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Faculty of Mechanical Engineering

Numerical simulation of the filling process in the pressure bottle.

Master thesis

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DIPLOMA THESIS ASSIGNMENT

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Rules for elaboration:

Numerical flow simulations in pressure bottles during the filling process, determination and testing of the simulation approaches, detections of the pressure and temperature distribution in the pressure bottle, investigation of the heat transfer generated by gas compression into the bottle material, validations of the pressure and temperature by the experimental results at the particular locations of the computational domain. The different materials of the bottle (metal or non-metal materials) will be considered for a numerical investigation.

Scope of graphic works: **20 pages**

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List of specialized literature:

[1] **CHUNG, T. J.,** *Computational fluid dynamics.* **Cambridge University Press, 2006, ISBN-13 978-0-521-59416-5.**

[2] **GRINSTEIN, F. F., MARGOLIN, L. G., RIDER, W. J.,** *Implicit Large Eddy Simualtion.* **Cambridhe University Press, 2007, ISBN 978-0-521-86982-9.**

[3] **KRAUS, A. D., AZIZ, A., WELTY, J.,** *Extended surface heat transfer.* **John Wiley & Sons, 2001.**

[4] **STEPHEN, B. Pope,** *Turbulent flows.* **Cambridge University Press 2000, ISBN 978-0-521-59125-6.**

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ABSTRACT

This work deals with the research and the development of a pressurized air bottle by creating a numerical model, and using this model to develop it. The model is planned to be used further to decrease the weight of the breathing flask used by the fire-fighters.

Failure experiments can be hazardous to perform in labs, that's why if a numerical model that can be reliable enough, simulating an experiment would be more preferable rather than putting anyone at risk. But with that comes a need to validate the simulation results in order for them to be usable.

A Numerical Model was setup for a Flask getting filled with Nitrogen and was validated through an experiment to compare the margin of error between Temperature results, an error less than 10% was achieved. The model shows good prospects for further usage into the advancement of the flask used in firefighting, the model is concerned mainly with the temperature and pressure distribution inside the flask using adequate turbulence models, and real gas equation models.

ANSYS workbench was used for simulating the gas filling of the flask, at first a steady-state simulation was used to calculate initial conditions that were later incorporated in the transient simulation. SST K-ω turbulence model proved to be best fit for the filling process, external heat transfer with the walls of the flask was assumed to be free convection with an ambient room temperature.

The Experiment was done at the federal institute for material testing in Berlin, and the institute provided the experimental data for the simulation to be validated.

Several models were tested starting from a simple compressible ideal gas model to more complex models for turbulence, real gas state equations and inlet conditions were changed to reach a model with most similarities with the experimental results.
The model used assumes specific aspects of the boundary conditions, for the example the filling of the flask being done at a linear rate of increasing pressure through a User-defined function, also Soave-Redlich–Kwong equation of state is being incorporated as to describe the different state of nitrogen during the flask filling, as it yielded the most similar results to the experiment. This model can be used further in testing different materials for the lining of the flask, also examining the thermal and mechanical stresses induced in the flask in case it’s exposed to fire.

Keywords: CFD; ANSYS; Fluid Dynamics; Simulation; Thermals

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Also **M.Eng. Thorsten Schonfelder** for showing me the firefighting department in Berlin, and providing me with the experiment data.

List of abbreviations

CFD	Computational Fluid Dynamics
RMS	Root mean square
BAM	Bundesanstalt für Materialforschung und -prüfung
TKE	Turbulent Kinetic Energy
. SST K-ω	Shear stress transport
MSc	Master of Science
DIN	Deutsches Institut für Normung eV (German Institute for Standardization)
min.	minute
sec.	second
t	time
K	Kelvin
TUL	Technical University of Liberec
SST	Shear stress transport
al	Auminium
Cu	Copper
sim.	simulation
abs	absolute
EXPE	Experiment

Contents

1. Introduction: Case study and collaboration

One of the leading causes of traumatic injuries among firefighters in the United States is falls and loss of balance on the fire ground. These events lead to over 11,000 injuries per year or more than 25% of all fire ground injuries, [1] Accidents due to falls typically account for the longest work absences for firefighters [2]. In 2003, a study determined that the mean total worker's compensation claim per slip, trip or fall injury was $8662, which is well above the mean of all claims – $5168 [3] - Thus, slip, trip and fall injuries are not only one of the most common, but also one of the most costly on the fire ground.

The virtual world is continuously taking over the real world, CFD has been growing in the past years due to several reasons, whether it is for cost efficiency, the experiment being too dangerous or for the sake of trying too many design options, CFD has provided a good environment for trial and error, or for elaborate designs that could be put to the test at the expense of only some processing power.

Computational fluid dynamics is a relatively new science, and as Academics we should pave the way for such software to be more reliable to be used by engineers, during my MSc thesis I was working on a Case study involving several partners, also it was the continuation of some experiment carried out by a colleague, the main goal was stimulating an experiment and validating the results in order to create an engineering approach to a model that would be used for further developing the studied product.

The air bottle configuration (mass and size) used with a firefighter's self-contained breathing apparatus may affect functional gait performance and slip/trip/fall risk, contributing to one of the most common and costly fire ground injuries to this population.

.An experiment made at BAM, and it was the base of the Diploma work of a colleague was used as the base for the simulation and research work.

Flows can usually describe using partial differential equations, by using the numerical simulation we can obtain an approximate solution, the solution is usually approximate to a certain degree, which means there's usually an error. The method of approximation is due to discretization, so as the accuracy of experimental data relies on the quality of measuring devices used, we can also say that the quality of the numerical simulation results can rely on the discretization method used.

Since there's always a margin of error, we need to have the ability to be able to analyze and judge the results, the complexity of the simulated model influences directly the results we have, for example solving Navier-Stokes equation for incompressible Newtonian fluids could achieve accurate results in principle, but moving on to simulate more complex models like combustion or multiphase could leave to a much bigger margin of error, at the end the user of a commercial software is trying to find the right combination of a Mathematical Model, Discretization method, adequate mesh, solution method to target a convergence criteria. And as a salesman might always have unlimited ambition, the average user might be stuck with results that lacks validation [4].

2. Experiment and previous work

2.1 Experiment preparation[1]


Figure 1 breathing air bottle

For the experiment temperature development inside breathing air bottle shall be recorded during filling. The experiments were carried out on the actual filling process presented in the experiment at the Berlin fire brigade. And the results were provided by BAM. During the filling measurements are to be made to the temperature inside the breathing air bottle in order to determine the maximum occurring temperature.

In addition, the experiment was carried out to examine influencing factors which the experiment operator can influence during the filling process, and it shall be used further for this thesis work to validate the results obtained from the simulation model.

Plotting of temperature profiles at the inlet of bottle during the filling process are recorded. The pressure and temperature profile is then could then be saved in order to be used later on to validate the simulation model.

[1] Most of the experimental data was provided by BAM.

2.2 Test planning - Temperature measurement in breathing air cylinders

The practical implementation of the temperature measurement in the breathing air bottle provides a special focus within the scope of the work. For this purpose a breathing air bottle (Type III) is equipped with temperature sensors which can then be used during a complete filling process, the temperature development can be recorded. [5] (see appendix A)

Figure 2 - drilled bottle with sensors

Conceptual idea of how the test should work

For the practical implementation of the temperature measurement, a concept must first be developed, such as the temperature inside and the breathing air bottle at different points.

When designing the test, it should be noticed that the temperature sensors in the bottle are minutely affected by the air flow only little.

Also the stability of the breathing air bottle must be guaranteed.

One possibility would be to provide appropriate temperature sensors on the outer surface of the Breathing air bottle and using the thermal conductivity coefficients for temperatures at the inside of the breathing air bottle.

The disadvantages of this are the direct additional temperature influence from the environment and the missing possibility to measure the temperature at different depths of the pressure bottle.

As a final concept, the variant chosen, in which the pressure bottles were drilled and

With temperature sensors from the outside through the bottle wall, because here the

Temperature inside the breathing air bottle can be measured and the inflow

In the bottle is not affected, that had the downside on having possibility of air escaping if the bottles are not well isolated.

The diameter of the holes should be as small as possible in order to minimize the effect on the breathing air bottle. In addition an adhesive with bond resistant to the pressure should be achieved. The temperature sensor is to be selected in such a way that an influence of the sensors on the flow is avoided.

The variant was chosen, in a way that the pressure bottles were drilled and temperature sensors inserted from the outside through the bottle wall, because in this method the temperature inside the breathing air bottle can be measured and the inflow in the bottle would not be affected.

2.3 Preliminary tests for concept selection

To ensure the stability of the pressure bottle and the safety of the test performers, it was mounted on a special platform, to carry out preliminary tests. The putty used with the sensors must be able to withstand the pressure of 300 bar.

In the bursting test, the pressure bottle is placed in a secured place [figure 3]

Environment filled with water-glycol mixture and the internal pressure of the cylinders steadily

Elevated. Breathing air bottles of the same type without glued temperature sensors which

At the time of the experiment at the Berlin fire brigade they usually burst at more than 1000 bar.

In the preliminary experiments which have been carried out, it is to be clarified whether weakening of the Breathing air bottle through the holes represents a safety risk and whether the adhesive putty spots can withstand the pressure of 300 bar. A total of three preliminary tests were carried out, the adhesive site for each preliminary experiment as described below has been optimized.

After Preliminary tests. This resulted in an increase in the maximum pressure of 450 bar, before again some hole starting leaking as it is the weakest point.

Figure 3 - testing area for pressurized flasks

2.4 The experiment

The air used at the Berlin fire brigade is compressed directly from the environment. Efforts are made to ensure that the air is free from contamination such as exhaust gases or dust.

The exact requirements for breathing air are set out in DIN EN 12021. The typical Composition of natural air is to be found in DIN EN 12021 [5]. When considering physical properties of air, it becomes clear that air in the experiments and simulation cannot be assumed as an ideal gas. As filling the gas bottle at 300 bar with ideal gas would give a different volume than when it is filled with real gas.

The breathing-air bottles with 6.8 liters would be produced according to the law of Boyle [6], assuming air as the ideal gas at 300 bars, a breathing air volume of 2,040 liters. However, this is not the case; rather, air must be considered here as a real gas, this allows a breathing air capacity of only about 1,854 liters.

Figure 4 - filling process

2.5 Filling process at the Berlin fire brigade

At the Berlin fire brigade, there are several thousand breathable bottles in use. Each is refilled after each use. A filling process at the Berlin Fire Brigade takes place as follows; first, the breathing air bottles are attached in series to the connections of the filling station and the valves of the pressure bottles are opened. Each of the six ports has its own Valve. Now the filling of the pressure bottles takes place.

Due to the pipe diameter between the compressor and the filling station as usually 6 bottles are filled at the same time, it takes up to 600 seconds until bottles are completely filled with breathing air and required pressure is reached. The Berlin fire brigade assumes that the minimum pressure for filling the bottles is at least at least 30 bar / min.

To check the current, an analogue manometer is installed at the filling station. As soon as uniform required pressure has been set, the valves of the filling station are closed.

2.6 Influencing factors of the user on the filling process[2]

Figure 5 - filling station manometer

The filling process is consciously and unconsciously influenced by the user. Factors by which the user can influence filling the breathing air bottle, Such as cylinder internal pressure at the beginning of the filling process, fill duration or mass flow, room temperature and temperature of the incoming air. The breathing air bottle is usually not completely emptied and thus a there is a residual pressure in the Breathing air bottle. Bottles are refilled immediately after use, without being completely emptied. It is not known how much residual pressure is present in the breathing air bottle. This raises the question as to the influence of the residual pressure on the temperature-development during filling.

[2] Photo was captured by myself in the visit to the berlin fire brigade

The user might perform the filling process by opening the valve to a certain degree, this leads to changing the filling duration. At the same time this changes the mass flow, a different filling time due to different mass flows also occurs when less than 6 air flasks are used, this influences the pressure. Other factors influencing the filling process like: room temperature at the beginning of the filling process and temperature of the incoming air.

Within the scope of the experimental investigations, the influence of the bottle-Pressure at the beginning of the filling process as well as the influence of the filling duration, the same filling volume or the mass flow of the temperature development inside the breathing air bottle during a filling process. For this purpose, a number of assumptions are assumed and that would be expressed later as the simulation covers one case.

3. Theoretical background and Models

3.1 Theoretical concept

Temperature development during the filling process during the filling process, a measurable, short-term occurrence shows temperature increase of breathing air inside the breathing air bottle as well as the container wall. Temperatures inside the breathing air bottle. The theoretical model for considering assumptions of the temperature increase of air in breathing air bottle by heating of the air during filling is due to two effects. First, the Kinetic energy E kin of the air is converted into internal energy U during the filling process.

