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Use of open-source software in Computational Fluid Dynamics - Thermal compartment model

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ABSTRACT

There are several concepts involving fluids that can be tested, validated and simulated in laboratories of Physics, Chemistry and Engineering courses. In industry, these concepts find applications, and before being used in practice, they can be simulated with computational tools. The application of Computational Fluid Dynamics (CFD) allows a more efficient and optimized experimentation, reducing costs and increasing reliability in the final product. As a practice, the present study models, investigates and optimizes the behavior of the air flow inside a refrigerator used to accommodate immunizers, modifying its air intakes, analyzing the temperature gradients on the shelves, making it possible to give an indication of the positioning of products that need better management due to thermal variations and product conservation. With the open-source programs OpenFOAM, Salome and Paraview, it was possible to develop experiences contributing to the establishment of theoretical knowledge. The model was developed with a steady state solver for fluctuating, turbulent and incompressible flow. The data reinforce the view that the results with CFD are fundamental for the development of more personalized models and values the possibility of using free tools in undergraduate courses.

KEYWORDS: open-source programs; computational fluid dynamics; refrigerators.

INTRODUCTION

Fluid Dynamics involves studies of heat transfer and related phenomena, such as chemical reactions, combustion, hydraulics, aeroacoustics, among others [1]. Research in these areas is under increasing development, from experimentation and validation to the development of theoretical computational methods [2]. Computational Fluid Dynamics (CFD) is part of the capillarity of Fluid Dynamics, which uses the Navier-Stokes equations as rulers to simulate by numerical solution, providing the possibility of modeling systems to analyze real problems and/or performed in didactic laboratories, for example, in addition to processes applied in industry and research. The CFD proves to be an inexpensive and quick practice of experimenting with fluid flow systems enabling the recovery of the Physics of the system [3].

In [4] basic systems of heat transfer and fluid dynamics are solved, analyzing the uncertainty between the numerical and the analytical solution, therefore a complementation between the methods, making the modeling accepted as an option. Therefore, with the CFD it becomes possible to idealize and apply themes developed in classroom in Physics, Chemistry and Engineering courses [5] [6].

With the evolution of machine power and the popularization of free tools, the modeling processes went to another level [7]. Simulating more complex systems that required greater machine power became possible for various technological applications, in agriculture, biology, physiology, aerospace, environment and product design, from idealization to the development of the final product.

The open-source programs are free of licenses, allowing autonomy in the execution of the simulation, in addition to not needing bureaucratic obstacles of local and/or virtual access in educational or business institutions. The main idea behind this article is to encourage the use of free software in CFD, from pre-processing, processing to postprocessing, with the programs Salome, OpenFOAM and Paraview, respectively [8] [9] [10].

The numerical simulation is a very efficient and comprehensive tool for Computational Fluid Dynamics. In this sense, Erick C. and Bruno Guedes developed work regarding the observance of practices to minimize the impacts of the pandemic on the air conditioning and refrigeration system in environments prone to the spread of diseases [11].

Regarding refrigerator optimization studies, as in the analysis by Juan M. Belman-Flores et al. [12], the performance of these machines is directly linked to their design, moreover, as demonstrated by Gupta et al. [13] in their studies, the CFD model of refrigerators is very similar to the experimental models, that is, the CFD has proven reliability. Reference [14] discusses the experimental simulation and numerical analysis of a refrigerator developed using a commercial program. In an analysis with CFD in a domestic refrigerator [15], the analysis was performed considering three different turbulence models for a fresh food compartment, verifying the cooling time rate of fresh food in the compartments, as well as representing the distribution of air and temperature gradients, observing an inhomogeneous distribution, therefore, temperature sensitive perishable foods should be stored on the highest shelf.

However, when it comes to immunizations, these temperature differences should be well investigated, as directed in the Cold Network Manual - Ministry of Health [16].

In the Immunization Program, the storage, conservation, handling, distribution and transport processes of immunobiologicals must comply with adequate refrigeration conditions throughout the process, from the producing laboratory to the moment the vaccine is administered [17]. According to the manual, vaccines should generally be carefully transported and stored isolated from light with their temperature limit between 265.5 K and 248.15 K (8°C and -25°C), as in the product specifications, from production to administration. Also according to the manual, with each exposure to a temperature outside the range recommended by the producer laboratory, there is a cumulative reduction in the potential of the product.

With the emergence of the pandemic and the development of its vaccination plan, questions about the storage process were evidenced regarding the planning of a structure that would guarantee the thermal stability for the conservation of the vaccines.

