inlet boundary conditions for the primary model called “main model”.

Since the only interest about the inlet development model is for its outlet condition it is possible to give simple inlet boundary condition. In this case there will be an entrance effect but then the flow will develop along the pipe length and will get a developed profile at the outlet surface.

Using this developed profile as new inlet boundary condition for droplets injection in the main model, the deposition entrance effect is reduced considerably. In fact the droplets injected in this way have both axial and radial velocity components with radial distribution.

The sensitivity analyses have shown that other inlet boundary conditions can affect the flow condition with an entrance effect. The one with the biggest effect is the steam inlet velocity.

Steam inlet velocity was previously given a uniform value everywhere in the pipe inlet cross section. However, flowing inside the stabilization wall a turbulent axial velocity profile was created before the steam entered the annular wall. The removal of the stabilization wall described in section III.3.1 inhibits this development of the steam flow. So a counter measure has to be taken in order to be able to remove the stabilization wall without creating an entrance effect due to the undeveloped velocity of the steam.

Also in this case the inlet development model is used. The same model used to create the inlet boundary conditions for droplets is used to create the inlet velocity boundary condition for steam. The only difference is that the steam boundary condition is passed to the main model via a profile file. Profile files are type of files that can be created and used in ANSYS Fluent containing different information about the main phase. In our case the parameters which are saved in the profile file and used as inlet boundary conditions are: steam axial and radial velocity components, turbulent kinetic energy and specific dissipation ratio.

These changes described in the last two sections increased considerably the accuracy of the model. The main improvements achieved are shown in the next chapter.

Chapter IV. - Results and Discussions

IV.1. Experimental Data from Adamsson and Anglart

In order to assess the accuracy of the model, experimental data taken by Adamsson and Anglart in 2006 are used [10]. A sketch of the experimental test section from the high-pressure two-phase flow loop at the Royal Institute of Technology (KTH) in Stockholm is shown in Figure 5.

The test section consists of a heated tube 3.65 m long and with a diameter of 14 mm. Flow conditions are typical for BWRs: 70 bar operating pressure, 10 K of inlet subcooling, mass flux variable from 750 to 1750 kg/m²s and mean heat flux around 1 MW/m². Four different axial power distributions have been used: uniform, inlet peaked, middle peaked and outlet peaked.

As can be seen in Figure 5 the measurements of the film mass flow rate done by the extraction of the film via the use of porous media is done in the last part of the test section.

Figure 5 - Schematic of Adamsson and Anglart test section

The onset of annular flow happens around one third of the total length of the test section, however to extract the liquid film at the beginning of the annular flow is technologically challenging because of the thick, highly unstable film. Hence, the measurements are done only in the last 0.8 to 1.39 meters of the test section where the annular flow is already developed and it is easier to do measurements of the film flow rate.

Figure 6 shows the four different axial power distributions used during the experiments. The black vertical lines mark the part of the test section in which extraction of film mass has been done in the cases with inlet, outlet and middle peaked distributions.

Figure 6 - Axial relative power distribution along the test section

IV.2. Improvement of Entrainment and Deposition

Before showing the validation of the model with the experimental data, a comparison of the modeling of entrainment and deposition before and after the changes described in section III.3 is done. In order to compare the two results and see the improvements done, the entrainment and deposition mass fluxes through the film-steam interface as functions of the axial position in the pipe are shown in Figure 7. This simulation is run using flow conditions analyzed in the experiments by Adamsson and Anglart.

The axial locations refer to the last 1.06 m of the test section. It is important to note that these results are instantaneous result from a transient simulation. This explains why the deposition curves are not smooth but instead they oscillate. Deposition is calculated by the LPT and at each instant the number of droplets deposited in a certain point of the wall can vary around a mean value.

Figure 7 - Deposition and entrainment mass flux versus axial distance from inlet of the model

Figure 7 also shows the results obtained by running a 1D code written in MATLAB, see Appendix C. In fact for single pipe geometries a 1D code using Okawa's correlation both for entrainment and deposition is a good reference for comparison. It is not assumed that the 1D code results are absolutely right and that they should be used to validate a CFD code. On the contrary a CFD code is supposed to be more precise than a 1D one. The aim of this comparison is just to have a general overview of the results. The correlations developed by Okawa were developed for this type of code so it is assumed that they give reasonable results when used in a 1D code.

The first thing to notice in this plot is the difference in entrainment mass flux. After the change of steam velocity used in the correlation from the film-steam interface to the bulk value the entrainment mass flux more than double, as expected. Besides comparing the CFD results with the 1D code, after the change the curves match in the majority of the points, meaning that now the Okawa's correlation is implemented correctly in the UDF of the CFD model.