The kinetic energy is generated by the high energy at the beginning, as well as pressure difference between the compressor and the breathing air bottle, in which atmospheric pressure prevails. The mechanical work supplied to the system is found on the compressor instead. The compression of the gas during the filling process in the breathing air bottle is the second factor which determines the temperature increase.

Secondly, the heating process which is caused by heat transfer to the environment caused by temperature differences between the temperature in the breathing air bottle and room temperature.

If the filling process takes place at a very high speed, i.e. faster than the filling process, heat can be dissipated, the initial heating can be adiabatic.

The consideration of the heat transfer from the respiratory air in the respiratory air bottle to the Framework of this methodology.

The heat transfer takes place from the breathing air onto the surface of the aluminum liner. Thus, the resulting heat flow occurs at the inner surface A, the Temperature difference ΔT between the air and the aluminum liner as well as a gas-and-material-dependent heat transfer coefficient α. This represents a proportionality-factor which decisively determines the strength of the heat transfer.

The heat conduction within the wall of the breathing air bottle is dependent on the thermal conductivity λ of a material. Type III air flasks are made of layers of different materials the heat conduction is different from layer to layer. Generally speaking.

$$\frac{dQ}{dt} = -\lambda A \frac{dT}{dl}$$

Equation 1 - Heat transfer equation

Heat conduction, described as thermal energy passing through the container surface is dependent on time dt. As well as temperature difference over the length certainly

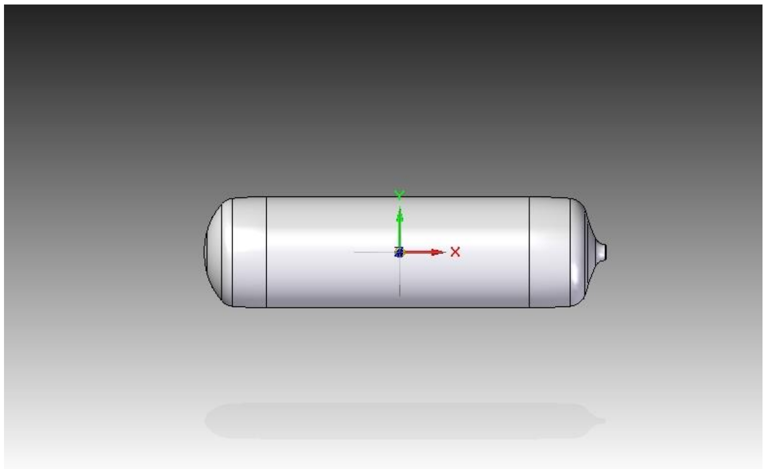
Furthermore, in heat transfer from the surface of the breathing air bottle to the ambient air; at a certain point in time the air becomes warmer as a result of compression. There is no further temperature increase than the maximum temperature of the breathing air and the breathing air bottle are reached, some heat is accumulated in the body of the cylinder as much as some is transferred to the external environment.

In the following stage, thermal equilibrium settles again, as we find that heat exchange takes place so that the temperature in the breathing air bottle is same as that of the ambient air temperature.

It is thus necessary that heat transfers in the environment are computed for a more realistic CFD model to be developed within the framework of the numerical investigations, in addition to heating being calculated.

3.2 Simulation

In order to achieve this calculation several different models were used and those will be analyzed, the model with the best results shall be discussed first. ANSYS WORKBENCH was used and the latest version available was 17.2



3.3 Mesh

Figure 5 - geometry used

ANSYS Mesh tools were for meshing as quadrilateral elements were used, and using an axisymmetric mesh shape (Figure 6) decreased the time of simulation by almost half. Several element layers were made close to the walls of the flask as it was observed in earlier simulations that the flow is more complex by the boundary layer close to the wall, other than that the geometry of the flask can be considered simple and the filling process of the flask yielded acceptable results.

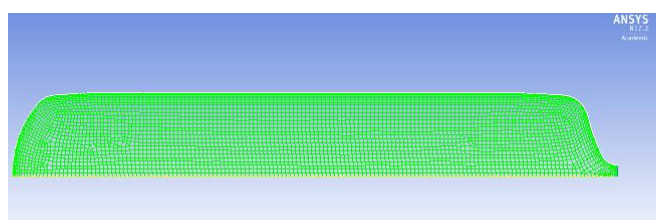


Figure 6 mesh

Mesh Quality:

Minimum Orthogonal Quality	0.031106
Maximum Ortho Skew	0.75387
Maximum Aspect Ratio	15.1371
Number of Nodes	8546
Number of Elements	4104
Wedges	11

3.4 Solver

ANSYS fluent version 17.2 offers 2 different types of solvers Density based and Pressure based, and while as the software is getting more advanced they are trying minimize the gap between the two solvers, yet the two solvers operate with an intrinsically different nature, the density based solver couples equations of Energy, momentum and continuity together and solves them simultaneously[8] which requires more time and memory, yet could provide more accurate results for simulations with supersonic velocities and highly varying density. For our simulation here we assumed the pressure increase at inlet is of linear function increase, so the difference between pressure at inlet and pressure inside the bottle is low enough for us to use the pressure-solver, which should need less time for the calculation to be finished; A variant of the pressure solver shall be used, by the name of The Pressure-Based Coupled Algorithm, this solver couples the momentum and continuity equations, then solves the rest of the governing equations sequentially in a segregated method that means it doesn’t require as much memory as the density based solver

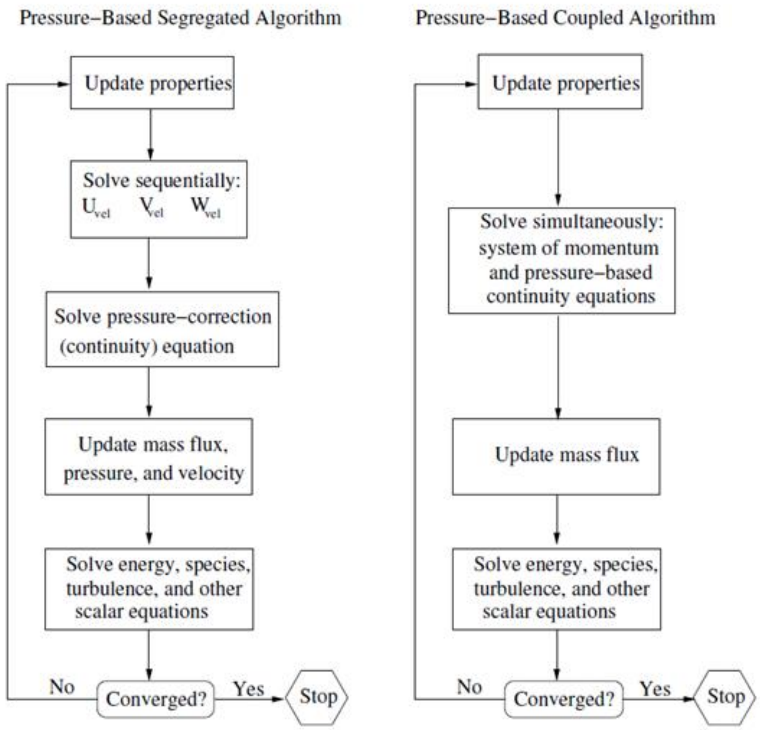


Figure 7 – Difference between solvers from ANSYS Documentation

Velocity Formulation

It is usually advised to use a velocity formulation that would result in low velocity differences in that frame, causing a decrease in the numerical diffusion in the solution, thus in the given case it was appropriate to calculate relative velocity if the change in the velocities in the vessel is huge[8]

3.5 2D – model

The geometric model was chosen to be a 2D mesh, and in relative to the original flask geometry the Axisymmetric mesh was considered to be the most describing to the current case, the symmetry of the flow and pressure distribution has been considered which has led to axisymmetric geometry, as when switched from planar mesh to asymmetrical mesh the calculation time was decreased drastically.

Energy Model:

ANSYS FLUENT solves the energy equation in the following form:

$$\frac{\partial}{\partial t}(\rho E) + \nabla.\left(\vec{v}(\rho E + p)\right) = \nabla.\left(k_{eff}\nabla T - \sum_j h_j\vec{J_j} + \left(\overline{\overline{\tau_{eff}}}.\vec{v}\right)\right) + S_h$$

Equation 2

(ANSYS HELP FILE: 5.2.1.1. The Energy Equation)

Where k_{eff} is the effective conductivity (sum of K and $k_{turbulent}$). $k_{turbulent}$ is the thermal conductivity according to the turbulence model used, and J is the diffusion flux, the first three terms on the right-hand side of Equation 2 represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively.

$$\mathbf{E} = \mathbf{h} - \frac{\mathbf{P}}{\boldsymbol{\rho}} + \frac{\mathbf{v}^2}{\mathbf{2}}$$

Equation 3

3.6 Turbulence model

The SST k-ω turbulence model is a two-equation eddy-viscosity model [9] which has become very popular. The shear stress transport (SST) formulation combines the use of a k-ω formulation in the inner parts of the boundary layer makes the model directly usable all the way down to the wall through the viscous sub-layer, hence the SST k-ω model can be used as a Low-Re turbulence model without any extra damping functions. The SST formulation also switches to a k-ε behavior in the free-stream and thereby avoids the common k-ω problem that the model is too sensitive to the inlet free-stream turbulence properties. Authors who use the SST k-ω model often merit it for its good behavior in adverse pressure gradients and separating flow. The SST k-ω model does produce a bit too large turbulence levels in regions with large normal strain, like stagnation regions and regions with strong acceleration. This tendency is much less pronounced than with a normal k-ε model though.

Model's Equations:

Kinematic Eddy Viscosity

In the analytical treatment of turbulent shear flows, the local shear stress may by expressed as the product of an eddy viscosity and the local velocity gradient by analogy with the laminar flow representation. However, while the molecular viscosity for laminar flow depends only on the fluid properties, the eddy viscosity is related to the structure of the turbulence in the shear flow. At present, turbulent flow phenomena are not well understood, so that empirical hypotheses are utilized to create a mathematical basis for the investigation of turbulent motion. These phenomenological theories lead to a formulation of the kinematic eddy viscosity (eddy viscosity divided by local density) which may be used with the equations of motion and a suitable equation of state to determine the local time-average conditions throughout a flow field. [7]

$$\upsilon_T = \frac{a_1 k}{\max(a_1 \omega, SF_2)}$$

Equation 4

Turbulence Kinetic Energy

TKE is usually means of measuring the kinetic energy of a non-constant fluid velocity by acquitting the RMS of the different velocities.

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[(\upsilon + \sigma_k \upsilon_T)\frac{\partial k}{\partial x_j}\right]$$

Equation 5

Specific Dissipation Rate

The specific turbulence dissipation, is the rate at which turbulence kinetic energy is converted into thermal internal energy per unit volume and time. This should give us means to calculate the temperature more accurately.

$$\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j}\left[(\upsilon + \sigma_\omega \upsilon_T)\frac{\partial \omega}{\partial x_j}\right] + 2(1 - F_1)\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial \omega}{\partial x_i}$$

Equation 6

Closure Coefficients and Auxiliary Relations

$$F_2 = \tanh\left[\left[\max\left(\frac{2\sqrt{k}}{\beta^*\omega y}, \frac{500\upsilon}{y^2\omega}\right)\right]^2\right]$$

$$P_k = \min\left(T_{ij}\frac{\partial U_i}{\partial x_j}, 10\beta^* k\omega\right)$$

$$F_1 = \tanh\left[\left\{\min\left[\max\left(\frac{\sqrt{k}}{\beta^*\omega y}, \frac{500\upsilon}{y^2\omega}\right), \frac{4\sigma_{\omega 2}k}{CD_{k\omega y^2}}\right]\right\}^4\right]$$

$$CD_{k\omega} = \max\left(2\rho\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial \omega}{\partial x_i}, 10^{-10}\right)$$

$$\phi = \phi_1 F_{1+}\phi_2(1 - F_1)$$

$$\alpha_1 = \frac{5}{9}, \alpha_2 = 0.44$$

$$\beta_1 = \frac{3}{40}, \beta_2 = 0.0828$$

$$\beta^* = \frac{9}{100}$$

$$\sigma_{k1=0.85, \sigma_{k2}=1}$$

$$\sigma_{\omega 1=0.5, \sigma_{\omega 2}=0.856}$$

3.7 Fluid and material models:

Nitrogen compressible using the Soave-Redlich-Kwong gas model [10]

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m(V_m + b)}$$

Where:

$$\alpha = (1 + (0.480 + 1.574\omega - 0.176\omega^2)\left(1 - \sqrt{T_r)}\,\right)^2,$$

$$a = \frac{1}{9(\sqrt[3]{2} - 1}\frac{R^2T_c^2}{P_c} = 0.42748\frac{R^2T_c^2}{P_c},$$

$$b = \frac{\sqrt[3]{2} - 1}{3}\frac{RT_c}{P_c} = 0.08664\,\frac{RT_c}{P_c},$$

T_r is the reduced temperature of the compound, and **ω** is the acentric factor: is a conceptual number introduced by Kenneth Pitzer in 1955, proven to be very useful in the description of matter. [11] It has become a standard for the phase characterization of single & pure components. The other state description parameters are molecular weight, critical temperature, critical pressure, and critical volume (or critical compressibility).The acentric factor is said to be a measure of the non-sphericity (centricity) of molecules. [12] As it increases, the vapor curve is "pulled" down, resulting in higher boiling points.

