

Seminar Nasional Tahunan Teknik Mesin (SNTTM) VIII

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M5-020 Study of the numerical simulation of fluid flow and heat flow distribution in a CO₂ condenser using Open Source CFD Codes

Nugroho Adi Sasongko¹⁾ and Jafar Mahmoudi²⁾

¹⁾ Department of Mechanical Structural Engineering and Material Science
Universitetet i Stavanger, Norway

²⁾ Departement Gas and Energy Technology
International Research Institute of Stavanger, Norway
Phone: +47-99495379, E-mail: na.sasongko@stud.uis.no

ABSTRACT

A literature survey of experimental data (density, enthalpy, entropy, viscosity, thermal conductivity and solubility of CO₂ in water) for CO₂/H₂O mixtures has been conducted in the Preliminary Survey of the Thermophysical Properties of Carbon Dioxide-Water Mixtures as a prior research by Li, H., et al, in 2008. As a continued research, mathematical models describing physical behavior are developed and implemented in the dynamic simulation on the thermophysical properties of CO₂ - H₂O. The numerical simulation was carried out by computational fluid dynamic (CFD) modeling. OpenFOAM as the open source software that has source code freely available was tried to use in this study.

- *Keywords: CO₂ capture and sequestration, Condenser, Computational fluid dynamic, Heat transfer, OpenFOAM*

1. Introduction

To have an extremely high concentration of CO_2 , we need special equipment to separate CO_2 from other flue gases. Condensers for separation of CO_2 and water vapor are central devices in oxygen-fired power plants with CO_2 capture, so called Oxy-Fuel processes. Condensation by condenser is the most common used method due to the cost benefit and easy operated. The need of pure CO_2 product is important due to the next utilization such as transportation, storage or as feed to chemical industries. The combustion exhaust mainly consists of CO_2 and water vapor. In the post combustion capture of CO_2 using chemical solvents, the waste gas from the stripper mainly contains CO_2 . Good understanding on separation of CO_2 and steam mixtures is important to design more efficient condenser and further safe and low risk during operation of our condenser. A condenser involves the transformation of water vapor to liquid by mechanical means. The thermophysical properties of $\text{CO}_2\text{-H}_2\text{O}$ mixtures play an important role in the condenser design.

The purposes of this study are:

- To study the numerical simulation of fluid dynamic on CO_2 and water vapor in the modeled condenser, the system of governing equations is solved numerically by the finite volume approach for fluid flow.
- To visualize the CO_2 and water vapor fluids behavior inside the proposed condenser model by using CFD code. The geometry variations are detail simulated thereby help to understand the thermophysical characteristic of the modeled condenser.
- To get and produce some necessary data in order to estimate potential performance of $\text{CO}_2\text{-H}_2\text{O}$ modeled condenser compare to recent available condenser.
- To investigate the possibilities to use Open Source CFD software OpenFOAM. Further, we expect to gain some knowledge and can compare or validate to other available CFD code, especially the commercial software of CFD^[1].

Since in the OpenFOAM has no available solver for doing phase change simulation, the approaches used in this study is for both gases are assumed as non condensable gas, and both gases are treated separately. Build up understanding of the separation process at varying thermal conditions and with varying fluid compositions is needed since the quality of produced CO_2 can be a critical factor for the next processing of CO_2 . Figure 1 presents the first proposed condenser for study in the CO_2 condenser research project. All components that display in here are assumed represent the main part to conduct the investigation.

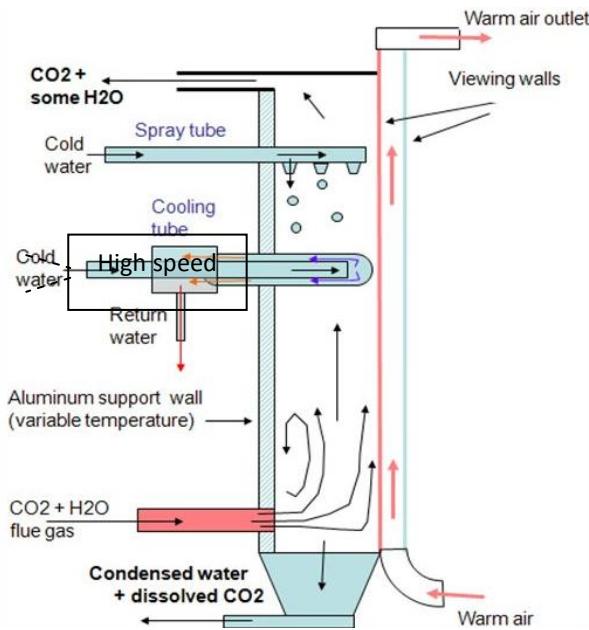


Figure 1. Illustration of the first geometry proposed for study^[2]