Looking now at the deposition mass flux curves one can see that after the changes made to the inlet boundary conditions for droplets and steam velocity, the entrance effect is reduced significantly. After 0.5 m the results of the three models are basically the same, however in the entrance region the previous model is underestimating the deposition source. After the changes made the deposition mass flux passes from values in the entrance region near zero to values around $0.5 - 0.6 \text{ kg/m}^2\text{s}$.

It is important to stress again the fact that the 1D results should not be taken as the right ones, however in a developed annular flow region it is physically reasonable to think that the deposition mass flux has a constant or monotonic shape like the 1D results.

Even if an entrance effect is still visible in the new results, it is less than before the changes, so it is possible to conclude that the new inlet conditions are closer to the real ones.

Ideally if perfect inlet conditions are given no or very little entrance effect will be seen.

IV.3. Droplet Diameter

A flow parameter which deserves to be discussed separately is the droplet diameter. In annular flow the size of droplets can change significantly with the diameter varying from tenths of a millimeter to a few millimeters.

The size of the droplets depends on different flow conditions in the near-wall zone. In fact considering that the droplets are created during the entrainment process based on shearing off of roll-waves, it is clear that their size is given by a balance between surface tension and drag forces.

Different correlations have been developed starting from these mechanistic considerations. However, to implement these correlations in the CFD model is quite complicated, especially considering that the entrainment is modeled with the Okawa's correlation which does not depend on local interfacial parameters.

Using a droplet size distribution would be better but is quite complicated. As a first approach it is reasonable to use a fixed value of the droplet diameter for the whole dispersed phase. The problem now is to choose a value which describes well the majority of the droplets in the flow. Since the area of interest for this project is annular flow in BWRs, this choice is done looking at the work done by Le Corre et al. in 2015 [11]. They carried out experiments at the Westinghouse FRIGG facility in Västerås in which they measured the droplet size distribution in annular flow considering typical BWRs operating conditions.

The main outcome of Le Corre et al. work is that 99% of the droplets mass is made of droplets with a diameter between 0.2 mm and 2 mm and that the arithmetic mean of the droplet mass distribution (de Brouckere mean) is 1.2 mm. This means that the majority of the dispersed phase mass is carried by droplets of 1.2 mm diameter. Hence this value is chosen for the CFD simulations done in this project.

Besides, these results justify the choice of removing the stabilization wall presented in section III.3.1, since a diameter of 0.1 mm is unreasonable to use to model the whole liquid dispersed phase.

It is of interest to know how much the solution is sensitive to the droplet diameter value. Therefore a sensitivity analysis is done. For this purpose the flow conditions from the Adamsson and Anglart experiments are taken into account and five different simulations, where only the droplet diameter is differing, are run. The five values are chosen in the interval given by Le Corre et al.: 0.2, 0.3, 0.7, 1.2 and 2 mm.

In Figure 8 the results of the sensitivity analysis are compared with the experimental data from Adamsson and Anglart. The first evidence from this study is that the model is very sensitive to the value used for the droplet diameter. Considering that evaporation and entrainment are calculated via correlations which do not depend on the droplet diameter this sensitivity has to be caused by the deposition simulation via the LPT model.

Figure 8 - Sensitivity analysis on droplet diameter ($P=70$ bar, $G=1250$ kg/m²s, uniform heat flux)

This phenomenon can be easily explained thinking about the turbulence in the steam flow. The liquid droplets are travelling in the steam core where vortices are created due to turbulent phenomena. The smaller the droplet the more its flow is affected by these vortices because of the lower inertia. Therefore small droplets gain more radial velocity and they are more likely to travel into the liquid film and being deposited. On the contrary, large droplets possess big inertia and their trajectory is less influenced by the steam flow, leading to lower deposition and therefore to a faster decrease of the film mass flow rate, as shown in Figure 8.

The second useful result obtained by this sensitivity study is that the curve obtained using a value of 1.2 mm approximate better the experimental data than the others. So, the choice of using this value is endorsed by these results. It is important not to be misled by the fact that the purple curve, obtained for a value of 0.7 mm passes through all the experimental points. In fact, when looking at the slope of the curves it can be seen that the 0.7 mm curve decreases at a slower rate than the experimental data while the 1.2 mm has the same rate.