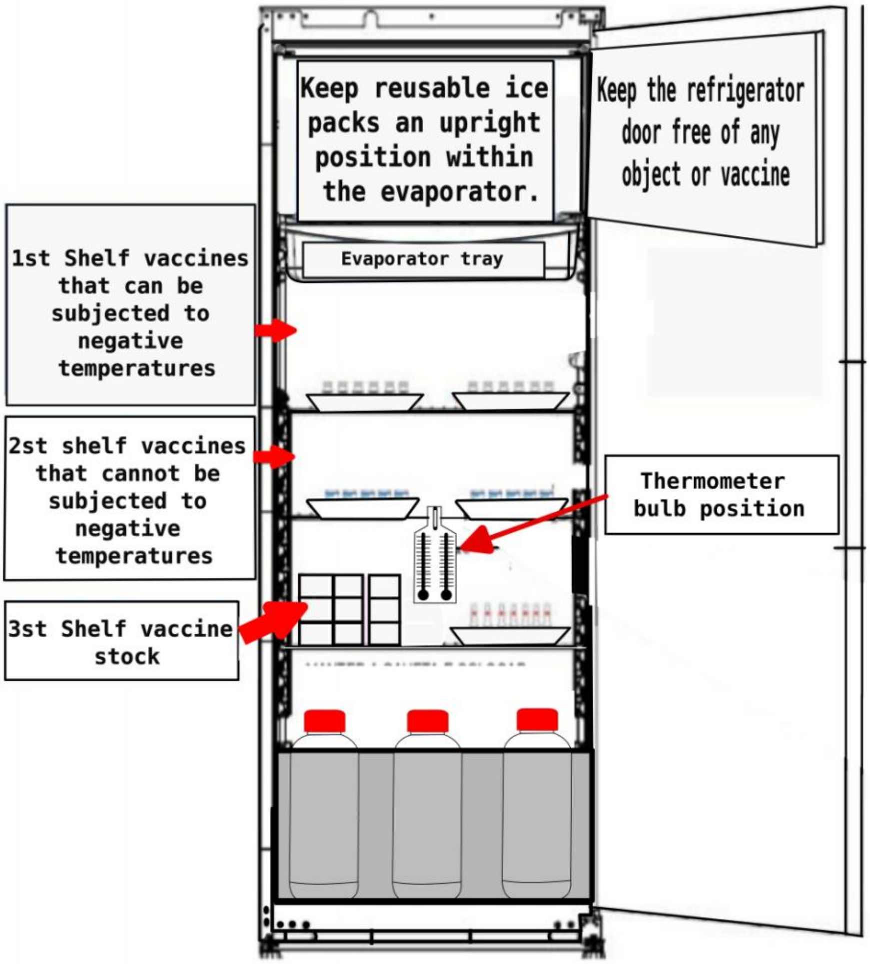
In this article we aim to stimulate research, with teaching topics covered in undergraduate courses, applying in this case the development of topics with simulation of three models of fluid inlet in the refrigerator compartment. The fluid inputs were modified and analyzed, via computational fluid dynamics, to maintain the smallest possible temperature variation in the cooling process and its faster re-stabilization. For that, we used the open source programs Salome, Openfoam and Paraview that are in section 2 (Model and Simulation).

CASE OVERVIEW

In this work, velocity and temperature maps were analyzed as a function of geometry, boundary conditions and numerical parameters. The hospital refrigerator was used as a model, in order to generate geometry and propose optimizations when possible.

To motivate the learning of CFD, this model was chosen due to its geometric simplicity of the upper internal compartment of three shelves with dimensions of 0.532 m wide, 0.550 m deep and 1.2 m high. Examples of product allocations related to immunizing agents are highlighted in **Figure 1** and following the recommendations of [16][17].

Figure 1 - Internal organization of a refrigerator

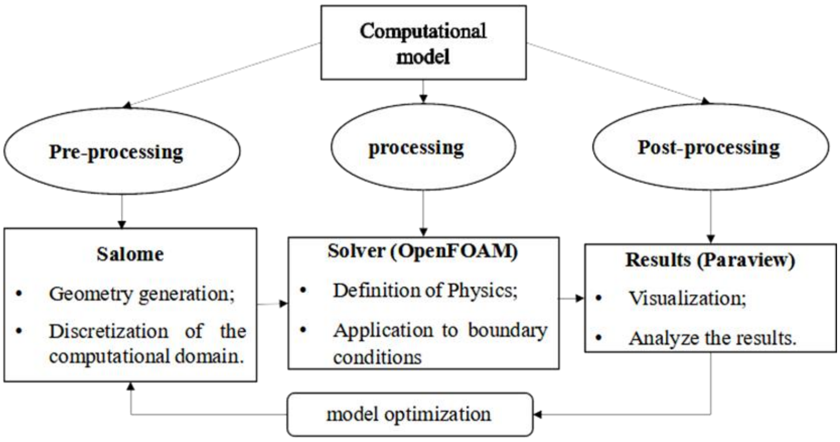


Source: Adapted from the Ministry of Health. National Health Foundation [16].

The CFD is an important tool for investigating the conservation processes of immunizers, such as vaccines against COVID-19, making it possible to visualize the distribution of the fluid flow and consequently the temperature in each compartment, proposing allocations that are appropriate for each product. However, in our work, we will encourage the use of open-source programs to enhance and disseminate their use, complementing experimental analyses.

In **Figure 2**, we employ a representation with adaptations of stream inputs, describing the stages of computational modeling development, progressing from pre-processing, through processing, to post-processing, and ultimately reaching the results and analysis phase.

Figure 2 - Flowchart of development of the computational model.



Source: adapted from Opencfd user guide [18].

MODEL AND SIMULATION

CFD is a field of scientific computing that simulates problems involving fluids in motion, with or without heat transfer. The integration with experimental practice becomes significant and complementary for the areas of Physics, Engineering, and related disciplines, as it allows the execution and visualization of more complex experimental practices, recovering the physics of the analyzed process. In this work, CFD is developed with assumptions and numerical approximations in the pre-processing and processing stages.