2. Fluid dynamic and heat transfer in CFD simulation

In fluid dynamic, a flow considered to be a compressible if density of the fluid changes with respect to pressure or temperature variation the flow field. The pressure, density and temperature of a substance may be related by an equation of state. For the ideal gas equation state shows that

$$p = \rho RT \quad (1)$$

This equation links the mass conservation and momentum equations to the energy equation, making it possible to calculate temperature changes, for example, from changes in density when two of the state variables are known (i.e. density and pressure). To govern the basic law for compressible flow, we need following general equation,

- mass conservation (continuity)
- momentum equation
- energy equation
- equation of state

Continuity equation

In OpenFOAM, the simple continuity term for steady state compressible flow uses following equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (2)$$

In the continuity equations, the changing of density is calculated each time iteration. ∇ is a nabla vector operator, represented in index notation as

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$$\nabla \equiv \partial_i \equiv \frac{\partial}{\partial x_i} \equiv \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right) \quad (3)$$

Momentum equation

From the basic equation of momentum, a simple standard momentum equation based on velocity vector that solved in the OpenFOAM, is shown below:

$$\frac{\partial \rho \vec{U}}{\partial t} + \nabla \cdot (\phi \vec{U}) - \nabla (\mu \nabla \vec{U}) = -\nabla p \quad (4)$$

This is represented in the numerical code as^[3]:

solve

```
(  
    fvm::ddt(rho, U)  
    + fvm::div(phi, U)  
    - fvm::laplacian(mu, U)  
===  
    - fvc::grad(p)  
)
```

Energy equation

Following the heat transfer on per relative unit mass and unit enthalpy, this is formulated as:

$$\nabla \cdot (\Phi \cdot h) - (\nabla \cdot \Phi)h - \nabla \cdot \alpha \nabla h = \nabla \cdot \left(\frac{\Phi}{\rho p} \right) - p \nabla \cdot \left(\frac{\Phi}{\rho} \right) \quad (5)$$

Above equation expresses the fact that heat transfer changes the total energy (the sum of thermal energy h , and kinetic energy) of the modeled fluid. This energy equation is converted to C++ codes as shown below:

```
(  
    fvm::div(phi, h)  
    - fvm::Sp(fvc::div(phi), h)  
    - fvm::laplacian(turbulence->alphaEff(), h)  
    ===  
    fvc::div(phi/fvc::interpolate(rho)*fvc::interpolate(p,  
    "div(U,p)"))  
    - p*fvc::div(phi/fvc::interpolate(rho))  
)
```

Navier-Stokes equations and compressible flow of Newtonian fluids

The Navier-Stokes equations are nonlinear partial differential equations in almost every real situation. The derivation of the Navier-Stokes equations begin with an application of the conservation of momentum (often alongside mass and energy conservation) being written for an arbitrary control volume. In an inertial frame of reference, the most general form of the Navier-Stokes equation ends up being:

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \right) = -\nabla p + \mu \nabla \cdot \mathbf{T}_{\text{stress}} + \mathbf{f} \quad (6)$$

\mathbf{f} represents body forces (per unit volume) acting on the fluid and ∇ is the del operator.

Each term in the above equation has the units of a volume force or equivalently, an acceleration times a density. Each term is thus dependant on the exact measurements of a flow.

Turbulence modelling

In the implementation of turbulence models, OpenFOAM has its own way to formulated in C++ script. For example, the turbulence kinetic energy has following equation:

$$\frac{\partial k}{\partial t} + \nabla \cdot (\mathbf{U}k) - \nabla \cdot [(\nu + \nu_t) \nabla k] = \nu_t \left[\frac{1}{2} (\nabla \mathbf{U} + \nabla \mathbf{U}^T) \right]^2 - \frac{\epsilon_o}{k_o} k \quad (7)$$

and representation differential equations in OpenFOAM natural language is:

```
solve
(
    fvm::ddt(k)
    + fvm::div(phi, k)
    - fvm::laplacian(nu() + nut, k)
    ==
    nut*magSqr(symm(fvc::grad(U)))
    - fvm::Sp(epsilon/k, k)
);
```

In this study, k-epsilon turbulence model is used in the simulation. Following script is represent turbulence numerical calculation of k-epsilon,

```
volScalarField
G = nut_*2*magSqr(symm(fvc::grad(U_)));
nut_ = Cmu*sqr(k_)/(epsilon_ + epsilonSmall_);
```

Where, Cmu is an empirical constant specified in the turbulence model (approximately 0.09).