Besides, if the curve starting point is moved upwards, the 1.2 mm will perfectly match the experimental data. This could seem like a trick, but after speaking with the author of the experiments he agrees that the first data point is in disagreement with all the other data points and that maybe an error happened during the measurement process.

Even if using a fixed value of 1.2 mm seems to be a good choice as a first approach, if the flow conditions are changed it might not be the case anymore and a different value might have to be used instead. Besides it is still important to keep in mind that given the high sensitivity of the model to this parameter, a better solution has to be implemented in the future, possibly one with a diameter distribution obtained by interfacial wave properties.

IV.4. Validation of the Model

Different data sets corresponding to different flow conditions taken by Adamsson and Anglart are used to validate the model. All the following simulations are run using a fixed value of droplet diameter of 1.2 mm, unless differently specified.

First, the same flow conditions used for the droplet diameter sensitivity analysis are considered. For these flow conditions ($P=70\text{bar}$ and $G=1250\text{ kg/m}^2\text{s}$), four different power axial distributions are analyzed: uniform, middle peaked, inlet peaked and outlet peaked. Being able to model different power distribution is relevant for this study because of the different axial power distributions used during BWRs operation.

It is important to stress that since the measurements are taken in the last part of the experimental test section, only the end part of the axial power profiles is affecting the model results. Hence, the evaporation rate is higher in the case with uniform axial power than in all the other cases.

The terms middle peaked, inlet peaked and outlet peaked refer respectively to the middle, inlet and outlet of the test section described in Figure 5 and not of the mesh used in the CFD model.

In order to change the power axial distribution in the model, the part of the UDFs concerning the evaporation mass and momentum sources has to be changed. Besides each different case has different inlet conditions of film and droplets mass flow rate so the inlet boundary condition for these two parameters have also to be changed accordingly from case to case.

CFD modeling of annular flow with a three-field approach

Figure 9 - Validation for $P=70$ bar, $G=1250$ kg/m²s and four different axial power distributions: uniform (top left) –middle peaked (top right) – inlet peaked (bottom left) – outlet peaked (bottom right)

Figure 9 shows the results of the simulations run to validate the model with the four different axial power distributions. The model is well approximating the majority of the data point in all the different cases analyzed.

An important outcome of this study is that with a uniform power distribution the decreasing of the film mass flow rate is mainly driven by evaporation while entrainment and deposition have a secondary role. Whereas in the other cases, the evaporation rate is lower and the contribution of deposition and entrainment becomes more important. In fact it is possible to see that the film mass flow rate is decreasing linearly in the uniform power case, while the slope is flatter in the other cases.

To validate the model with different flow conditions, four of the other experimental data sets by Adamsson and Anglart are chosen. These cases differ from the ones in Figure 9 mainly for the total mass flux while pressure and mean heat flux remain almost the same.

CFD modeling of annular flow with a three-field approach

The first two cases in Figure 10 show the results obtained for a total mass flux $G=1750 \text{ kg/m}^2\text{s}$ with a uniform and an inlet peaked axial power distribution.

Figure 10 - Validation for $P=70$ bar, $G=1750 \text{ kg/m}^2\text{s}$, uniform (left) and inlet peaked (right) axial power distributions

The other two cases shown in Figure 11 are instead obtained for a total mass flux $G=750 \text{ kg/m}^2\text{s}$ with inlet and outlet peaked axial power distributions.

Figure 11 - Validation for $P=70$ bar, $G=750 \text{ kg/m}^2\text{s}$, inlet peaked (left) and outlet peaked (right) axial power distributions

Looking at these last results it is possible to see that the model is not working as well as for the cases analyzed in Figure 9. These last four simulation results are slightly underpredicting the experimental data, except for the one at $G=1750 \text{ kg/m}^2\text{s}$ and with an inlet peaked axial power distribution for which an overprediction is instead noticed.

Hence, it can be concluded that the model cannot be used as it is for a wide range of flow conditions, especially if the total mass flux is changed.

There are different reasons why the model is not responding well when changing the flow conditions. First of all it could be that the way the inlet conditions are calculated is not good for every flow condition. In fact the length needed in the development model could be dependent to flow parameters such as the axial velocity. A slower flow could require a longer pipe to develop the inlet conditions.

It could also be that some parameters which have not been taken into consideration during this master thesis influence the model results, for example some constants used in the Okawa's entrainment model could also depend on the flow conditions.

However, the main hypothesis is that since the droplet size depends on the flow conditions, as said in section IV.3, the value chosen of 1.2 mm is only valid for a total mass flux of $1250 \text{ kg/m}^2\text{s}$ but it should be changed for lower or higher mass fluxes.