THE COMPUTATIONAL METHOD

In the Fundamental Laws of Physics, mathematical models are established based on the equations of conservation laws; Conservation of mass, Newton's Second Law and First Law of Thermodynamics, which can be applied in terms of fluid flow [5]. In Newton's second law we have,

$$\sum \vec{F}_R = m.\vec{a} = \sum \vec{F}_p + \sum \vec{F}_{visc} + \sum \vec{F}_g \tag{1}$$

With the acceleration vector $\vec{a}$ (m/s^2) and the resultant of the forces $\vec{F}_R$ (N) acting on a mass m (kg), where the acceleration is described as follows.

$$\vec{a} = \frac{d\vec{u}}{dt} = \frac{d\vec{u}}{dt} + \vec{u}.\nabla\vec{u} \tag{2}$$

With $\rho = m/V$,

$$\frac{\sum \vec{F}_R}{dV} = \frac{\sum \vec{F}_p}{dV} + \frac{\sum \vec{F}_{visc}}{dV} + \frac{\sum \vec{F}_g}{dV} \tag{3}$$

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The sum of pressure forces per volume,

$$\frac{\sum \vec{F}_p}{dV} = -\nabla . p \tag{4}$$

The sum of viscosity forces per volume,

$$\frac{\sum \vec{F}_{visc}}{dV} = \nabla . \tau \tag{5}$$

And the force due to gravity is,

$$\frac{\sum \vec{F}_g}{dV} = -\rho g \vec{k} \tag{6}$$

From **Equation 2,**

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u} . \nabla \vec{u}\right) = -\nabla p + \nabla . \tau - \rho g \vec{k} \tag{7}$$

Where the symbols for quantities and operators are defined by:

V =Volume (m^3);
ρ = Specific mass (kg/m^3);
$\frac{\partial}{\partial t}$ = Partial derivative;
$\vec{u}$ = Velocity (vector) (m/s);
∇ =Nabla operator (vector operator);
p = Pressure (Pa);
τ = Viscosity stress matrix;
g = gravity acceleration;
$\vec{k}$ = Unit vector on the z axis (vertical).

The Navier-Stokes equations solved in CFD describe the behavior of a compressible or incompressible Newtonian fluid, involving pressure and viscous stresses. In its general form, it considers a scalar field Φ, being possible to write the presented equations as a general transport equation. These are the basis for the CFD that uses a method of solving partial differential algebraic equations [19], **Equation 8**.

$$\underbrace{\frac{\partial(\rho\emptyset)}{\partial t}}_{unsteady\ term} + \underbrace{\nabla . (\rho\vec{v}\emptyset)}_{convection\ term} - \underbrace{\nabla . (\Gamma\nabla\emptyset)}_{diffusion\ term} = \underset{source}{S} \tag{8}$$

Where, ∅ is the scalar variable of interest to represent different conservation equations. Only three components of the equation are changed, the variable ∅, the diffusion coefficient Γ and the source term S.

As an example, to obtain the equation conservation of mass, we have that ∅ = 1 e Γ = 0 and S = 0.

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho.\vec{v}) = 0 \tag{9}$$

These equations, when subjected to appropriate boundary conditions, which will be discussed later in the text, will mathematically represent the problem at hand. Solving these equations analytically is only possible for very simple flows.

In order to model cases involving fluid dynamics, it is necessary to fragment (discretize) the domain into control volumes (CV), then apply the conservation equations in each of the control volumes that constitute the mesh, which will be treated by a numerical method, Method of Finite Volumes (MVF), integrating the governing differential equations, **Equation 8**, in each control volume [18]. To represent the entire domain, we have integration of **Equation 8**, with A representing the surface of the CV [19].

$$\underbrace{\frac{\partial}{\partial t}\left(\int_{CV} \rho\phi dV\right)}_{time} + \underbrace{\int_{A} \boldsymbol{n}.(\rho\vec{v}\phi)dA}_{advective} = \underbrace{\int_{A} \boldsymbol{n}.(\Gamma\nabla\phi)dA}_{diffusive} + \underbrace{\int_{CV} SdV}_{source} \tag{10}$$

To generate the computational domain with geometries of the refrigerators and subsequent construction of the mesh, we used the open-source program Salome [20].

PRE-PROCESSING – COMPUTER DOMAIN AND MESH GENERATION

To achieve a reduction in computational cost, mesh generation and simulation in a thermal analysis of a given system, the simplification can be done by reducing the geometric complexity, as done in the reduction in the model, and/or disregarding the heat transfer equations, as described by [21][22].

Figure 3 represents the models of the refrigerant air inlets in the compartments. **Figure 3-1** represents initial geometry based on real model, where the air inlet is 0.528 m wide and 0.06 m high, and the air outlet is 0.528 m wide and 0.09 m high. However, in the structures in **Figures 3-2** and **3-3**, the air inlets have been modified to 0.155 m wide and 0.05 m high. Changes in the geometries were made in order to analyze them, keeping the dimensions and position of the air outlet.