3. Modeling procedure in OpenFOAM

The OpenFOAM (Field Operation And Manipulation) code is an object-oriented numerical simulation toolkit written in C++ language. The toolkit implements operator-based implicit and explicit second and fourth-order Finite Volume (FV) method in three dimensional spaces^[4].

The governing equations are solved on discrete control volumes. FVM recasts the PDE's (Partial Differential Equations) of the Navier-Stokes equation in the conservative form and then discretize this equation. This guarantees the conservation of fluxes through a particular control volume. Though the overall solution will be conservative in nature there is no guarantee that it is the actual solution. Moreover this method is sensitive to distorted elements which can prevent convergence if such elements are in critical flow regions. This integration approach yields a method that is inherently conservative.

$$\frac{\partial}{\partial t} \iiint Q dV + \iint F dA = 0 \quad (8)$$

Where

- Q is the vector of conserved variables
- F is the vector of fluxes
- ∇ is the cell volume
- A is the cell surface area

OpenFOAM is based on a three dimensional platform and utilizes tensor of different ranks to describe the physical entities. The basic approach is to set up a given case and solve this by applying a specific solver to the case.

The OpenFOAM software used in this project is version 1.5-dev which is installed on the Linux Ubuntu 8.10 Platform 32 bit and using ParaView version 3.3 (Open Source) as a post processing GUI.

Pre-processing

Pre-processing refers to the operations carried out prior to the calculations. This covers mainly geometry production, meshing, and setting up the boundary condition or initial condition variables for the calculations.

Geometry production

Building 3D geometry and mesh are generated by Salomé Open source software version 4.1.4. sp2, a complete version for Debian Etch 32 bit. Salomé uses millimeter as a default dimension.

The 3D geometry is made to visualize and simulate the behavior of the fluids in a real size condenser model. The dimensions of the 3D condenser model are 500 mm x 150 mm x 2700 mm, with inlet tube is in the same direction as y ordinate. The diameter of the inlet and outlet tubes is 100 mm. For each cooling tubes has 50 mm diameter and placed approximately in the middle of condenser. The configuration of the cooling tubes is managed, so that their position is assumed effective to cool down the temperature of the gas flow. In this geometry, the spray tubes are not included in the geometry build up, numerical simulation and analysis. The reason is just to simplify the first simulation using OpenFOAM. Figure 2 presents the 3D model of condenser in this primary study.

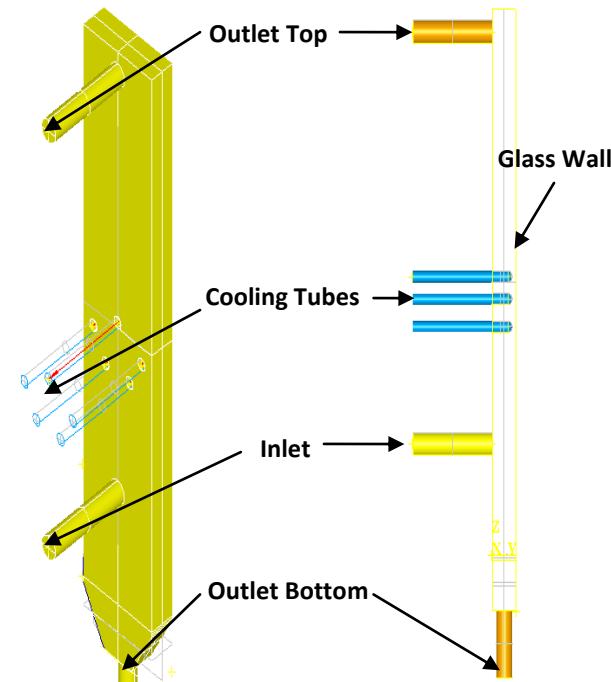


Figure 2. 3D model of condenser

Meshing production

Algorithm used in the mesh or sub-mesh is 1D-2D-3D by Netgen 3D parameters hypothesis. Fine of mesh can be adjusted by hypothesis construction, by changing maximum size value, put second order Netgen 3D parameter, and fineness custom, after that choose optimize option.