To study this hypothesis a simulation of one of the last four cases analyzed ($G=750 \text{ kg/m}^2\text{s}$ and inlet peaked axial power distribution) is done reducing the droplet diameter from 1.2 mm to 0.3 mm. The results are shown in Figure 12.

As expected from the sensitivity study on droplet diameter, when using a smaller value of the droplet size, the deposition rate increases leading to a higher film mass flow rate. The underprediction noticed before is no longer seen and the experimental data are very well approximated by the model results.

However, even if the hypothesis of the droplet diameter seems to be correct it cannot be stated with 100% confidence that this is the only reason leading to the underprediction of the experimental data for $G=750 \text{ kg/m}^2\text{s}$ or to the overprediction of the experimental data for $G=1750 \text{ kg/m}^2\text{s}$. Besides even if it is known from the studies presented in section IV.3 that the droplet size is affected by different flow parameters, there is no evidence of why a value of 0.3 mm is appropriate for the particular flow case analyzed.

Figure 12 - Validation for $P=70 \text{ bar}$, $G=750 \text{ kg/m}^2\text{s}$ and inlet peaked axial power distribution with a droplet diameter of 0.3 mm

IV.5. Onset-to-Dryout Simulation

All the validation cases shown above refer to a model which describes a portion of an already developed annular flow, in which film and droplets inlet conditions are known and the inlet boundary conditions are calculated in order to meet these conditions. However, it is of interest to model not only part of the flow but the entire annular flow starting from the Churn-Annular transition and modeling until dryout happens. The Churn-Annular transition is also referred to as onset of annular flow and that's why the term Onset-to-Dryout simulation is used.

When modeling the whole annular flow starting from the onset, the choice of inlet boundary conditions becomes complicated. In fact the only thing that can be known with a certain precision is the steam quality. Therefore it is possible to know the amount of vapor and liquid in the flow but it is difficult to know which fraction of the liquid is dispersed as droplets or travel on the wall as liquid film. Besides, the transition zone is a highly chaotic one and the creation of steam velocity profile and droplet injection file from outlet condition of another model cannot be done.

On the other hand, when modeling annular flow from the onset to dryout or near dryout conditions the length of the channel is long and the entrance effects are less important. In fact for such long distances the flow can develop properly even if the inlet boundary conditions are far from the real ones. Of course the results in the initial part of the channel would not be accurate but, since the major interest is on the final part of the channel, it is a good compromise.

Given that the inlet boundary conditions of droplets and steam velocity are not as important as for the partial flow modeling, one should still determine the onset entrainment fraction, which is the fraction of liquid in the form of dispersed droplets. Some research has been done in this direction, and a few correlations have been developed with the help of look-up tables. Such tables collect experimental data of Critical Heat Flux for different flow conditions and can be used to develop correlations for different parameters. However, even if these correlations have been validated in a wide range of conditions, the look-up tables are not globally accepted and their results still have uncertainties [12].

Since it is not easy to find a proper value and given the complexity of the transition phenomenon it is reasonable to assume that the entrainment fraction in reality is constantly varying. It is then important to know how much the solution of the model depends on this parameter.

To do so, three different simulations are run for different onset entrainment fraction. For this purpose the mesh used previously has been scaled in order to have a three meter long annular region. The flow conditions are taken as common BWR operational ones: $G=1250 \text{ kg/s}$, $P=70 \text{ bar}$ and uniform heat flux $Q''=0.98 \text{ MW/m}^2$. The flow quality at the churn-annular transition is taken using Mishima and Ishii criterion [13]. Finally the values of the entrainment fraction chosen for the three simulations have been taken close to the one obtained using the correlation developed by Jiao et al. [12].

The results of these simulations are shown in Figure 13.

Figure 13 - Sensitivity to onset entrainment fraction E_0 in onset-to-dryout simulation

The main outcome of this study is that the results are very sensitive to the onset entrainment fraction. By changing this value only from 0.51 to 0.60, the dryout position, which in the figure is the point in which the curves intersect the horizontal axis, is reduced by around 0.3 meters.

Unfortunately it is not possible to know with the current knowledge on annular flow, if such sensitivity is reasonable or if it is a flaw of the model.

Chapter V. - Conclusions and Follow-Up

Modeling annular flow with CFD codes turns out to be quite challenging. There are many boundary conditions and computational settings that have to be analyzed properly and tuned. Besides there is not a unique way of doing it, many different approaches can be tried and none of them is with certainty better than the others.