3.8 Boundary conditions

The filling experiment had a flask being filled uniformly with a filling station [Figure 9] it was hard to predict which model would fit a good simulation for the current case, on visiting the lab in Berlin, Germany and monitoring the filling process. It was best thought that a pressure inlet with a user defined function cause the pressure to increase linearly. The inlet temperature was considered to be -8 °C.

The flask material was first considered to be aluminum,

Figure 8 - filling station

3.9 UDF code used:

```
/*********************************************************************/
/* unsteady.c                                                       */
/* UDF for specifying a transient pressureprofile boundary condition */
/*********************************************************************/

#include "udf.h"

DEFINE_PROFILE(unsteady_pressure, thread, position)
{
  face_t f;

  begin_f_loop(f, thread)
    {
      real t = RP_Get_Real("flow-time");
      F_PROFILE(f, thread, position) = 200000. + (50000.*t);
    }
  end_f_loop(f, thread)
}
```

In order to be able to control the pressure increase inside the flask the above UDF code was used to make the simulation closer to the experiment [Figure 16]

External wall were assumed to be of 3 mm thickness, with an overall heat transfer coefficient of 50 $\frac{watt}{m^2K}$ was assumed to simulate the external environment. (See Appendix C)

4. Results

In this chapter features shall be discussed as follows: how different modules and solution methods were used and how they were overcame, several simulations were made and since we can always get results that look colorful with all the color gradients, validation of those results might be the trickiest issue facing the average simulation engineer.

The first set-up to be discussed is the latest used model which incurred good results when compared to the experimental results which were obtained as part of my stay at BAM[3].

The idea of the simulation is to have the same sensors in the bottle as surface monitors on the mesh (Same position) and by comparing the readings from the sensors and the surface monitor at the same time instant, the average value of the error can be obtained and from that place we can validate how far-off reality the simulation is.

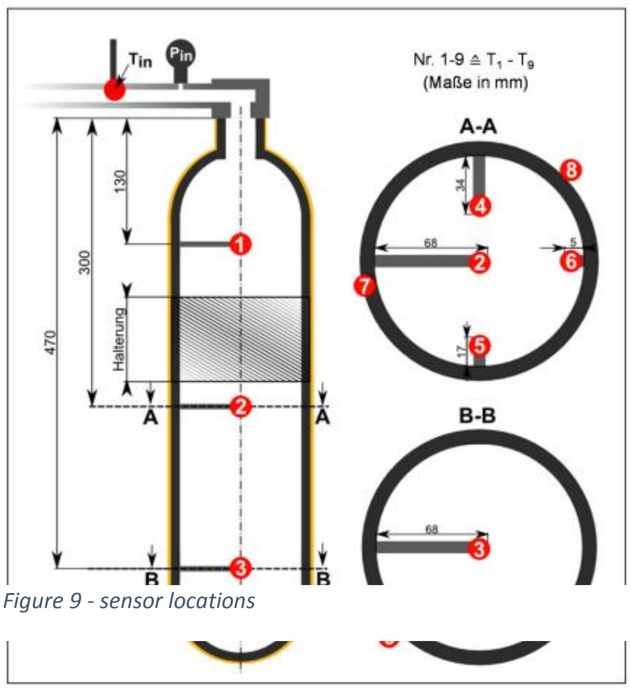


Figure 9 - sensor locations

Since the mesh used for the simulation was axi-symmetric, we were not able to have all the sensors simulated, since we are dealing with basically one lateral plane of the flask. So surface monitors labeled (T1, T2, T3 & T4) corresponding to the same sensors depicted in figure 1. Also one of the big indicators of how good the simulation was going is the pressure rise inside

[3] (Bundesanstalt für Materialforschung und –prüfung) with the help of Dr.-Ing. Frank Otremba and Thorsten Schönfelder, M.Eng.

the bottle, comparing the pressure rise according to the simulation and the experiment was permitted us to know how the UDF function used are simulating the pressure increase inside the bottle.

4.1 Validation of the results:

<u>Temperature sensor 1</u>

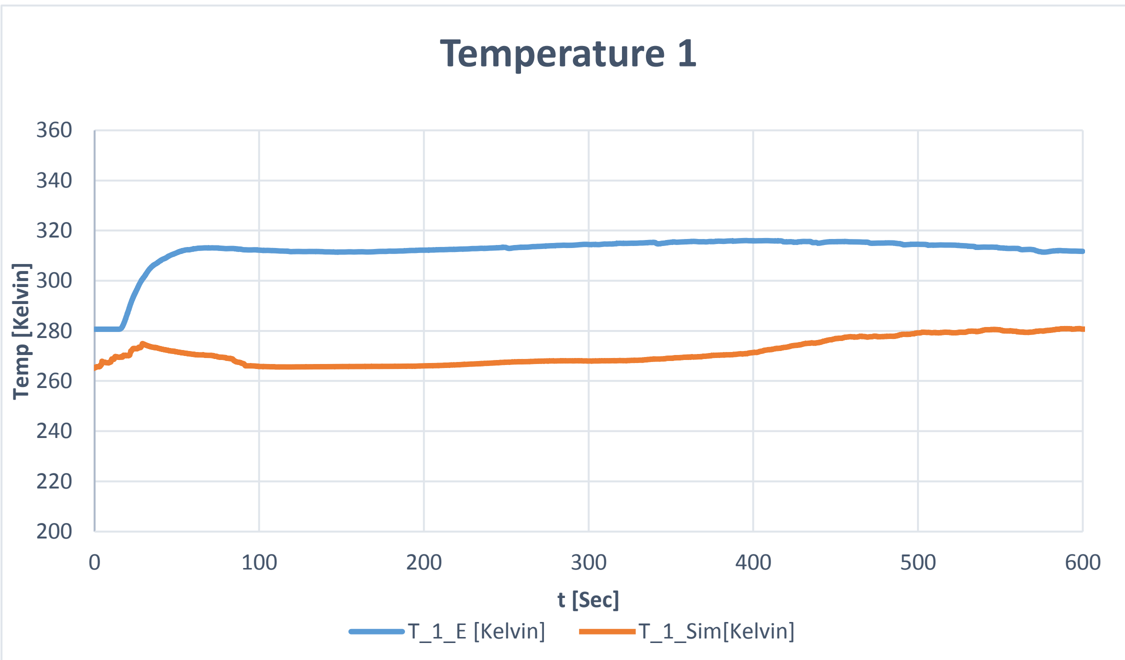


Figure 10 temperature sensor 1 comparison between experimental results and the simulation

It is observed as closer the sensor is to the inlet of the cylinder the error increases, making sensor T1 having the biggest error among sensors them the simulation results and the experimental results, but we can say the error is varying between 3.8% and 14.8% and even for the maximum error the results could be considered accurate, for the error percentage [equation 11] was used and how error changes with time check [figure 12]

$$Error = \frac{|T_{exp} - T_{sim}|}{T_{exp}}$$

Equation 7

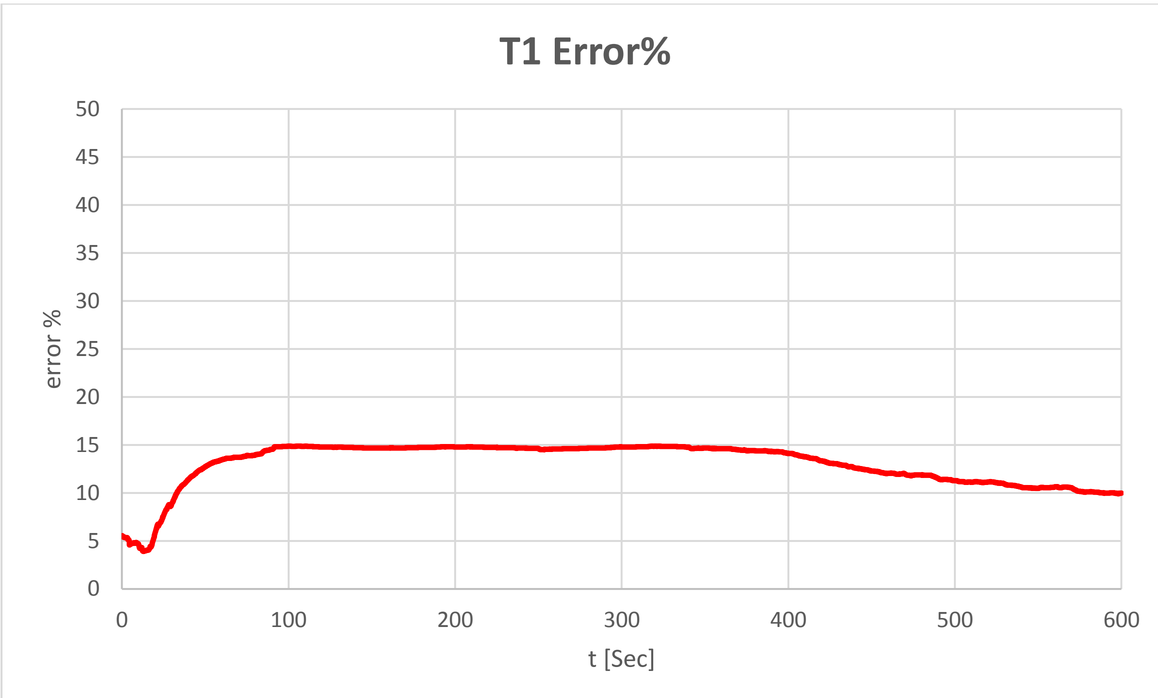


Figure 11 - error percentage of sensor 1 changing with simulation time

It is notable that the different at the start between the experiment and the simulation is small (less than 5%), which is due to the position of T1, it is close to the inlet where we know the boundary condition of T in is about -8 °C, which makes the case quiet simple to simulate till approach t = 50 sec, that is when the experiment and simulation start diverging till the error reaching the maximum which is about 14.8% and the error deviates around this value till it decreases again towards the end.

Temperature sensor 2

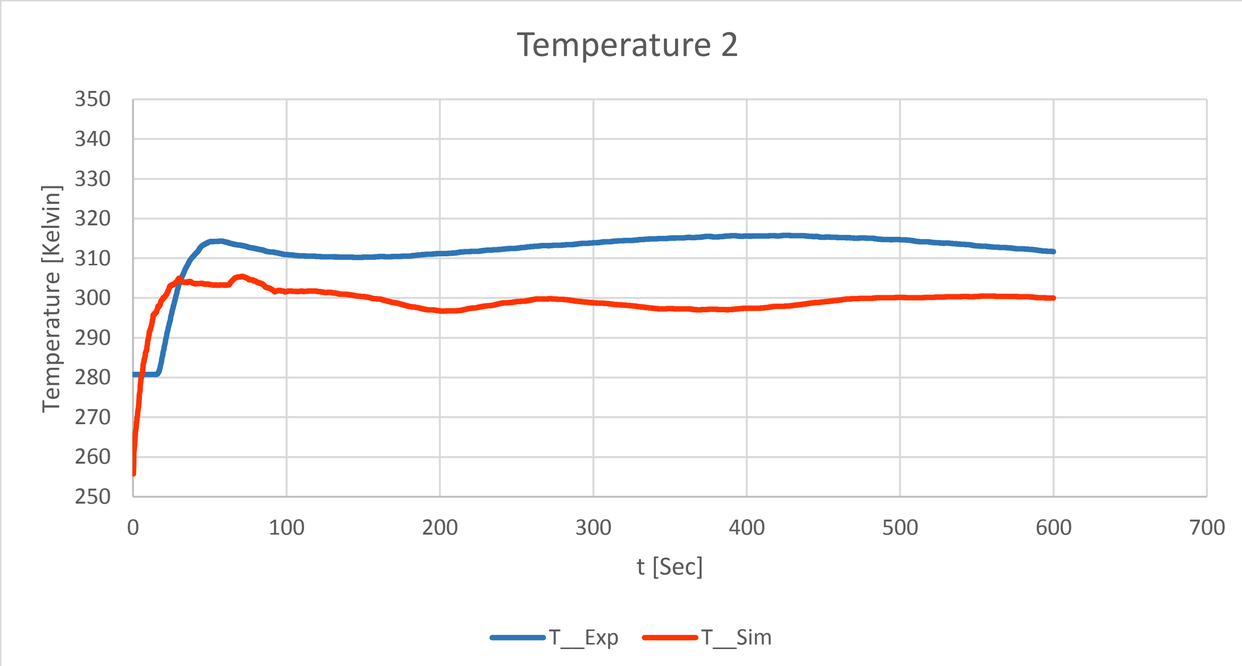


Figure 12 – temperature sensor 2 comparison between experimental results and the simulation

It is observed that in the simulation it is calculated that the inlet temperature stays the same till it reaches sensor 2, which is somewhere in the middle of the bottle while the experiment shows that at the beginning the sensor could read some higher temperature (280 °K) and this could be due to the fact that in the simulation the air bottle was assumed to be empty, while that couldn't have been the case in the real-life experiment, it is also observed that the 2 readings catch up as time goes by reaching an error of zero somewhere around t = 40 seconds and then the difference in error is maintained till the end of simulation with a maximum error of about 6%, which is shown in [figure 13].