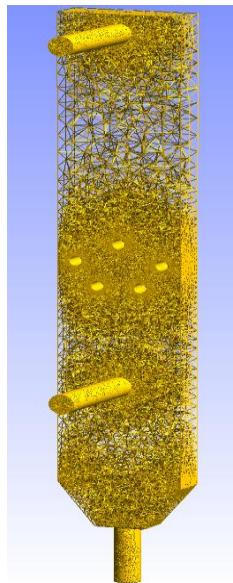


Figure 3. 3D mesh (viewing by GMSH meshing tool)

Salomé will generate mesh automatically based on our input. The meshing can be checked by typing checkMesh command in shell to see that there are no errors in the mesh. Keep in mind that OpenFOAM uses meter as a default length dimension, so a dimension adjustable is needed. Meshing that is shown in figure 3 has 350.070 cells.

Cooling tubes

Comprehensive analysis on cooling tubes is necessary due to the importance of knowing the effective heat transfer around the cooling tubes wall. To have a very fine mesh is extremely essential, so manipulated meshing is needed. For non orthogonal mesh, EnGrid software could be a good choice to refine our mesh. The latest version of this software (EnGrid 1.0) can be downloaded from SourceForge, the “official” website for Open source software. Its package is available for both Linux and Windows platform. Following figure 4 shows a close view of produced mesh in cooling tubes.

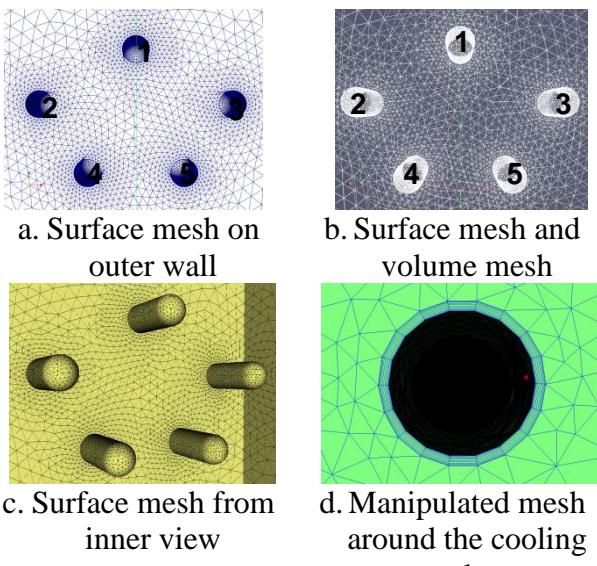


Figure 4. Cooling tube fine meshes

Solving

OpenFOAM defines its physical parameters by using simple single matrix. For example *nu* as a dynamic viscosity symbol will be written in the script as *nu* [0 2 -1 0 0 0 0], which is represent its metric units [kg m s K A mol cd]. In this simulation, we tried to use several generic solvers that we look into and used as a based solver for comprehensive calculation and investigation.

1. simpleFoam, related to validation of the simulation. This is an incompressible solver without heat transfer or energy equation calculation.
2. rhoSimpleFoam, for steady state compressible flow simulation with heat transfer or energy calculation based on Reynolds Average Simulation.
3. rhoPimpleFoam, for transient state compressible simulation with heat transfer or energy calculation based on Reynolds Average Simulation.

Thermophysical properties

In general solver of OpenFOAM, rhoSimpleFoam and rhoPimpleFoam use similar thermo package to calculate rho, which is assumed the fluid flows as a prefect gas. The thermo type model using in these solvers is hThermo as shown a code below:

```
thermoType
hThermo<pureMixture<constTransport
<specieThermo<hConstThermo<perfectGas>>>>
```

In detail, this code tries to combine a complex thermo calculation based on:

- pureMixture, a mixture property which solves a general thermophysical model calculation for passive gas mixture
- constTransport, a transport coefficient which has constant transport properties (i.e. viscosity and thermal conductivity models)
- specieThermo, a derived thermophysical property of species, derived from C_p , h
- hConstThermo, a basic thermophysical property which has constant specific heat (C_p) with evaluation of enthalpy h
- perfectGas, a perfect gas equation of state

In OpenFOAM, compressible solver wall heat transfer will be calculated as

$$q = \text{alphaEff} * \text{snGrad}(T) \text{ and} \\ \text{temperature} \quad \text{gradient} \quad = \\ q/(\text{alpha_eff} * \text{Cp0} * \text{rho0})$$

where alphaEff is an effective thermal conductivity. alphaEff is differentiated from the turbulence model in the database and then it will ask the turbulence model for the near-weall heat transfer coefficient calculation. Heat capacity is assumed constant for both CO_2 and water vapor. Heat capacity (C_p) will not vary much with temperature, but density will change more than negligible. Heat capacity [$\text{m}^2/\text{s}^2\text{.K}$] at constant pressure $1 \times 10^{+05}$ Pa is set 840.4 for CO_2 and 2000.0 for water vapor (H_2O). rhoSimpleFoam works by a constant heat flux, since it is a steady state solver.