Within this project the main focus is put on the choice of proper inlet boundary conditions and computational settings in order to obtain valuable results using an Eulerian-Lagrangian approach. The Lagrangian Particle Tracking brings many complications since the results given by this method are very dependent on the inlet conditions. However, the LPT seems to be the best choice to model in 3D the flow of dispersed droplets within the steam core. This method is simply solving equations of motion for each parcel tracked so that you do not need to use any correlation to model deposition. In this way deposition modeling is quite general and applicable to different geometries and flow conditions.

It is also shown that the main parameters influencing the LPT results are the droplet inlet velocity, the steam inlet velocity and the droplet diameter.

There is one more inlet flow parameter that could affect the entrance region. This parameter is the droplet inlet spatial distribution. It has been noticed during the postprocessing of the different simulations carried out in this project that the droplets traveling in the steam core develop a certain spatial distribution in which the near-wall zone is slightly less dense of droplets compared to the inner part of the pipe. At the current state droplets are injected at the inlet with a uniform spatial distribution. This is thought to be the best solution at the moment because there are no experimental data to refer to. However, how this inlet parameter affects the results should be investigated with a sensitivity study. In fact it could be part of the reason why there is still some difference between the model results and the experimental data compared in section IV.4.

Regardless of the improvement done in the settings of the inlet boundary conditions and on the calculation speed of the model that has been noticeably increased, there are still many aspects that have to be studied and improved in order to have a model that can be trusted and used in design processes and safety analysis.

The difficulties in doing so are not only related to computational limitation or difficulties in using the CFD model but also and mainly to the current lack of knowledge about annular flow itself. This physical process has kept many scientists and researchers busy for decades but its complexity is so that many things still remain unknown and only correlations for particular flow conditions and simple geometries have been formulated so far. Anyway the interest shown on this topic by industries and academic institutions all over the world and the wider and wider use of CFD codes in many industrial processes let us hope for a faster and faster development of such models.

Regarding the model developed during this master thesis there are some recommendations that the author thinks can help for a future development.

First of all in order to be able to use the model for different geometries than pipes the entrainment modeling need to be changed. Currently the Okawa's correlation is used and its validity is restrained to pipe geometries. The best choice would be to use a correlation which does not depend on the geometry. To do so this correlation should be developed from only mechanistic consideration in order to give local results at each point of the liquid film. Using a local correlation that depends only on local flow parameters like film superficial velocity would also make it possible to use different values of the diameter of entrained droplets, positively affecting also the deposition modeling. If the droplet diameter is calculated locally the large sensitivity of the results due to the choice of a fixed value will also be avoided.

In the recent literature few studies on this topic have been done. Of particular interest is the work done by Liu and Bai [14]. They propose a correlation based on the interfacial properties of liquid film waves. Since this correlation is using a force balance on each wave crest to determine the maximum volume of entrained liquid from each wave, it could be applied to any geometry. Even though the correlation involves a lot of parameters which are difficult to get and seems to be quite complicated to apply in the ANSYS Fluent model via UDFs, it still seems to be the best alternative currently available.

Another useful article that can help in the development of entrainment modeling is the research done by Berna et al. in which the authors present and analyze most of the literature existing on droplets in annular two-phase flow and derive new correlations on important variables such as amount and size of entrained droplets. Even if Berna et al. studies refer to pipe geometries some interesting general results depending on local parameters are achieved [15].

The second main change to do to the model in order to be able to study more cases is to pass from a structured mesh to an unstructured one. Using structured mesh simplify the model because the cell faces are either parallel or perpendicular to the main flow direction. This leads to some simplification in the injection of droplets from a surface via UDFs or injection file. For example the entrainment mass flow rate is obtained in the UDF by multiplying the entrainment mass flux obtained from Okawa's correlation and the area of the local mesh element face. This can be done because the face of the element is parallel to the film surface. However, in an unstructured mesh this would not be true and the value of the area has to be properly calculated in a different way.

This example is not the only case in the UDFs in which the mesh element face area is used and all of these cases have to be taken into account and changed accordingly when using an unstructured mesh.

Apart from these main changes which are according to the author the two most significant ones there is one more change that has to be done especially if dryout and post-dryout conditions want to be modeled.

This change concerns the evaporation mass source. Since the current model studies only pre-dryout cases, it is assumed that the whole wall surface of the geometry is wet with enough film liquid to fully absorb the wall heat flux via evaporation. However, when simulating general annular flow where dryout can occur, it can happen that part of the wall is dry and evaporation does not occur leading to a local increase of temperature. To be able to model this phenomenon the mass source term in the UDF should be re-written taking into account a condition of sufficient liquid film. Besides the energy equation should be solved to be able to see the local increase of temperature.