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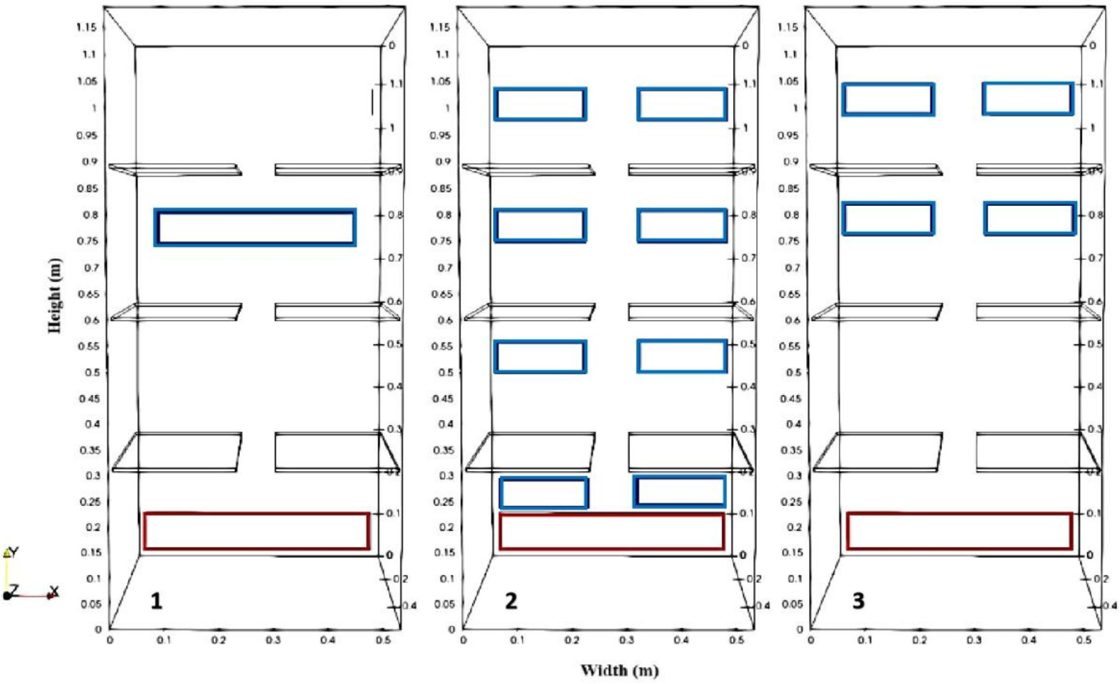
Figure 3 - Geometries of models 1 with a central air inlet, model 2 with eight and model 3 with four fluid inlets in blue, in red the output of the flow

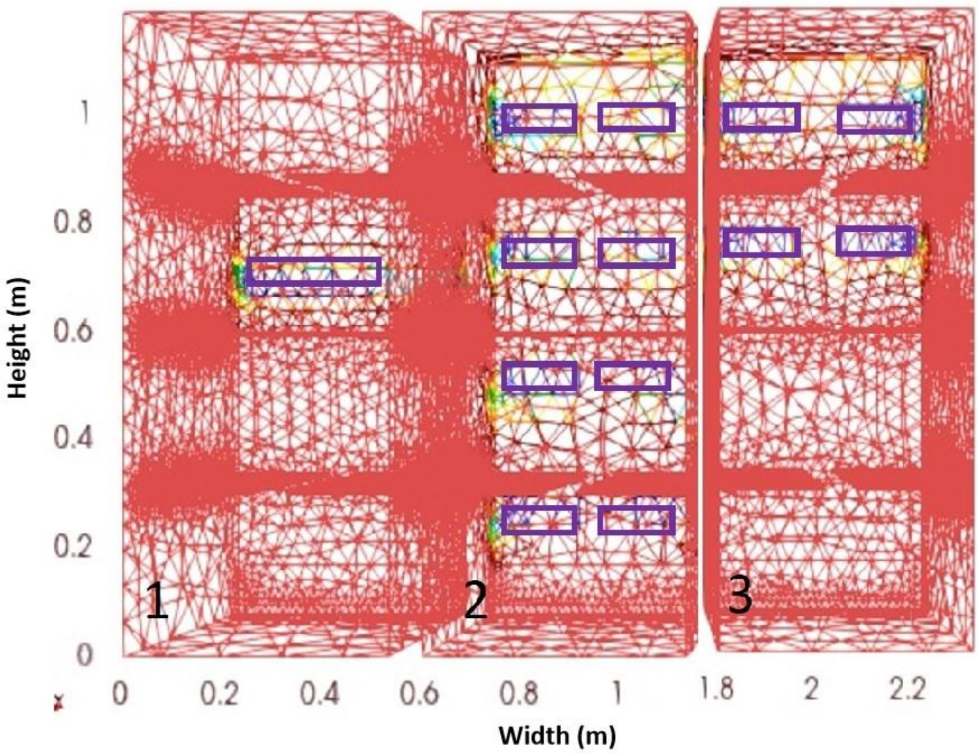


Source: Own authorship.

The division of the internal space of the refrigerator was made through shelves below the air inlets that will be used to accommodate the products.

Domain discretization was performed with Salome, that is, domain division into smaller subdomains (Control volume); through this process, the meshes shown in **Figures 4-1, 4-2** and **4-3** are obtained. Thus, it becomes possible to solve the partial differential **Equation 8** because through the discretization process, discretized structural units are originated, possible for computational analysis with the desired recovery of physics.

Figure 4 - Mesh generated from the geometry of Figure 3.



Source: Own authorship.

To check the quality of the meshes, we use checkMesh, an Openfoam command, with specific data about the mesh generation, **Table 1.**

Table 1 - CheckMesh of Openfoam utility for statistical analysis and evaluation of quality parameters

Mesh:Tetrahedral Meshes	**1**	**2**	**3**
Dots	32577	21208	32781
Faces	315198	191518	317466
Cells	150799	90055	151924
Max skewness	0.966808	0.986066	0.891237

Source: Own authorship.

The meshes were directed to the OpenFOAM solver, where were used the properties of the fluid and the boundary conditions.