A thermal conductivity (k) is the quantity of heat transmitted through a unit thickness in a direction normal to a surface of unit area, due to a unit temperature gradient under steady state conditions. In temperature 373 K and pressure $1 \times 10^{+05}$ Pascal, the thermal conductivity for CO_2 is 0.023 W/m.K and water vapor is 0.016 W/m.K. This thermal conductivity of the fluid flows will be updated each time step.

Water vapor - H_2O - is composed of one Oxygen atom and two Hydrogen atoms. With 18 atomic units water vapor is lighter than carbon dioxide with 44 units. Water vapor as a gas in air will replace other gases and reduce the total density of the mixture. Dry air is denser than humid air. The density (mass/volume) of water vapor is around 0.804g/liter, which is significantly less than that of dry air at 1.27g/liter at STP.

From the analytical calculation, we get that Prandtl number of gas flow in 373K and 1 m/s is around 0.7 for CO_2 and 35 for water vapor and also both fluids have Achimedes number around 0.860 which mean forced convection dominates.

Post processing

Post-processing refers to application used subsequent to the solving sequence. After generating the log file, it is necessary to extract the residual error trends over a long period of time. The foamLog and pyFoam scripts are therefore used to extract data of residuals velocity, pressure, turbulence parameters, iterations, Courant number, and other defined parameters from a log file and present them in a set of files that can be plotted graphically. The 3D simulations has an average clock time more than 500.000 seconds or 6 days per single simulation (transient solver can be more) that's mainly depend on the capability of computational machine. For further research, to anticipate too much simulation time, we can play around the under-relaxation factors, convergence parameters, schemes, and discretisation to reach a decent result, unless we're trying to do a couple of million cells on a single-CPU machine.

4. Numerical result and discussion

Several 3D cases are simulated by the chosen solvers. Physical properties such as velocity, temperature, pressure, turbulence and heat flux distributions will be tried to analyze in this section. CO_2 is assumed as a non condensable gas due to low condensation temperature and high condensation pressure. Water vapor (H_2O) is also assumed as a non condensable gas. One may argue that this is incorrect, but it is considered relatively simple to implement in the simulation (due to unavailable solver in OpenFOAM that can simulate phase change in multiphase compressible gas mixtures). These approaches are assumed can give preliminary information on thermophysical phenomenon in the condenser.

The simulation on 3D case was carried out by the initial condition of the pressure inlet, internal pressure and pressure outlet of the condenser in $1 \times 10^{+5}$ Pa. Except for heat flux analysis, fluid flow is set through the condenser by inlet velocity of 1 m/s and the glass wall has uniform temperature 323 K. For all simulations, temperature on the five cooling tube walls is uniform 288 K. Figure 5 illustrates the situation where the gases flow across a bundle of cooling tubes.

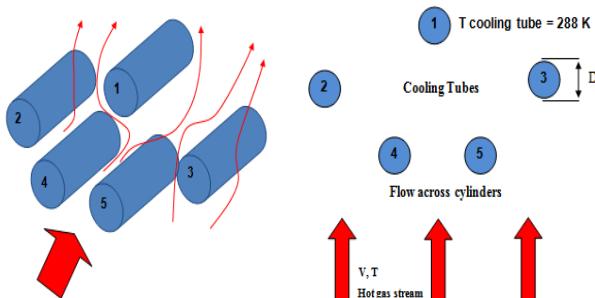


Figure 5. Illustration of flow across a bundle of cooling tubes inside the condenser

Velocity analysis

Figure 6 presents the condenser with only one of the outlets is opened. The reason why the bottom outlet tube is closed, it is because of condensation built up. In real experiment, the bottom outlet tubes will be closed to let all the gas experiences cooled by the cooling tubes. The bottom condenser is managed to collect liquid water from condensation process. When the bottom part is full by condensed gases, then the bottom outlet will be opened.