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Appendices

Appendix A – User Defined Functions

Below is an example of the User Defined Functions used during the simulations. To simulate different flow conditions a few parameters have to be changed and sometimes also entire part of the UDF has to be changed or deleted. The script presented in this appendix contains all the different UDFs used throughout the whole master thesis project. Therefore, pay attention when using them to be sure to make the right modification to fit the flow conditions you are simulating.

```
#include "udf.h"
#include "sg_film.h"

real hvap = 1504900;
real heat_flux_mean = 983443;
real n = 0.111;
real ke = 0.000479;
real rhovap = 36.525;
real rholiq = 739.72;
real dh = 0.014;
real r = 0.007;
real muliq = 0.000091249;
real Ref_crit = 320;
real sigma = 0.017633;
real p_diam = 0.0012;

DEFINE_PROFILE(film_mass_source,tf,i)
{
    real film_thickness, film_vel, vap_vel, Jf, Jg, fi, Ref, area_face,
    area[ND_ND], pos[ND_ND], r1, x_inj, y_inj, z_inj, evap_mass_source,
    evap_mom_source, ent_mass_source, distrib;
    face_t f;
    cell_t c;
    Thread *tc;

    begin_f_loop(f,tf)
    {
        film_thickness = F_EFILM_HEIGHT(f,tf);
        film_vel = F_EFILM_W(f,tf);
        c = F_C0(f,tf);
        tc = THREAD_T0(tc);
        F_CENTROID(pos,f,tf);
        vap_vel = 0.6543*pos[2]*pos[2]*pos[2]-7.706*pos[2]*pos[2]+
        32.44*pos[2]-28.95;
        Jf = 4*film_vel*film_thickness/dh;
        Jg = vap_vel;
        fi = 0.005*(1+300*(film_thickness/dh));
        Ref = (rholiq*Jf*dh)/muliq;
        if (Ref>Ref_crit)
```

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```

        ent_mass_source =
        ((ke*rholiq*fi*rhovap*Jg*Jg*film_thickness)/sigma)*pow
        (rholiq/rhovap,n);
    else
        ent_mass_source = 0.0;

    distrib=-0.041572*pow(pos[2],6)+0.43222*pow(pos[2],5)-1.5111
    *pow(pos[2],4)+1.7822*pow(pos[2],3)-0.036178*pow(pos[2],2)+
    0.094166*pow[2]+0.4022;

    evap_mass_source = distrib*heat_flux_mean/hvap;

    evap_mom_source = evap_mass_source*film_vel;

    F_AREA(area,f,tf);
    area_face = NV_MAG(area);
    r1 = r-5*film_thickness;
    x_inj = r1*(pos[0]/r);
    y_inj = r1*(pos[1]/r);
    z_inj = pos[2];

    C_UDMI(c,tc,0) = evap_mass_source;
    C_UDMI(c,tc,1) = evap_mass_source*area_face;

    C_UDMI(c,tc,2) = evap_mom_source;
    C_UDMI(c,tc,3) = evap_mom_source*area_face;

    C_UDMI(c,tc,4) = ent_mass_source;
    C_UDMI(c,tc,5) = ent_mass_source*area_face;

    C_UDMI(c,tc,6) = x_inj;
    C_UDMI(c,tc,7) = y_inj;
    C_UDMI(c,tc,8) = z_inj;

    C_UDMI(c,tc,12) = F_EFILM_DPM_MASS_SRC(f,tf)/area_face;
    C_UDMI(c,tc,13) = F_EFILM_WS(f,tf);

    F_PROFILE(f,tf,i) = -(ent_mass_source+evap_mass_source);
}end_f_loop(f,tf)
}

DEFINE_DPM_INJECTION_INIT(entrainment_inj,I)
{
    Particle *p;
    cell_t c;
    Thread *tc;