PROCESSING – THE OPENFOAM

To perform the processing, among the various solvers available by OpenFOAM to solve the case, the solver chosen was the buoyantSimpleFoam, which is a steady-state flux - turbulent fluctuating solver for incompressible fluids, which includes radiation, ventilation, and heat transfer, however, disregards buoyancy [23][24]. In our model we consider an incompressible Newtonian fluid. From the continuity **Equation 9**, for a fluid of an incompressible flow, ρ = constant.

$$\nabla.(\rho.\vec{u}) = 0 \quad (11)$$

For a Newtonian fluid, we show the relation to viscous forces as [25],

$$\frac{\sum \vec{F}_{visc}}{dV} = \mu\nabla^2\vec{u} \quad (12)$$

For Newton's viscosity equation, consider the dynamic viscosity coefficient. Assuming for a Newtonian fluid the shear stress (Matrix of viscosity stresses) τ given by (kN/m^2) [26].

$$\tau = \mu\frac{\partial u}{\partial h} \quad (13)$$

μ is the (N.s/m^2) and h is the transverse distance. In the present article we also consider a Newtonian fluid, disregarding viscous dissipation and radiation, thus, the governing equations (**Equation 7**) will be simplified in this model [26]. We soon arrived at,

$$\rho\left(\frac{\partial\vec{u}}{\partial t} + \vec{u}.\nabla\vec{u}\right) = -\nabla p + \mu\nabla^2\vec{u} - \rho gh \quad (14)$$

The solver uses the semi-implicit discretization method for pressure-bound equations, proposed by Caretto et al. [27]. The resolution starts from the moment equation in the OpenFOAM solver, a representation of the differential equation of **Equation 8** in its natural language and model considerations can be found in [28].

The momentum and continuity equations are used to construct an equation for the pressure. The pressure equation for the incompressible model can be derived from **Equation 14** [25],

$$\nabla^2\left(\frac{p}{\rho}\right) = -\nabla.(\vec{u}.\nabla\vec{u}) \quad (15)$$

In other words, the pressure equation relates the change in pressure in an incompressible fluid to changes in the velocity field in the fluid.

In the model, the thermophysical properties of the air were considered, while the boundary conditions were inserted according to **Table 2.**

Table 2 – Basic boundary conditions

Contour conditions	**Inlet**	**Outlet**	**fixedWalls**
Velocity (m/s)	fixedValue = 2.5 m/s	zeroGradient	noSlip
Pressure ($kg/m.s^2$)	fixedFluxPressure	zeroGradient	calculated
Pressure (Hydrostatic Contribution) ($kg/m.s^2$)	fixedFluxPressure	zeroGradient	fixedFluxPressure
Temperature (K)	fixedValue = 193.15K	zeroGradient	zeroGradient

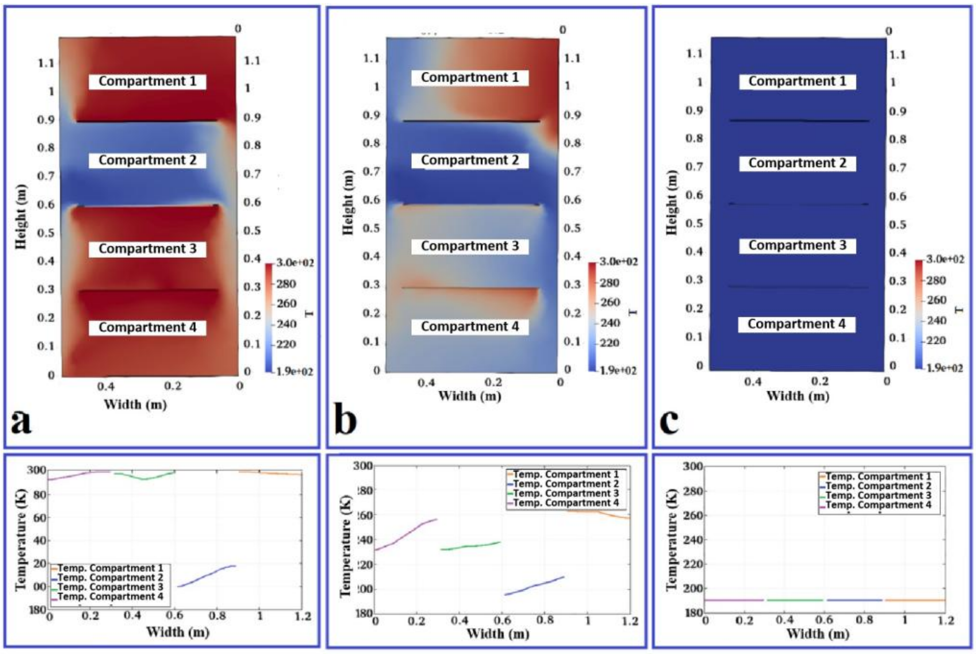
Source: Own authorship.

RESULTS AND DISCUSSION – POST PROCESSING

Paraview is the open-source program generally used by OpenFOAM to perform postprocessing, being compatible with several file formats, with filters providing a better interpretation and analysis of the results. In this study, we chose to use the Plot over line filter to represent the temperature gradients as a function of the height in the compartment.

Figure 5-a, **5-b** and **5-c** illustrate the cooling process of the model 1 (**Figures 3-1** and **4-1**). Figure 5a represents iteration 200, where it is possible to observe that the cooling process starts on the second shelf, which may imply difficulties in the cooling process of the first shelf (compartment 1), as naturally the cold fluid moves downwards.