The speed is reduced inside the condenser because of volume expansion that varies from small inlet tube into bigger volume (inner condenser). The minimum velocity region is located in the bottom of condenser, where situated between the inlet tube and bottom outlet. The flow is forced to the top of condenser as the only way out from the flow channel. For most of the slice part, ranges of velocity inside of the condenser are between 0 – 0.5 m/s before it reach the outlet tube. After passed the cooling tubes bundle, the flow slowly formed in laminar. The gradients in the flows will contribute to contour variation of velocities inside the condenser.

The figure 6 (b) and (c) show the close view of velocity vector around the cooling tubes. It can be seen that the biggest velocity magnitude flows around outside of the cooling tubes bundle, or close to side of the vertical wall of the condenser. The gas which flows across the cooling tubes bundle through the middle seems has relatively smaller velocity vector. This is predicted due to obstacle from each cooling tubes that makes the speed is declined.

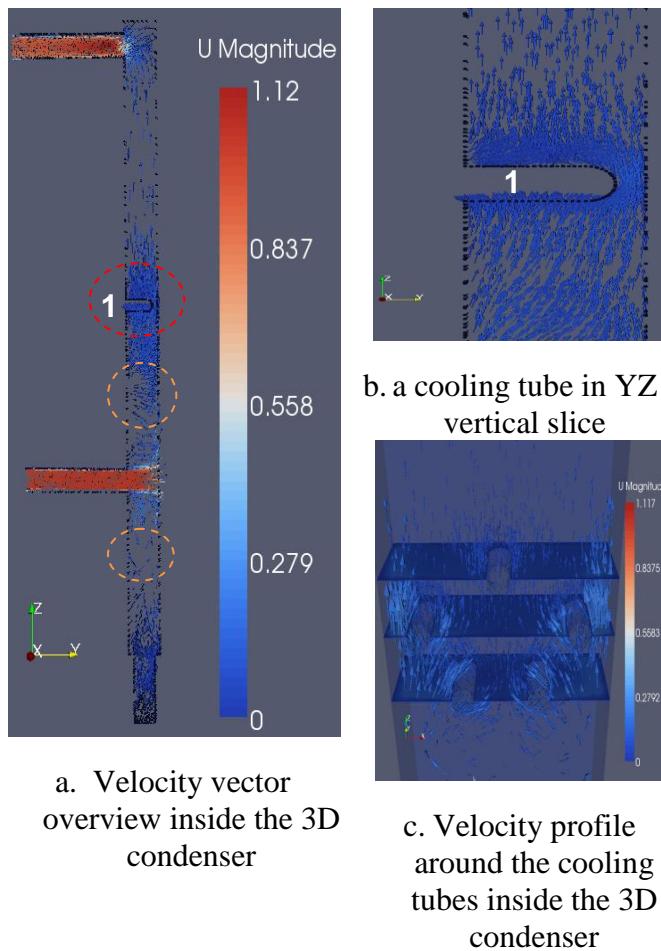


Figure 6. Close view of velocity vector

Turbulence analysis

Different flow regimes will consequence in different momentum transfer rates. The turbulent flow controls the transport momentum and energy of both species; therefore it is a great interest to take into account an accurate calculation and analysis in the turbulence flow field. The peak values of each turbulence parameters, can give us an idea, approximately on which location the turbulence is developed. Typically, the place of turbulence kinetic energy occurs in the same high as turbulence dissipation (epsilon). Figure 7 shows turbulence parameter k-epsilon profiles along the glass wall in the Z axis (height). The turbulence energy and dissipation rate decline become smaller on the highest glass wall. This is happening follows the laminar flow that is developed after the last remaining turbulence flow around the cooling tubes. From this figure, it can be found three crests that have possibility represent where the fully turbulences take place.