    loop(p,I->p_init)
    {
        c = P_CELL(p);
        tc = P_CELL_THREAD(p);
        P_POS(p)[0]=C_UDMI(c,tc,6);
        P_POS(p)[1]=C_UDMI(c,tc,7);
        P_POS(p)[2]=C_UDMI(c,tc,8);
    }
}

```

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```
P_FLOW_RATE(p)= C_UDMI(c,tc,5);
P_DIAM(p)=p_diam;
P_VEL(p)[0]=C_U(c,tc);
P_VEL(p)[1]=C_V(c,tc);
P_VEL(p)[2]=C_W(c,tc);

C_UDMI(c,tc,9)=C_U(c,tc);
C_UDMI(c,tc,10)=C_V(c,tc);
C_UDMI(c,tc,11)=C_W(c,tc);

}
}

DEFINE_DPM_INJECTION_INIT(inlet_inj,I)
{
Particle *p;
cell_t c;
Thread *tc;
face_t f;
Thread *tf;
int n;

real x[ND_ND],area_face,area[ND_ND];

loop(p,I->p_init)
{

c = P_CELL(p);
tc = P_CELL_THREAD(p);
real area_min=1;
c_face_loop(c,tc,n)
{
f = C_FACE(c,tc,n);
tf = C_FACE_THREAD(c,tc,n);
F_AREA(area,f,tf);
area_face = NV_MAG(area);
if(area_face<=area_min)
area_min=area_face;
}

C_CENTROID(x,c,tc);
P_POS(p)[0]=x[0];
P_POS(p)[1]=x[1];
P_POS(p)[2]=x[2];
P_FLOW_RATE(p)=581.1*area_min;
P_DIAM(p)=p_diam;
P_VEL(p)[0]=0;
P_VEL(p)[1]=0;
P_VEL(p)[2]=C_W(c,tc);

}
}
```

```

DEFINE_SOURCE(vapor_mass_source,c,tc,dS,eqn)
{
    real vol_cell,evap_mass_source;

    vol_cell = C_VOLUME(c,tc);
    evap_mass_source = C_UDMI(c,tc,1)/vol_cell;
    return evap_mass_source;
}

DEFINE_SOURCE(vapor_mom_source,c,tc,dS,eqn)
{
    real vol_cell,evap_mom_source;

    vol_cell = C_VOLUME(c,tc);
    evap_mom_source = C_UDMI(c,tc,3)/vol_cell;
    return evap_mom_source;
}

DEFINE_PROFILE(z_film_mom_source,tf,i)
{
    face_t f;
    cell_t c;
    Thread *tc;
    real drop_vel, ent_flux;

    begin_f_loop(f,tf)
    {

        c = F_C0(f,tf);
        tc = THREAD_T0(tc);

        drop_vel = C_UDMI(c,tc,11);
        ent_flux = C_UDMI(c,tc,4);

        F_PROFILE(f,tf,i) = -(C_UDMI(c,tc,2)+ent_flux*drop_vel);
    }end_f_loop(f,tf)
}

DEFINE_PROFILE(y_film_mom_source,tf,i)
{
    face_t f;
    cell_t c;
    Thread *tc;
    real drop_vel, ent_flux;

    begin_f_loop(f,tf)
    {

        c = F_C0(f,tf);
        tc = THREAD_T0(tc);

        drop_vel = C_UDMI(c,tc,10);
        ent_flux = C_UDMI(c,tc,4);
    }
}

```

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```
F_PROFILE(f,tf,i)= -ent_flux*drop_vel;
}end_f_loop(f,tf)
}

DEFINE_PROFILE(x_film_mom_source,tf,i)
{
face_t f;
cell_t c;
Thread *tc;
real drop_vel, ent_flux;

begin_f_loop(f,tf)
{

c = F_C0(f,tf);
tc = THREAD_T0(tc);

drop_vel = C_UDMI(c,tc,9);
ent_flux = C_UDMI(c,tc,4);

F_PROFILE(f,tf,i)= -ent_flux*drop_vel;
}end_f_loop(f,tf)
}
```

Appendix B – Injection File

The injection file is a way of defining the injection in the DPM. It is used to inject droplets specifying for each injected parcel its spatial coordinate, velocity components, diameter, temperature and mass flow rate. These files are text file in which each line corresponds to an injection. Here, it is shown the formatting of one line in an injection file.

```
(( x y z x-vel y-vel z-vel diameter temperature mass-flow-rate ))
```

In the model these values are extracted from the solution of the inlet development model. Using `File → Extract → Solution Data` it is possible to extract and save these values in a ASCII format. To convert this file into an injection file, a MATLAB and a C language script are used. In MATLAB it is possible to import the ASCII file and save it in a matrix where the values for the z coordinate and mass-flow-rate can be adjusted to meet the value needed as inlet condition for the injection of the main model. Once this is done, the matrix can be saved or simply copy pasted in a .txt file. The C script then reads the .txt file and creates a new .txt file called “nuovo.txt” with the right formatting of the lines (double brackets at the beginning and end of each line, space divided values). Finally the decimal sign has to be changed from coma to dot and the extension of the file has to be changed from .txt to .inj. This can be done simply renaming the file and changing the extension in the name.

To run the C script via the terminal go to the directory which contain the script and the injection.txt file and run the following command:

```
./nameofthescript nameotheinjectionfile.txt
```

The name of the script and the file commonly used in the project are respectively “injectionCprogram” and “inj.txt”. The final injection file is then called “injection0.inj”

Appendix C – 1D Code

The following MATLAB script is used to model in 1D the same flow modeled with ANSYS Fluent in order to have something else to compare the results with other than experimental data. This particular script refers to the following flow conditions: $P=70$ bar, $G=1250$ kg/m²s and uniform power distribution.

```
R=0.007;
A=pi*R*R;
dropd=0.0012;
muliq=0.000091249;
mugas=0.000018960;
rho=36.525;
rhol=739.72;
mldrop=4/3*pi*(dropd/2)^3*rhol;
D=0.014;
H=1504900;
q_sec=983443;
sigma=0.017633;
en=0.111;
ke=0.000479;
g=9.81;
vi=12.0352;
Z=1.06;
G=1250;
M=G*A;
h=0.001;
N=round(Z/h);
mvap=zeros(1,N);
mdrop=zeros(1,N);
mfilm=zeros(1,N);
filmthi=zeros(1,N);
filmvel=zeros(1,N);
ment=zeros(1,N);
mdep=zeros(1,N);
steamvel=zeros(1,N);
mdrop(1)= 0.0989;
mfilm(1)=0.0258;
mvap(1)=M-mfilm(1)-mdrop(1);
Mtot(1)=M;
steamvel(1)=vi;
Ment=0;
Mdep=0;
z=(h:h:Z);

film_vel1 = vi;
film_thickness1=R-(R*R-mfilm(1)/pi/rhol/film_vel1)^0.5;

Jf = 4*film_vel1*film_thickness1/D;
Jg = vi;
Ref = (rhol*Jf*D)/muliq;
fi1 = 0.005*(1+300*(film_thickness1/D));
film_thickness2 = 0.25*sqrt(max(16/Ref,0.005)*rhol/(fi1*rho))*Jf*D/Jg;
fi2 = 0.005*(1+300*(film_thickness2/D));
delta=abs(fi2-fi1);
```

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```

while delta>0.001*fil

    film_vel2 = film_vel1*(R*R-(R-film_thickness1)*(R-
    film_thickness1))/(R*R-(R-film_thickness2)*(R-
film_thickness2));
    Jf = 4*film_vel2*film_thickness2/D;
    fi1 = 0.005*(1+300*(film_thickness2/D));
    film_thickness1 = film_thickness2;
    film_vel1 = film_vel2;
    film_thickness2 =
0.25*sqrt(max(16/Ref,0.005)*rho1/(fi1*rho))*Jf*D/Jg;
    fi2 = 0.005*(1+300*(film_thickness2/D));
    delta=abs(fi2-fi1);
end

filmthi(1)=film_thickness1;
filmvel(1)=film_vel1;

for i=2:N

    mvap(i)=mvap(i-1)+(q_sec/H)*h*2*pi*R;
    steamvel(i)=mvap(i)/rho/A;
    Jf = 4*filmvel(i-1)*filmthi(i-1)/D;
    Jg = steamvel(i-1);
    Ref = (rho1*Jf*D)/muliq;
    fi = 0.005*(1+300*(filmthi(i-1)/D));
    ment(i-1)=ke*rho1*fi*rho*Jg*Jg*filmthi(i-1)*((rho1/rho)^en)/sigma;
    vd=steamvel(i-1)-0.23;
    C=mdrop(i-1)/(vd*A);
    mdep(i-1)=C*0.0632*((C/rho)^(-0.5))*((rho*D/sigma)^(-0.5));
    Ment=Ment+ment(i-1)*h*2*pi*R;
    Mdep=Mdep+mdep(i-1)*h*2*pi*R;
    mfilm(i)=mfilm(1)-Ment+Mdep-mvap(i)+mvap(1);
    filmthi(i) = 0.25*sqrt(max(16/Ref,0.005)*rho1/(fi*rho))*Jf*D/Jg;
    filmvel(i) = mfilm(i)/(rho1*pi*(R^2-(R-filmthi(i))^2));
    mdrop(i)=mdrop(1)+Ment-Mdep;
    Mtot(i)=mdrop(i)+mfilm(i)+mvap(i);
end

```