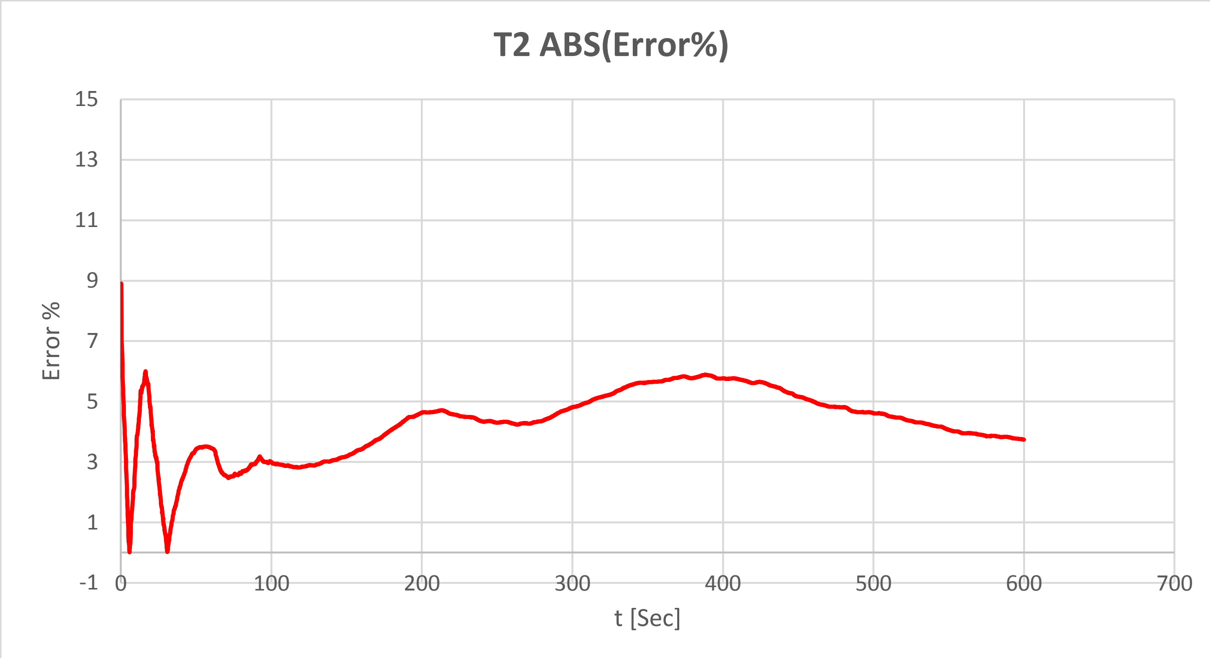


Figure 13 – error percentage of sensor 2 changing with simulation time

At the early start it is observed that there's a higher error (9%), the error seems to be varying violently all through the first 60 seconds, even reaching zero twice, which could be due to several factors include inaccurate results in the experiment itself, also at the beginning there is an assumption that might be causing the error, which is the initial pressure difference between the inlet and the pressure inside the bottle, the error seem to stabilize as we go further in the simulation with a maximum of 6% which could be considered accurate for a simulation. From here it is noticed that the difference between the experiment results and the simulation results increases where we would expect turbulence to be higher. As no matter how much simulation equations tend to describe turbulence, there is always factors that are hard to include in commercial simulation software.

Temperature sensor 3

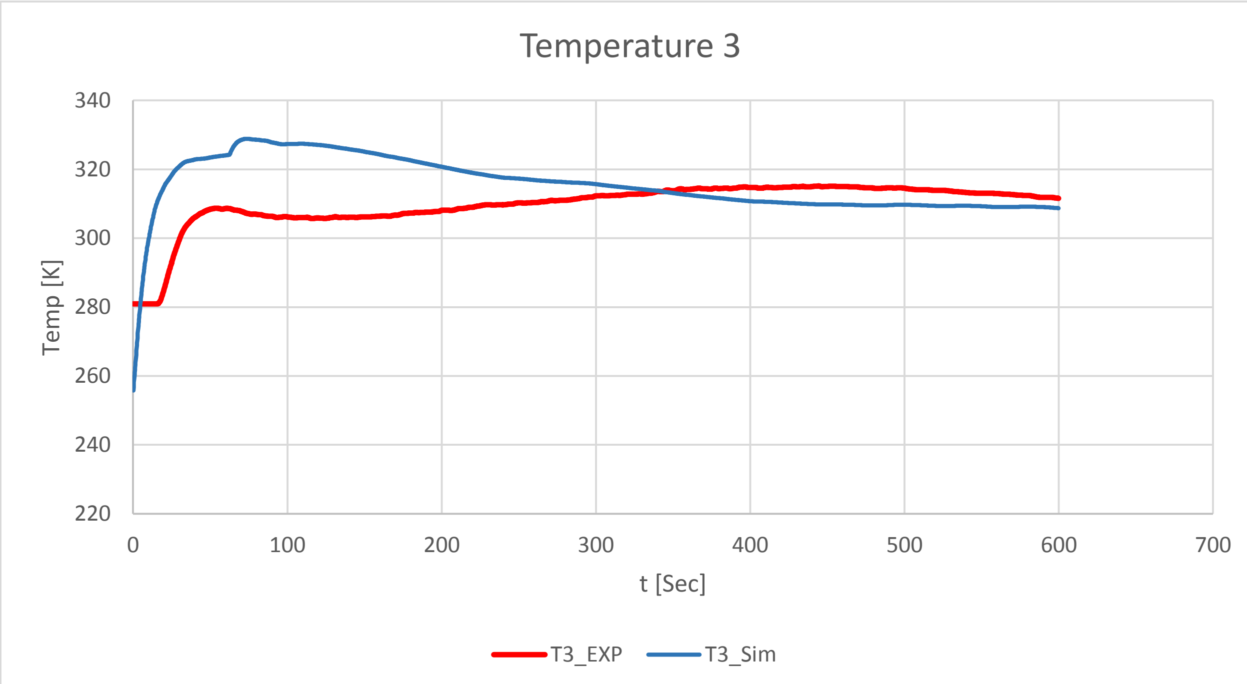


Figure 14 – temperature sensor 3 comparison between experimental results and the simulation

Temperature difference between the experiment and simulation is following the same form, where temperature difference is in the range 10 to 20 degrees where at the first seconds of the simulation there's a huge difference between the results, and as we move forward in the simulation the differences start closing onto each other giving more accurate results towards the end. It can be considered good that simulation predicted the time of highest temperature increase within a couple seconds, but it still remains that the actual experimental temperature showed lower temperature than that of the simulation for the first half, and then it's inverted for the second half.

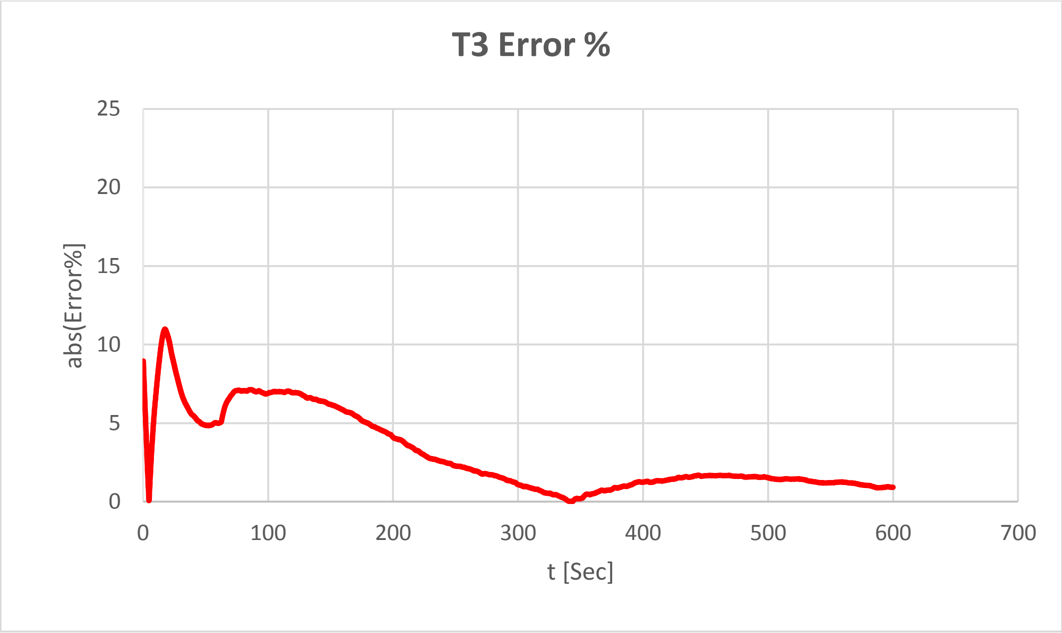


Figure 15 - error percentage of sensor 2 changing with simulation time

Sensor T3 is at the end of the flask, away from the inlet. It is also noticed that the further the sensor is placed away from the inlet, the solutions seems to stabilize and gives us a lower error%. It is also worth-stating that for the most of this specific sensor the margin of error lies below the 5% line, it could be due to the simple geometry of the gas flask, and the usage of appropriate models for simulation.

4.2 More Validation criteria

One of the validation criteria in order to compare how close we are to the experiment, was the usage of user-defined functions to simulate the same increase of pressure in the air bottle, a linear function was used to control the pressure at inlet, while the pressure in the experiment varied due to reasons to be discussed further.

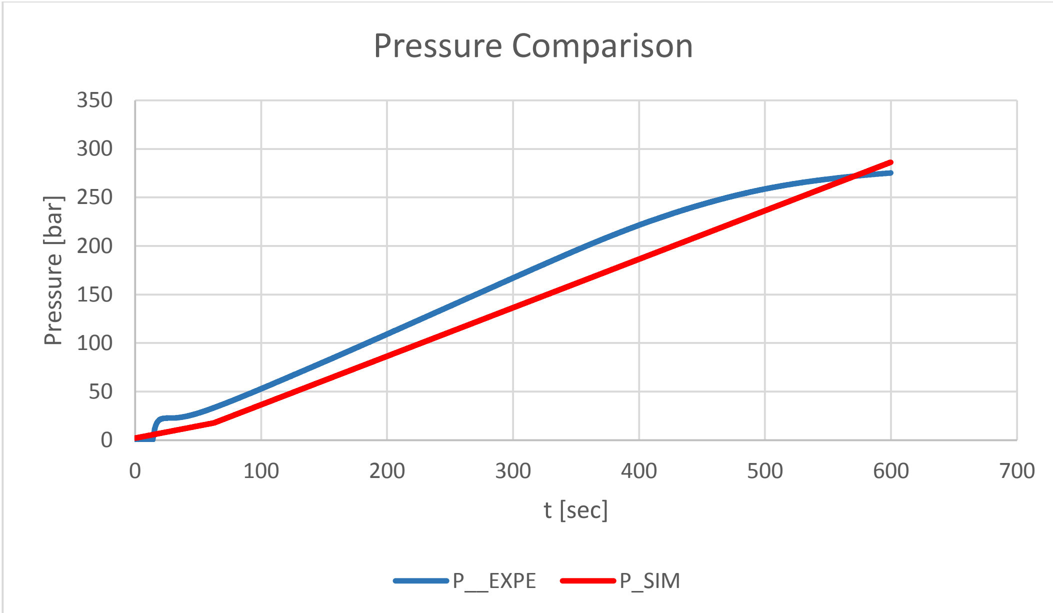


Figure 16 – comparison between experimental and simulation pressure change inside the bottle

Comparing the experiment pressure cure with the simulated on, we can observe that the experimental one has a curvature at the end, and a small hike at the beginning, those feature were simplified into the linear function at the inlet.