Figure 5: 200(a), 400(b) and 1300(c) stage iterations, referring to the model figure 3-1



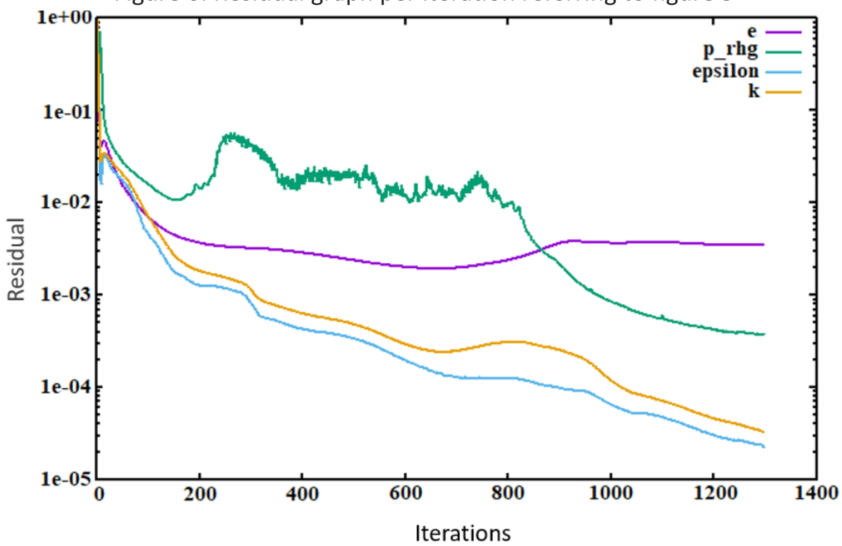
Source: Own authorship.

In **Figure 5b**, the stage of 400 iterations is represented, it can be seen that the second shelf (compartment 2) reached temperatures between 195 K to 210 K, still at this stage, the first shelf (compartment 1) still remains at temperatures between 257 K and 262 K, the third shelf (compartment 3) is at temperatures between 231 K and 238 K, and finally the fourth shelf (compartment 4) reached temperatures between 231 K and 256 K, as indicated in their respective graphs.

The delay of the flow of cold air in reaching the first shelf occurs because it tends to move downwards, thus persisting higher temperatures in the first shelf (compartment 1), that is, the initial configuration of the refrigerator delays the thermal equilibrium. Temperature uniformity is achieved in 1300 iterations (**Figure 5c**), reaching a minimum temperature of 195.15 K.

The graph in **Figure 6** represents the residuals per iteration, where e is the relative error, p_rhg is the pressure with hydrostatic contribution, ε is the viscous dissipation rate of turbulent kinetic energy and k is the turbulent kinetic energy, which are the turbulent variables. Through it we can verify the tendency of the parameter's convergence in the buoyantSimpleFoam solver.

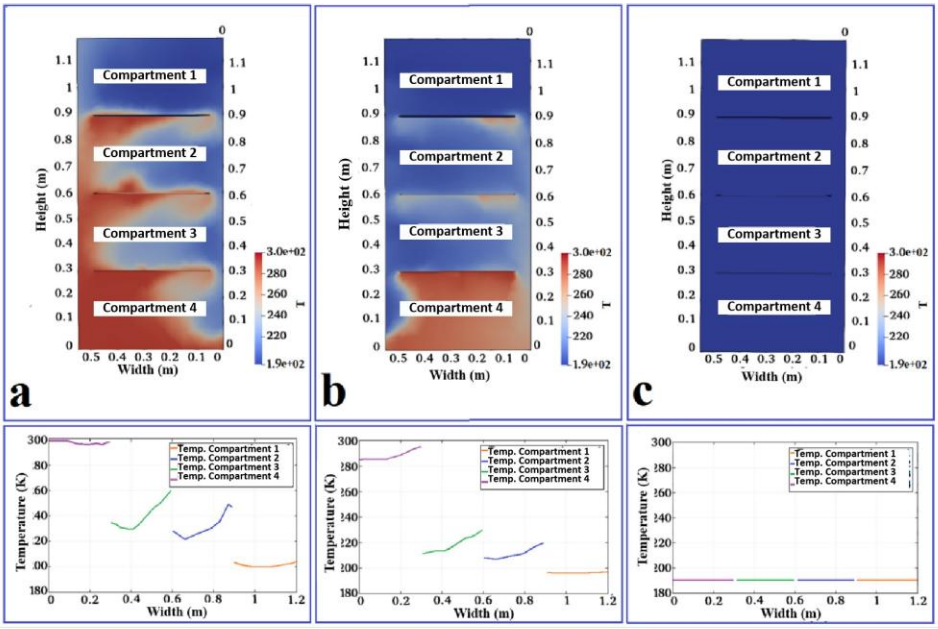
Figure 6: Residual graph per iteration referring to figure 5



Source: Own authorship.

The result of processing the model 2 (**Figures 3-2** and **4-2**) is represented in **Figure 7**. **Figure 7a** illustrates the iteration stage 100, where it is possible to notice the cooling process on the first shelf (compartment 1), second (compartment 2), third (compartment 3) and fourth shelf (compartment 4), so the flow of cold air is gradually distributed to the second, third and fourth shelves.

Figure 7: a) 100, b) 160 e c) 590 iterations, referring to the model in figure 3-2



Source: Own authorship.