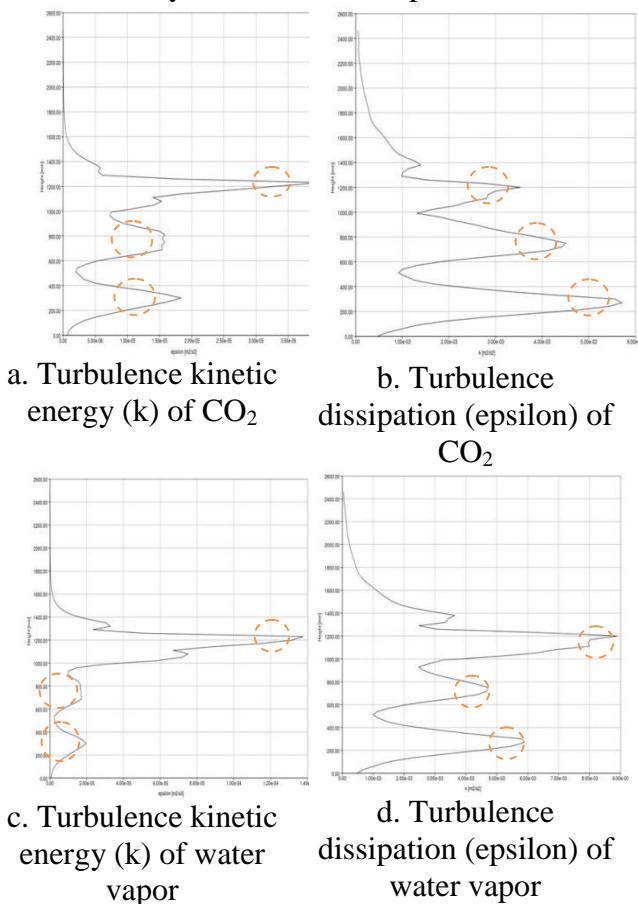


Figure 7. Turbulence k-epsilon profile along the height on glass wall

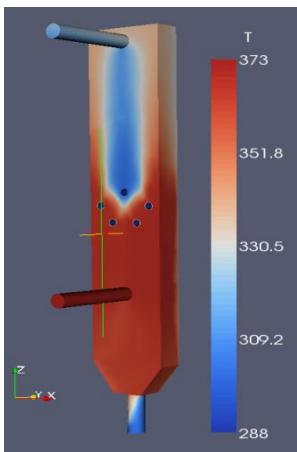
Temperature

Figure 8 displays the simulation results of the temperature distribution on the condenser wall affected by heat convection. Since the adiabatic boundary condition was not managed, this implies the

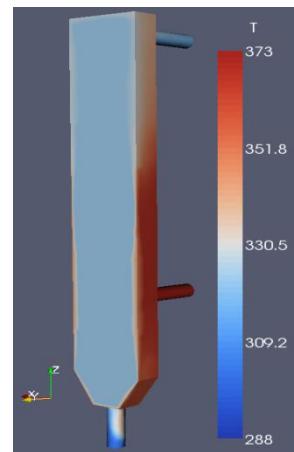
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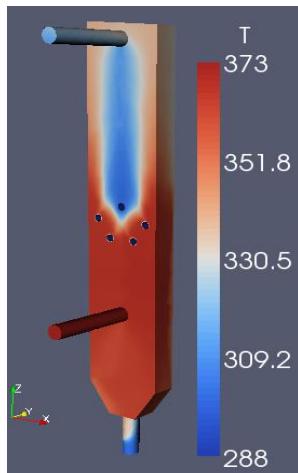
temperature variations on the walls. Some part of a half bottom condenser wall relatively has high temperature more than 360 K. A half bottom of the condenser has high temperature because of no cooling treatment. After the cooling tubes region to the top, the temperature shows a tendency to decline, mainly in the middle region, starting from the middle of cooling tubes. On the right side, the glass wall is conditioned by a uniform temperature 323K, flowing hot air from bottom right side of the condenser. This treatment is conditioned since we would like to reduce moisture builds up on the glass wall. This transparent wall further will be used to investigate inner condenser from outside by a high speed camera, to see the condensation process and distribution of the water droplets in the gas stream. Further this physical phenomenon will initiate the condensation process; because of the H_2O vapor possible to reach the situation that dealing to the phase change since it has relative low condensation temperature and pressure



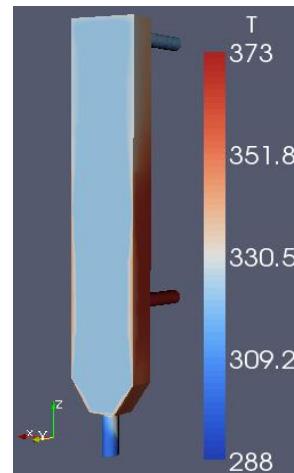
a. CO_2 flow simulation



b. CO_2 flow simulation



c. Water vapor flow simulation



d. Water vapor flow simulation

Figure 8. Temperature convective distribution on 3D geometry wall

Heat fluxes analysis

Heat fluxes around the cooling tubes

By varying the flow rates, we expect to see variations in average heat fluxes on each cooling tubes and glass wall against the Reynolds number. Increasing the velocity results rising of the momentum transfer between the fluids and the wall, and thereby increase the wall heat fluxes. In the following figure (9), presents the plot of average heat fluxes on each cooling tubes and glass wall. The negative value indicates the heat leaves out from the inner condenser. In the opposite, the positive value indicates the heat comes into the condenser absorbed by the gases flow. The heat from gas flow is released and transferred to the wall due to differential temperature. Interesting in here that the cooling tubes 2 and 3 have bigger magnitude values of heat flux compare to the cooling tubes 1, 4, and 5. In the region around cooling tubes 2 and 3 give relative strong forced convection compares to other cooling tubes walls.