In order to insert the sensors into the pressure vessel, the flask was drilled in several place to insert the sensors, and then the whole was closed with resign, which might have led to certain leakage especially at higher pressures, and could be one of the reasons the results between the simulation and the experiment are different.

Figure 17 – showing drilling of sensors in the flask

4.3 Results Visualizations

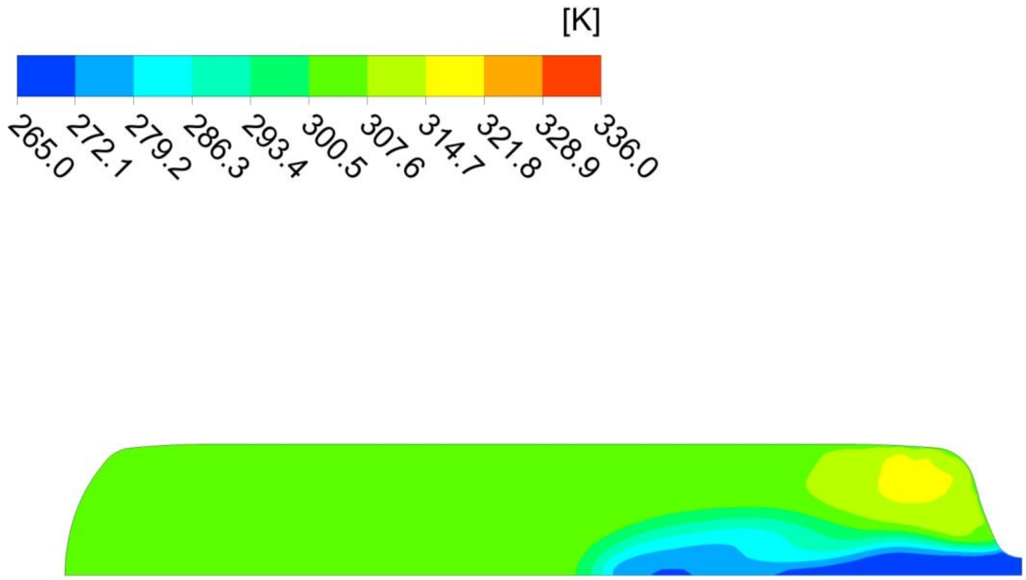


Figure 18 - Temperature at t = 5 sec

After validation of the results given for the several experiment and simulated sensors (temperature point monitors) we can consider our results accurate to a certain degree, since sampled results are within an acceptable margin of error we can further study results than can only be obtained by simulation, for example obtaining such contours via real-life experiment could be near impossible.

We can see the areas of higher temperature, and upgrade the inner lining of the pressure bottles accordingly.

The first 100 seconds usually have the highest temperature rise inside the bottle, probably due to the turbulence and high kinetic energy of the air.

Also the lab didn't have means of measuring velocity or mass flow rate, yet the results can be considered reliable given some amount of skepticism.

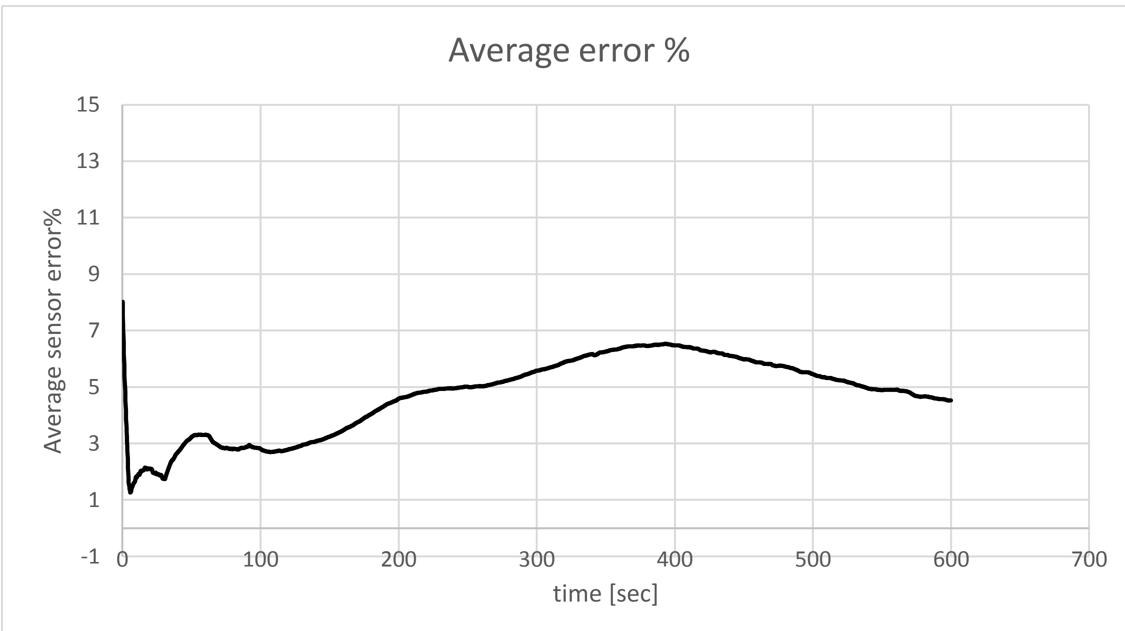


Figure 19 - Average sensor error %

The above graph when calculating the average of the whole simulation as compared to time where the maximum error is below 9% and

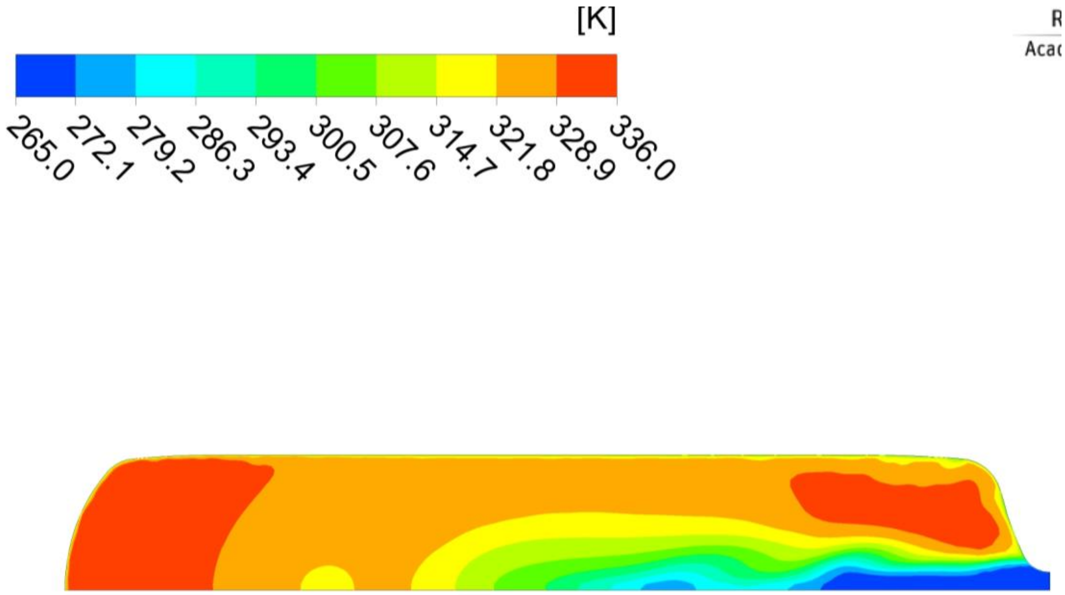


Figure 20 - Temperature at t = 20 sec

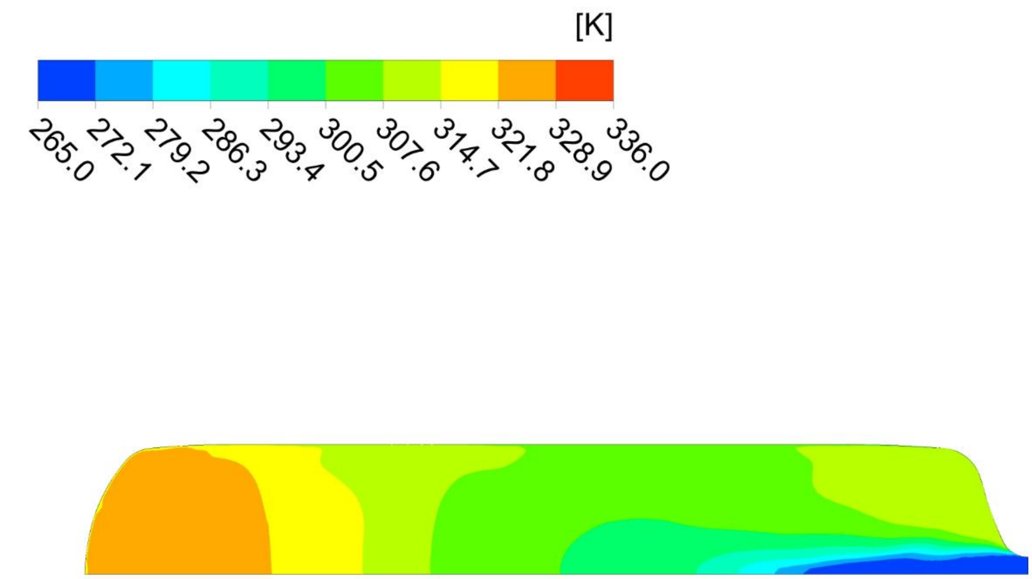


Figure 21 - Temperature distribution at t = 100 secs

Velocity at inlet

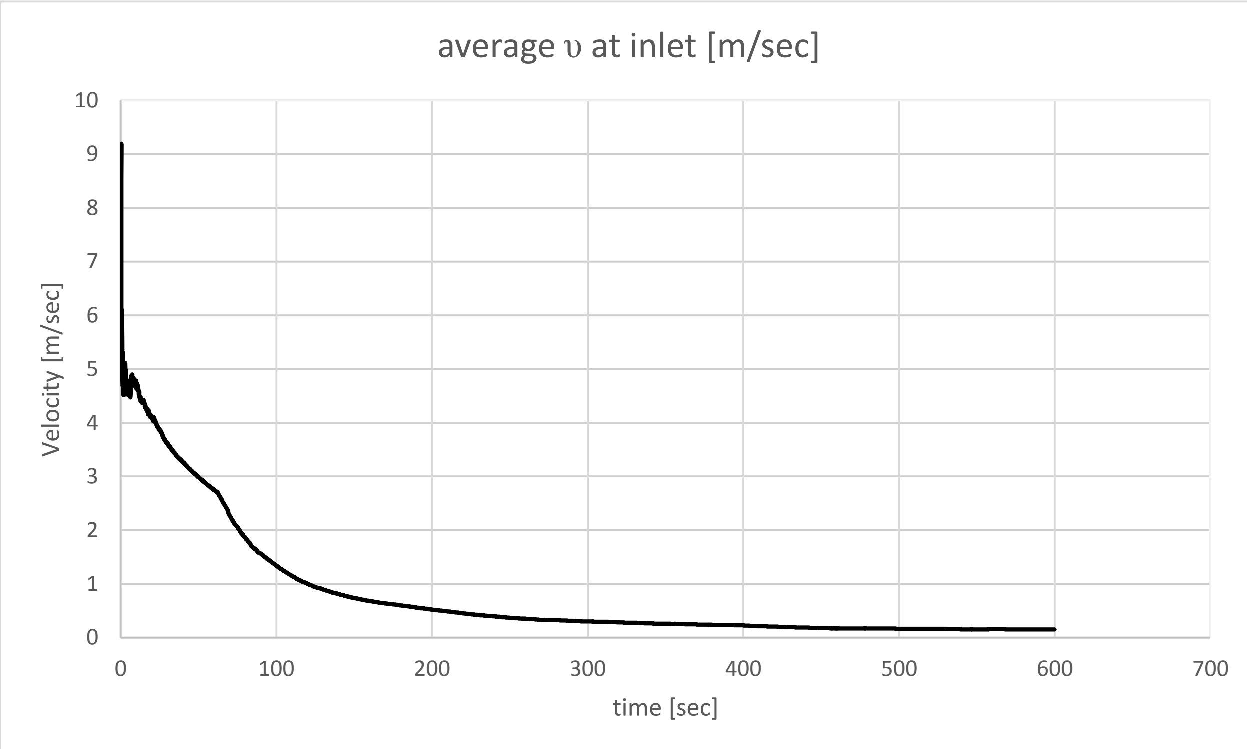


Figure 22 – time plot of velocity change with time during the filling process

It is observed that at the beginning of the filling process, the velocity is very high since the flask is assumed to be empty at the beginning of the filling process and then as the filling process keeps decreasing till it reaches near zero. (See Appendix B)