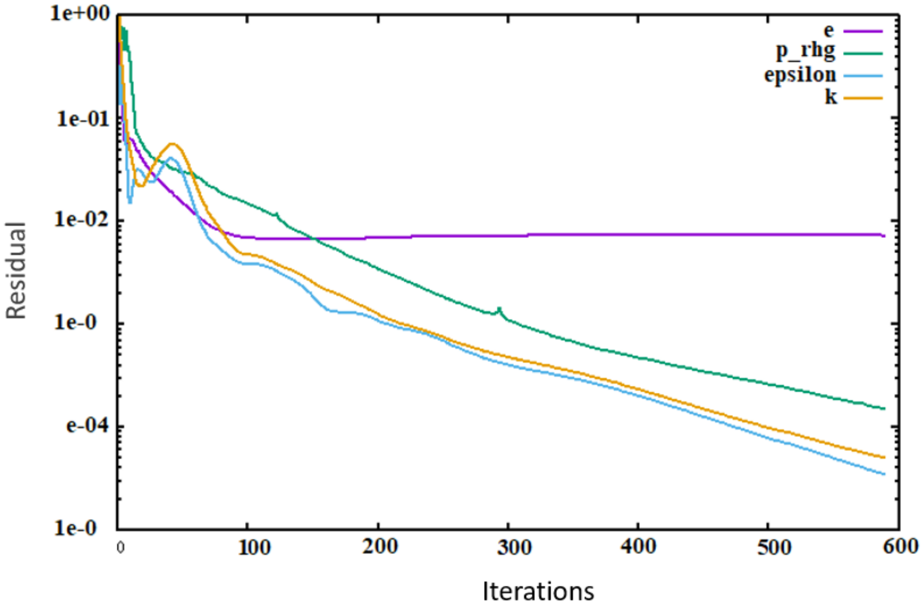
In **Figure 7b**, iteration 160 is illustrated, in which we can see that the first shelf (compartment 1) is close to the minimum temperature for the system

(195.15 K), the temperatures of the other shelves follow a gradual decrease, with the temperatures of the second shelf (compartment 2) between 207 K and 220 K, the temperatures of the third shelf (compartment 3) between 211 K and 230 K, and the fourth (compartment 4) with temperatures between 285 K and 295 K.

In **Figure 8c**, iteration 590 is shown, in which the refrigerator reached the minimum uniform temperature of 195.15 K; it is therefore noted that the refrigerator, with this configuration, reached the minimum temperature in a shorter time than the previous refrigerator.

The residuals per interaction plot illustrated in **Figure 8** also show that this configuration has a tendency to converge.

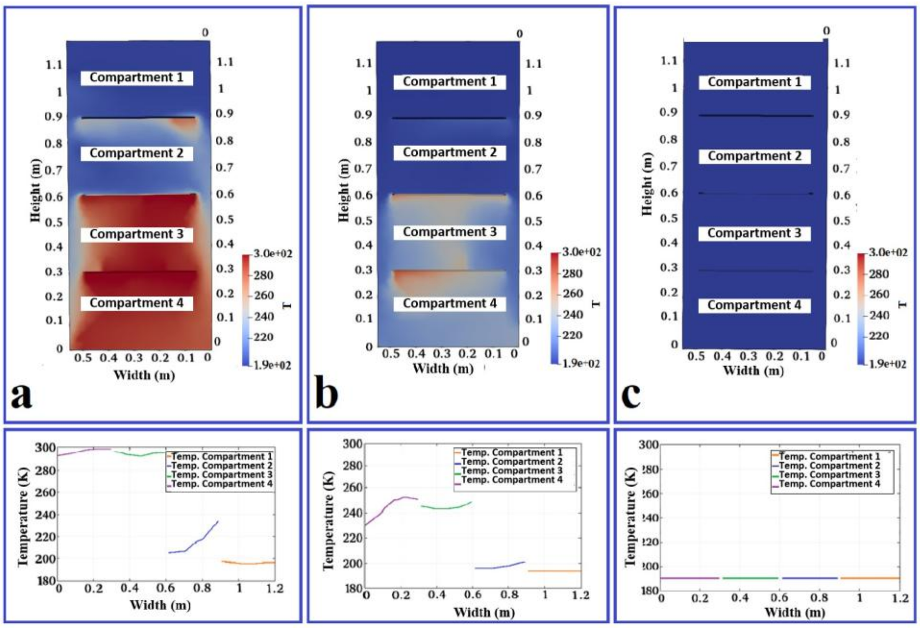
Figure 8 – Residual as a function of iterations referring to Figure 7



Source: Own authorship.

Figure 9 shows the cooling process related to model 3 (**Figures 3-3** and **4-3**). **Figure 9a** illustrates the process in 200 iterations; it is possible to notice that the first shelf (compartment 1) is close to the minimum temperature for the system (195.15K).

Figure 9 - a) 200, b) 400 e c) 1000 iterations, referring to the model in figure 3-3



Source: Own authorship.

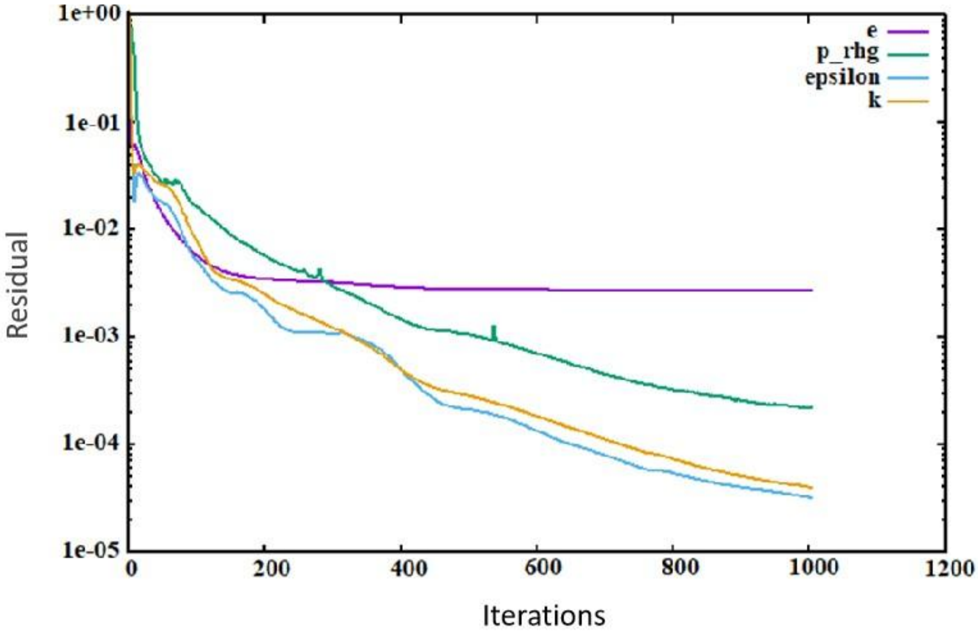
The second shelf (compartment 2) has temperatures between 205 K and 233.2 K. However, the third and fourth shelves (compartments 3 and 4) are at temperatures between 292 K and 300 K.