<u>Mass flow rate</u>

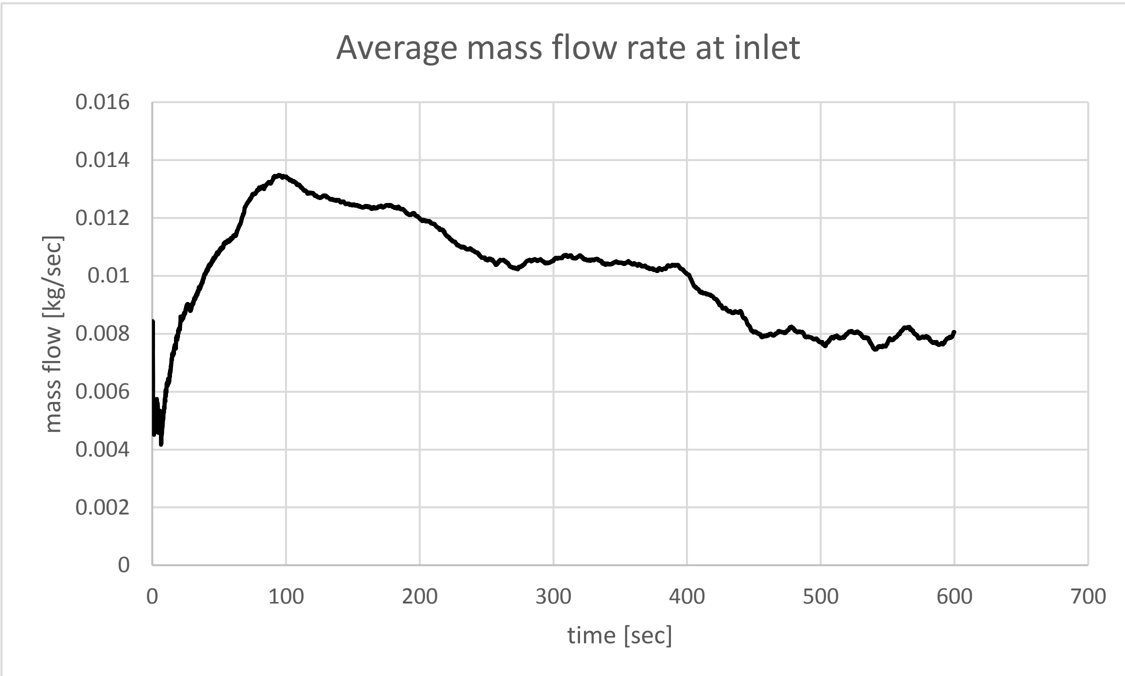


Figure 23 – time plot of average mass flow rate change with time

In order to have adequate initial conditions, a steady state simulation was performed for the initial time step of the transient simulation, since more inputs are needed it is always helpful to have initial results that could help the transient simulation to converge.

From the acquired simulation results, the mass flow rate started from the initial value acquired by the steady state simulation, and then started increasing steadily till t = 100 and then it started to decrease slowly.

5. Usage of Model for Research and Development

5.1 Material comparison

The next step after validation the simulation model is to use it for further enhancing the research and development of the breathing air bottle, and the following simulations are used for illustration of how by changing some of the parameter we can predict how the filling process can react to the different stimulants, like the air flask material shall be replaced instead of aluminum copper can be used, and there is mainly 3 parameters that change when a material is changed: Density, Specific heat (Cp) and thermal conductivity. In the following part, the change of temperature with time between the two material is compared, which opens the door for even more complex materials to be used, which eventually would help with the development of the bottle.

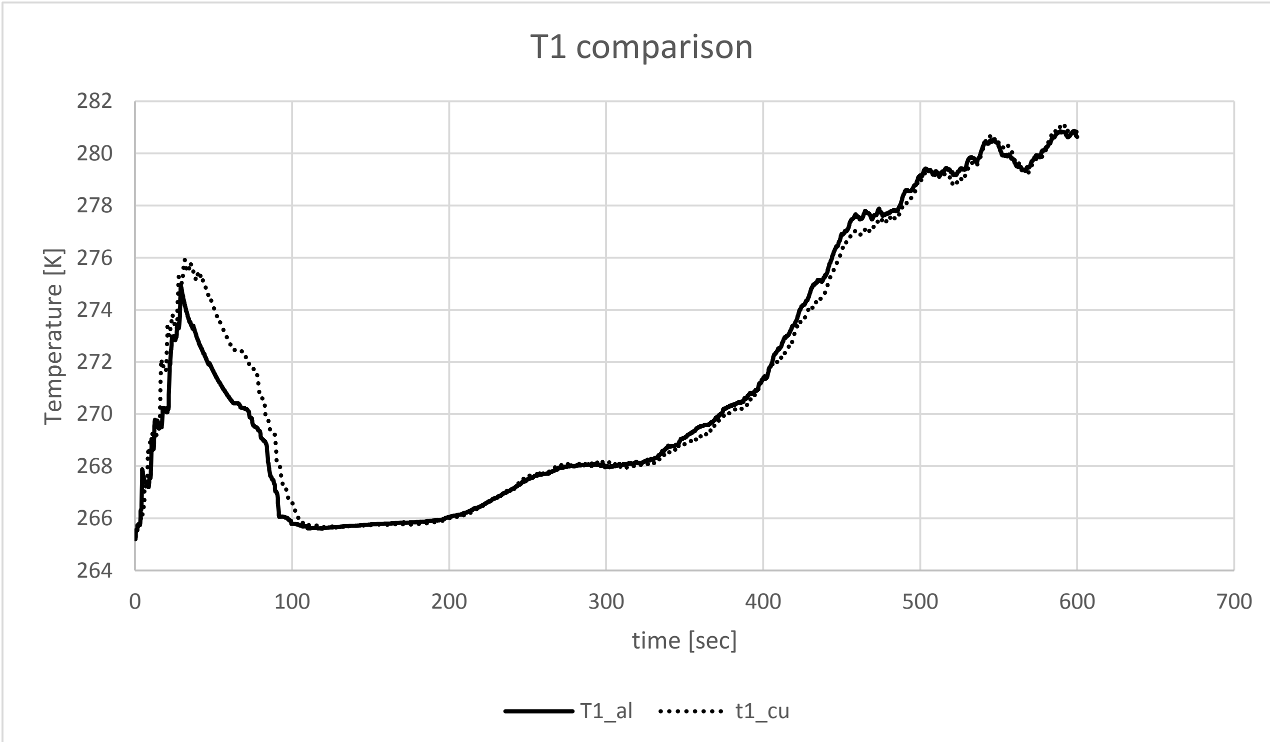


Figure 24 - Temperature comparison between Aluminum & Copper

This is an example for the usage of different material for the pressure flask, usually a composite material is used to manage to give the pressurized bottle a much lighter weight which maintaining the material properties, for the sake of simulation a different material copper was used instead of aluminum and there’s a minor change in the temperature.

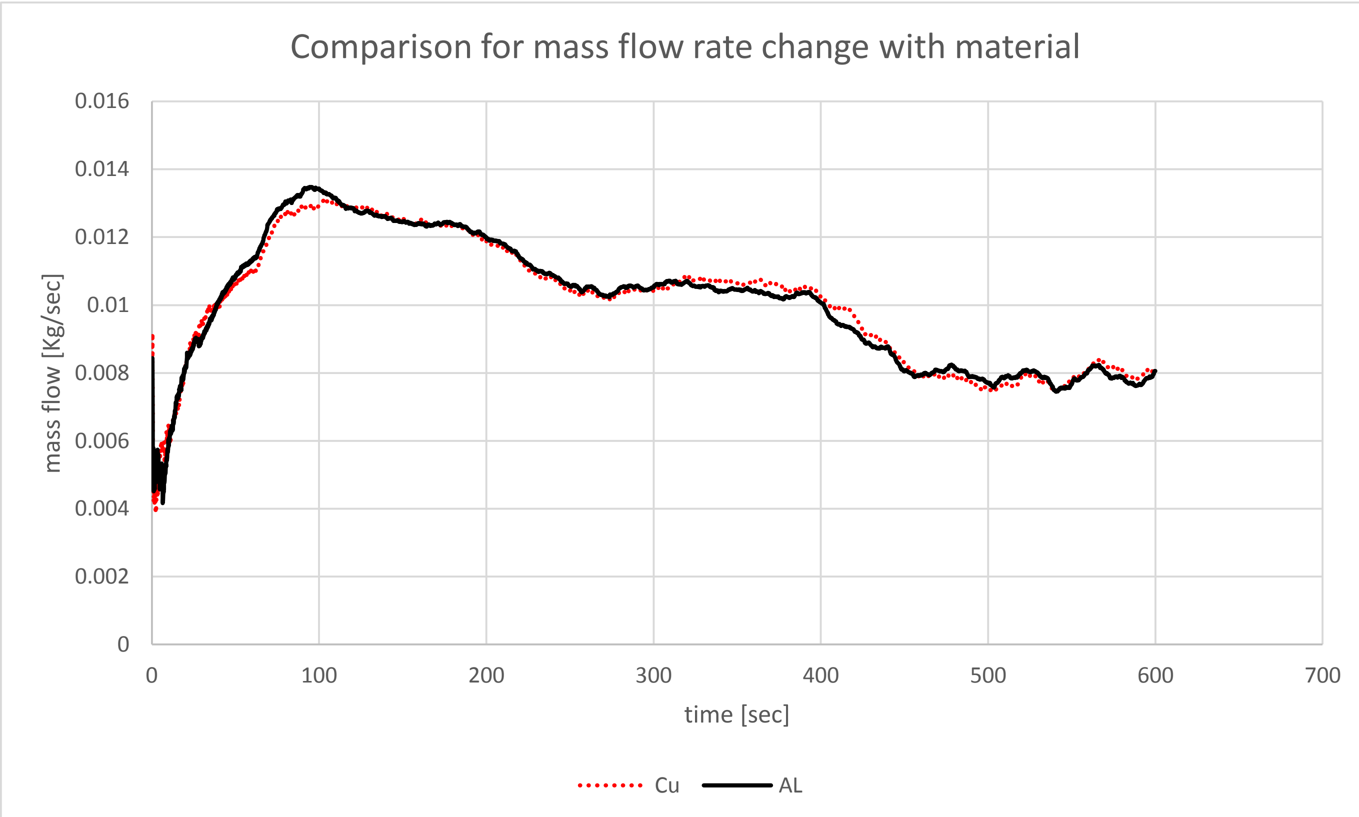


Figure 25 - mass flow rate in case of Al or Cu

It is indicated in [Fig 25] that 2 cylinders of 2 different materials might have a minor difference in the mass flow rate while both are of the same capacity, that shouldn't change that the area under both curves should be equal. Which could be simply explained that the difference in heat transfer coefficient should influence the temperature which is directly related to the velocity of fluid thus affecting the rate of flow, as well as the heat capacity leading to a different amount of head accumulation in the material.

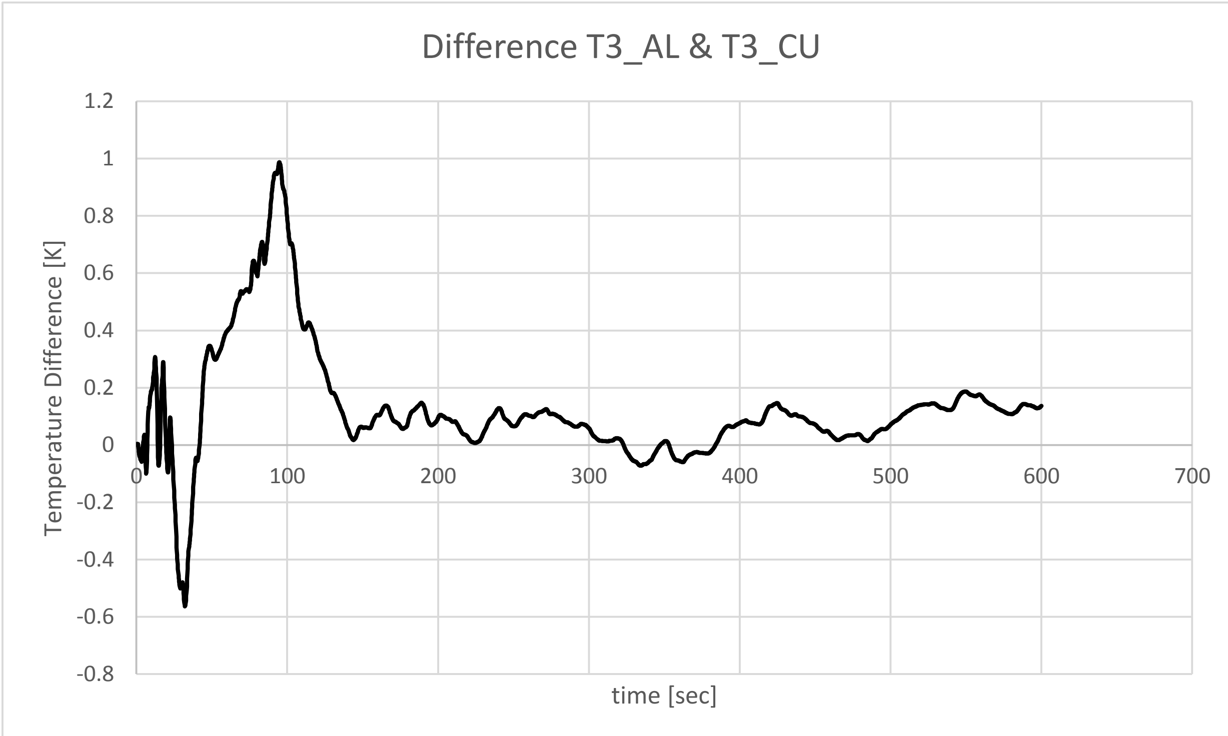


Figure 26 - Temperature difference for Aluminum & Copper

it was also observed that the further we went away from the inlet of the flask, the material doesn't make much difference as in order to plot a graph that reflects the difference between the 2 materials instead of plotting the temperature value we are plotting the difference between T_{cu} and T_{Al}, as the differences closer to the inlet was observed to be around 5° as we get further away from the inlet, where the velocities and Reynolds number is much lowers, it appears to be that the cylinder body has less influence of the temperature of the fluid inside.

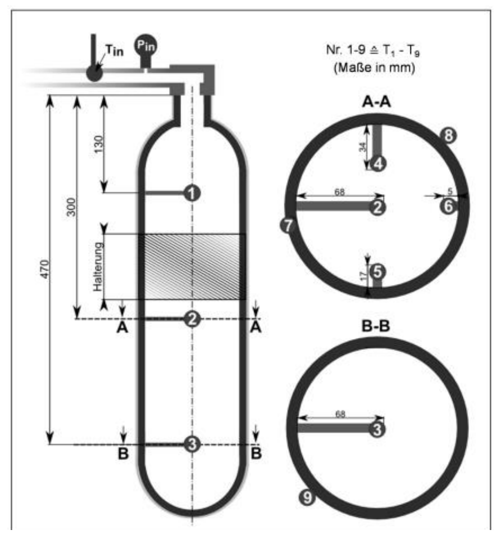


Figure 27 - sensor locations

5.2 Overview of some previous simulations

In order to be able to achieve the lowest error, several simulations were done aiming to get the best results, in some cases the solution never seemed to converge, while others gave inaccurate results, so it could be helpful to go through some the Workbench projects carried out and be able to see how the progression of simulation went.

Simulation case 1: was a transient simulation planar, using compressible ideal gas model.

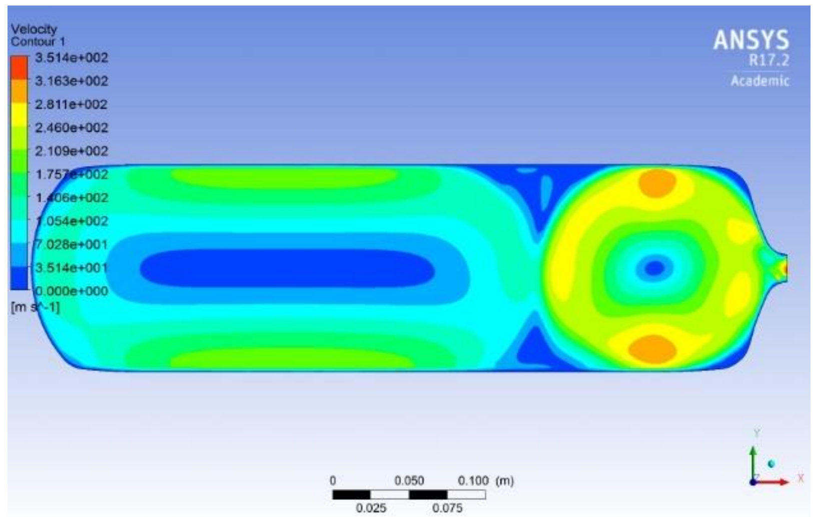


Figure 28 - project 1 Temperature contour

Simulation case 4

Axisymmetric model was used instead of planar, which lead to a drastic decrease in simulation time.

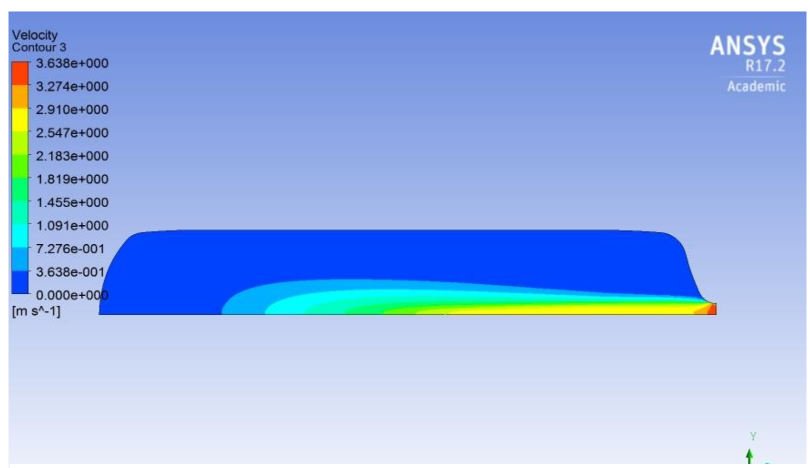


Figure 29 - Project 4 axisymmetric temperature contour

Simulation case 7

Is the project that is was relied on to get most of the results of the diploma work, using a UDF (User Defined Function) to define a changing inlet pressure to adapt more with the filling process. Point monitors were added to simulate the sensors used in the experimental results for validation. Velocity which was assumed based on previous simulations to be around 1.5 m/sec at inlet, at start, while an inlet pressure which is varied according to UDF. Turbulence model used was DES (Detached eddy simulation) and the margin of error was considered a bit higher.

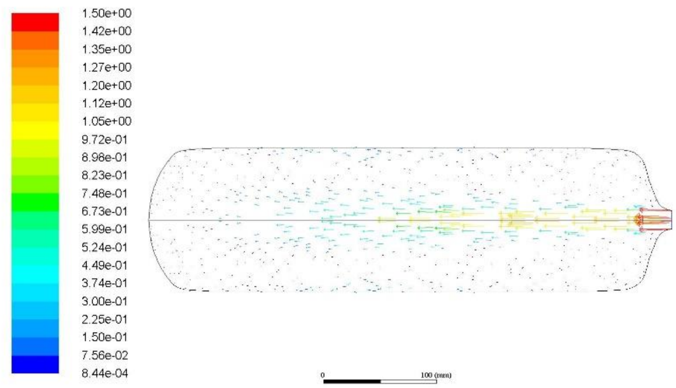


Figure 30 - velocity vectors from project 7

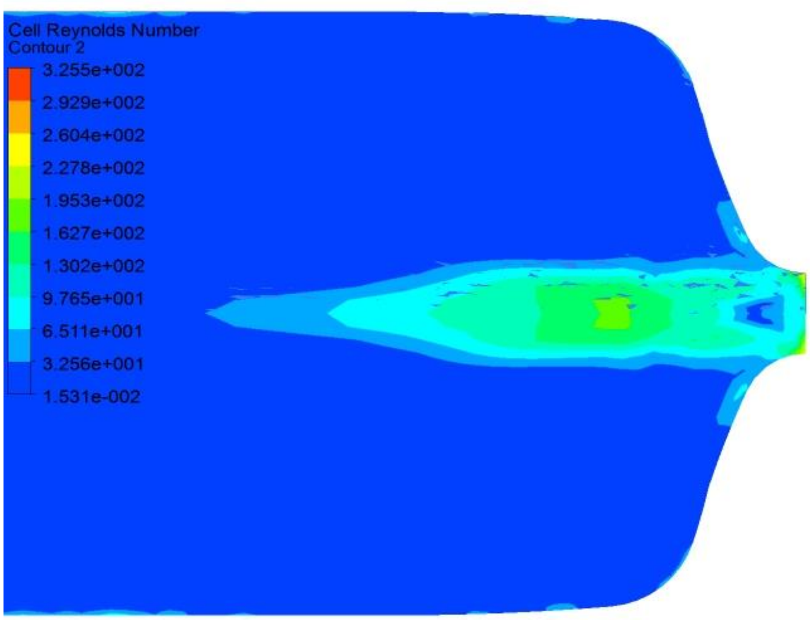


Figure 31 - Reynolds number at t = 5

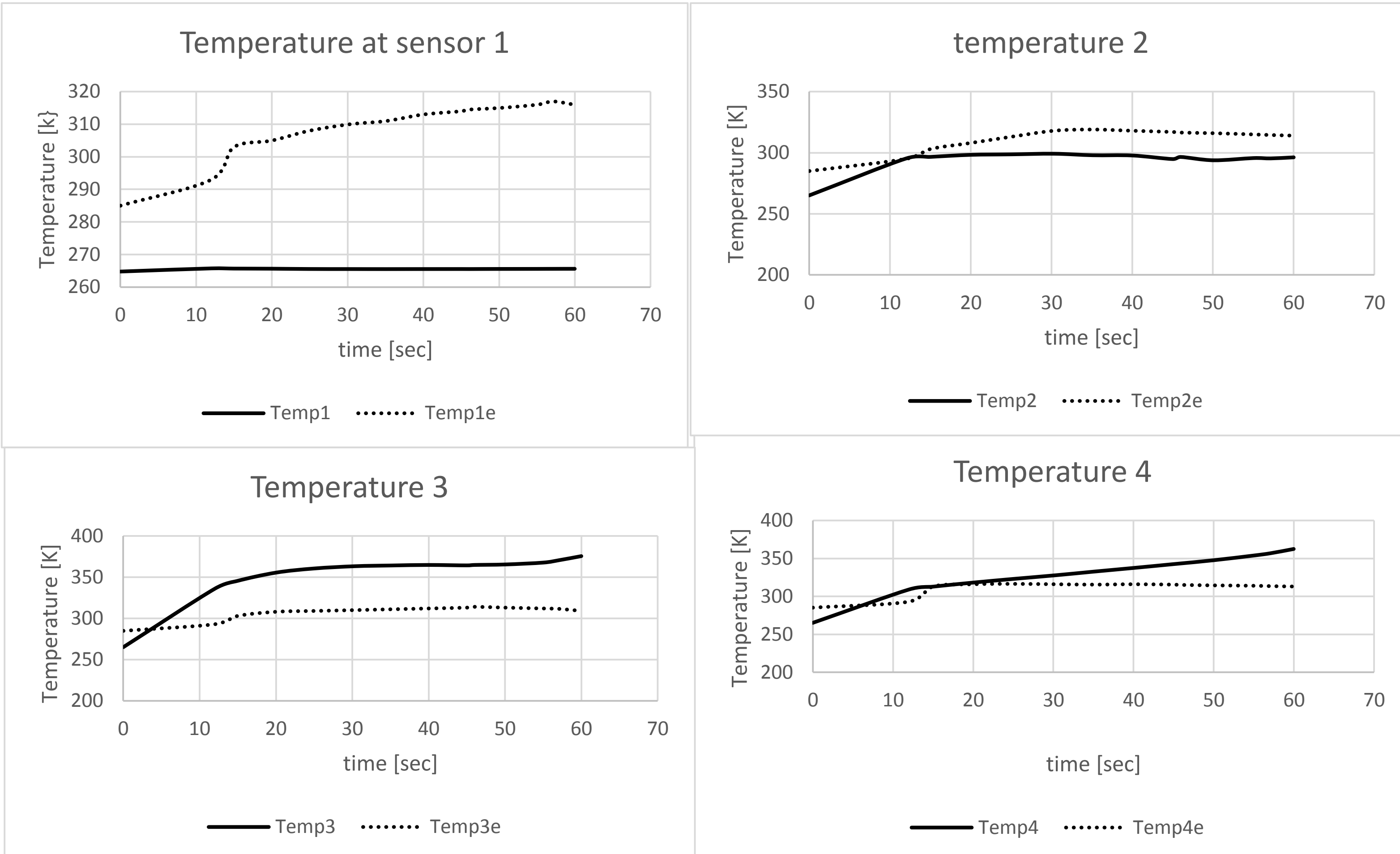


Figure 32 - comparison for error for case 7

In figure 33, it shows how the error was relatively higher than the results that were discussed and later on used to validate the model this diploma work is based on, and similar to previous realization it seems like sensor 1 usually has the highest error, due to the highest turbulence.