In 400 iterations, represented by **Figure 9b**, it is noted that the first shelf (compartment 1) reached the minimum temperature for the system, the second shelf (compartment 2) is between 196 K and 201 K, the third shelf (compartment 3) is at temperatures between 242 K and 248.5 K, and the fourth shelf (compartment 4) is at temperatures between 230 K and 252 K.

In **Figure 9c** the iteration 1000 is shown, at which the refrigerator has reached the temperature of stability of 195.15 K, showing that this model reached the minimum temperature with fewer iterations than **Figure 5c**.

Again, the residual plot shown in **Figure 10** indicates a trend towards convergence in processing results.

Figure 10 – Residual as a function of iterations referring to Figure 9



Source: Own authorship.

From these results, it was possible to abstract the idea of how the designer is relevant in refrigeration of thermal compartments and the importance in the distribution of fluid according to the placement of their entries. The allocation of air intakes in each of the shelves is an option to reduce the instability and contribute to a smoother cooling process. However, such modification may lead to an increase in the energy consumption.

CONCLUSION

The data reinforce the view that the results with CFD are fundamental for the development of more personalized models and values the possibility of using free tools. Furthermore, physical prototyping at the scale of this device is difficult to implement, as physical projects have more need for sensor points, making it difficult to locate critical points, temperature gradients. In addition, post-processing the simulation results in CFD provides a wealth of extra data and insights that may not be achieved using a physical experiment. With the introduction of Computational Fluid Dynamics in scientific initiation, it was possible to develop the model relating the theory developed in Physics, Engineering, etc., providing a better abstraction of the phenomena involved and topics discussed at graduation. In short, it is noted that the CFD provides the possibility of analysis before the conclusion of a design in choosing a better stability thermal according to the needs of the product.

Uso de programas de código aberto em Fluidodinâmica computacional - Modelo de compartimento térmico

RESUMO

Existem diversos conceitos envolvendo fluidos que podem ser testados, validados e simulados em laboratórios dos cursos de Física, Química e Engenharias. Na indústria, esses conceitos encontram aplicações e, antes de serem utilizados na prática, podem ser simulados com ferramentas computacionais. A aplicação da Fluidodinâmica Computacional (CFD) permite uma experimentação mais eficiente e otimizada, reduzindo custos e aumentando a confiabilidade no produto final. Como prática, o presente estudo modela, investiga e otimiza o comportamento do fluxo de ar no interior de um refrigerador utilizado para acomodar imunizantes, modificando suas entradas de ar, analisando os gradientes de temperatura nas prateleiras, possibilitando dar uma indicação do posicionamento de produtos que necessitam de melhor gerenciamento devido a variações térmicas e conservação do produto. Com os programas de código aberto OpenFOAM, Salome e Paraview, foi possível desenvolver experiências que contribuem para o estabelecimento de conhecimentos teóricos. O modelo foi desenvolvido com um solver de estado estacionário para fluxo variável, turbulento e incompressível. Os dados reforçam a visão de que os resultados obtidos com CFD são fundamentais para o desenvolvimento de modelos mais personalizados e valorizam a possibilidade de utilização de ferramentas gratuitas na graduação.

PALAVRAS-CHAVE: programas de código aberto; fluidodinâmica computacional; refrigeradores.

Uso de Programas de Código Abierto en Dinámica de Fluidos Computacional - Modelo de Compartimentos Térmicos

RESUMEN

Existen diversos conceptos relacionados con fluidos que pueden ser testeados, validados y simulados en laboratorios de los cursos de Física, Química e Ingenierías. En la industria, estos conceptos encuentran aplicaciones y, antes de ser utilizados en la práctica, pueden ser simulados con herramientas computacionales. La aplicación de la Fluidodinámica Computacional (CFD) permite una experimentación más eficiente y optimizada, reduciendo costos y aumentando la confiabilidad en el producto final. Como práctica, el presente estudio modela, investiga y optimiza el comportamiento del flujo de aire en el interior de un refrigerador utilizado para alojar inmunizantes, modificando sus entradas de aire, analizando los gradientes de temperatura en los estantes, permitiendo indicar la posición de productos que necesitan un mejor manejo debido a variaciones térmicas y conservación del producto. Con los programas de código abierto OpenFOAM, Salome y Paraview, fue posible desarrollar experiencias que contribuyen al establecimiento de conocimientos teóricos. El modelo fue desarrollado con un solucionador de estado estacionario para flujo variable, turbulento e incompresible. Los datos refuerzan la visión de que los resultados obtenidos con CFD son fundamentales para el desarrollo de modelos más personalizados y valorizan la posibilidad de utilizar herramientas gratuitas en la graduación.

PALABRAS CLAVE: programas de código abierto; fluidodinámica computacional; refrigeradores.

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