6. Conclusion

After several simulations, and testing of different models for real gas, and turbulence models, the filling process of the gas bottle was successfully simulated with a varying error between zero and 15% which from an engineering point of view could be an accurate and reliable model to help with the development of the researched pressure bottle.

Most satisfying results were obtained using shear stress transport K-ω for turbulence, and the Soave-Redlich-Kwong equation of state for real gas. It is also beneficial to have earlier simulations which had less accurate results and discuss why the used models weren't sufficient to get best results in order to have a reliable simulation model to aid with the further development of the air bottle, the usage of UDF code has major importance in achieving the pressure profile required, and it heat transfer between the bottle itself and the surroundings was taken into consideration which of course had a high influence on how the temperature of the air flask changes.

The thesis continues into validating the model and then takes it further into generating results that might have been hard to achieve in the lab, like for example how a different material composition of the cylinder can influence the rate of mass flow rate, or the temperature distribution.

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8. Appendix

Appendix A

Experiment Data

using the set-up in the picture, the bottle was kept in it's the experiment involve having 2 bottles make the same experiment as it was important to verify the error of the experiment itself.

Figure 33 - Keeping the flask in place

Appendix B

Velocity vectors

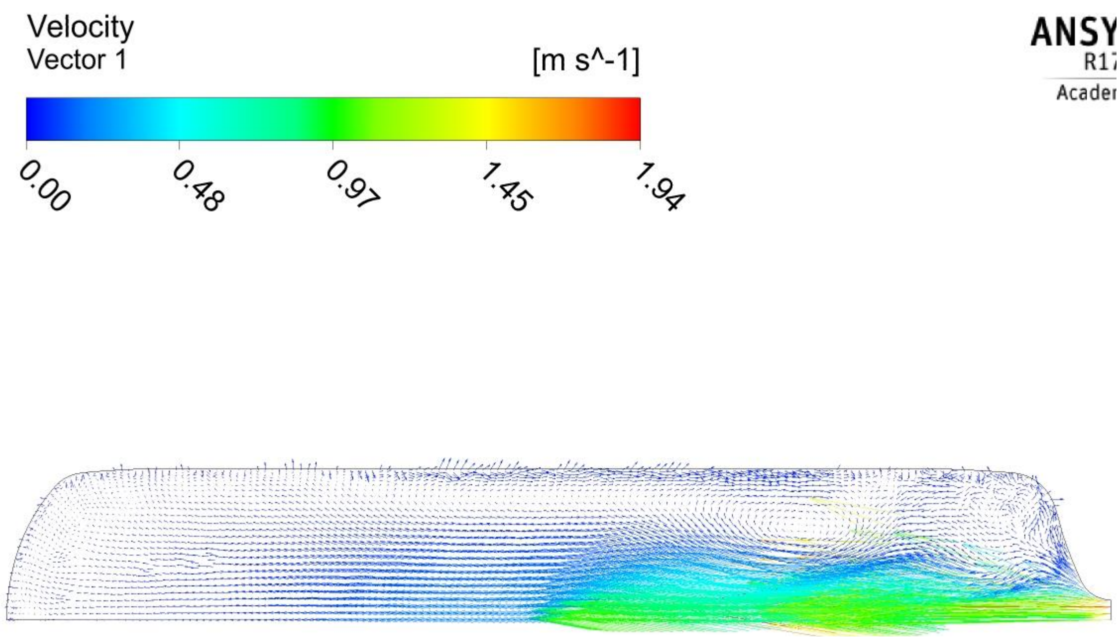

Figure 35 - velocity vector at t = 5 sec

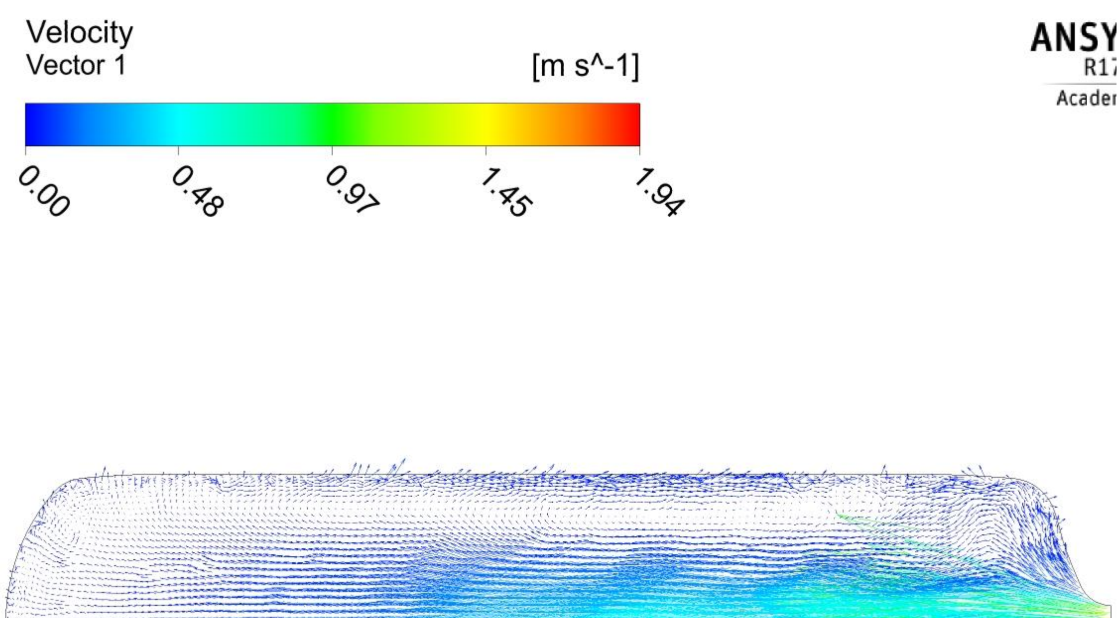

Figure 34 - velocity vector at t = 20

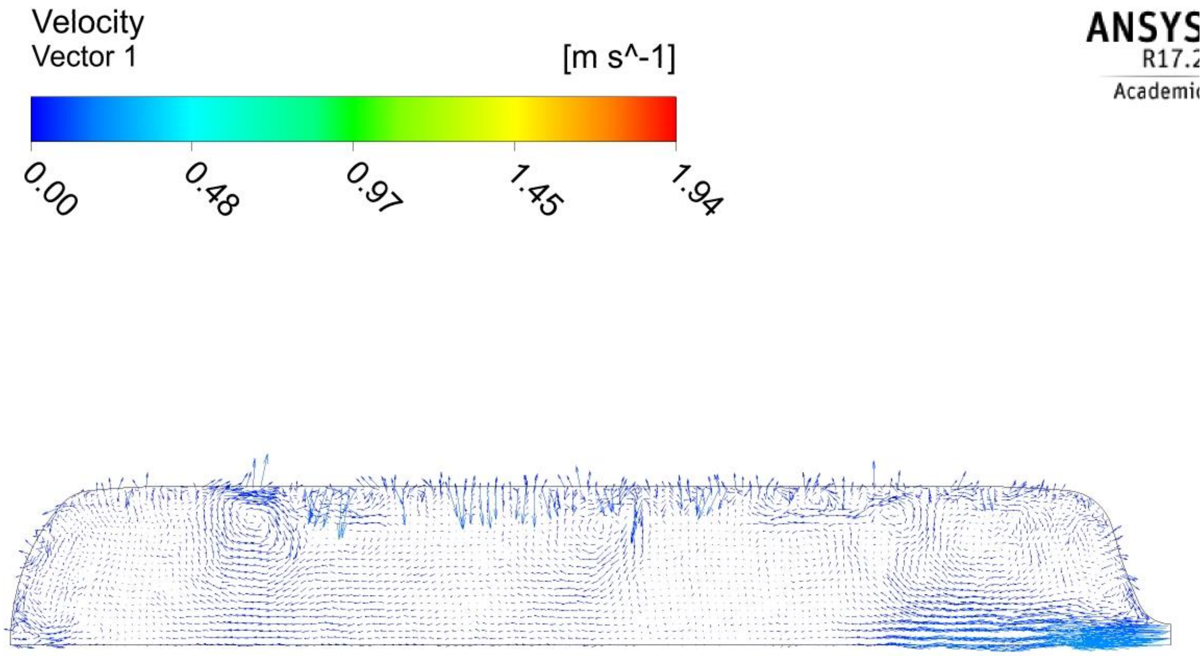

Figure 36 - velocity vector at t = 250 sec

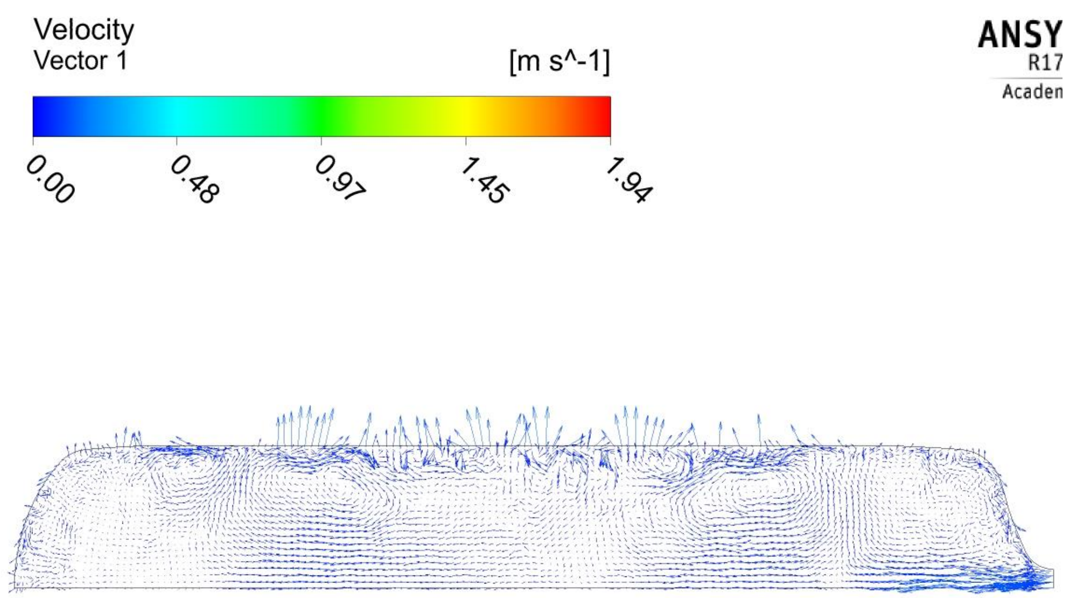

Figure 37 - Velocity vector at t = 600 sec

Appendix C

Details of the used model

Solver Type	Pressure based
2D Space	axisymmetric
velocity formulation	Absolute
Models	Energy Equation
Viscous	SST- K-Omega
boundary conditions	pressure inlet
solution scheme	coupled
Pressure	second order
Density	Second order upwind
Momentum	Second Order upwind
Turbulent Kinetic energy	Second order upwind
specific dissipation rate	First order upwind
Energy	Second order upwind
transient formulation	first order implicit
flow courant number	200
momentum relaxation factor	0.5
Pressure relaxation factor	0.5
under relaxation density	1
under relaxation body forces	1
under relaxation turbulent kinetic energy	0.8
under relaxation specific dissipation rate 0.8	0.8
under relaxation turbulent viscosity	1
under relaxation energy	0.75