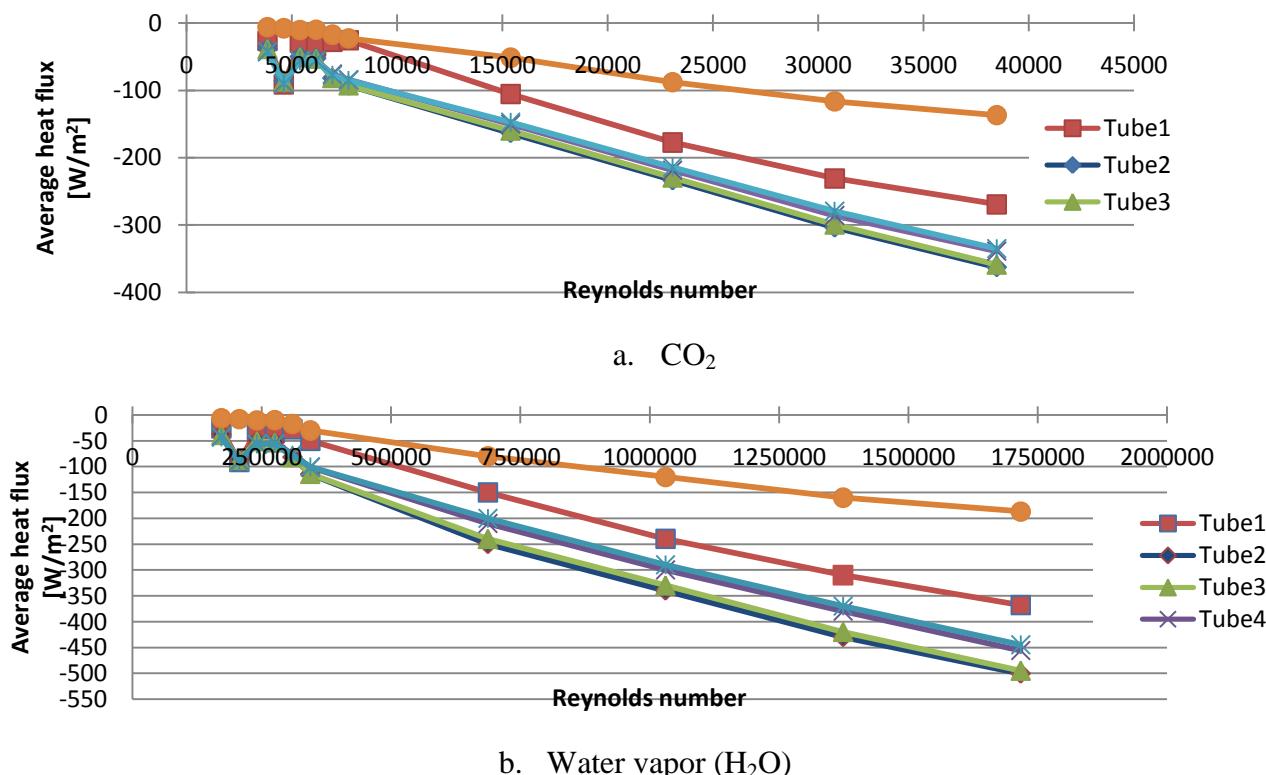


Figure 9. Average heat fluxes on the cooling tubes walls in different Reynolds number

Heat fluxes on the glass wall

In the figure 10, presents the distribution of the wall heat fluxes along the glass wall caused by convection. The major negative values of wall heat flux are occurred between height 200 – 400 mm and 600 – 800 mm. This is in the same location where turbulence flows occur in the condenser. Turbulences give a high contribution in the wall heat fluxes distribution. The heat flux curve is showed a small crest to the “positive” values that takes place approximately between height 400

to 600 mm. This area is located in the same height where the inlet pipe is placed. A relative strong forced convection from inlet flow is the main contribution, making relative lower negative value of the wall heat flux. The relative big positive values of the wall heat flux are occurred at the high between 1100 mm – 1500 mm. These areas are occurred at the same height where the cooling tubes are located. All of the different temperatures simulations in each gases has similar tendency and relate to each others.

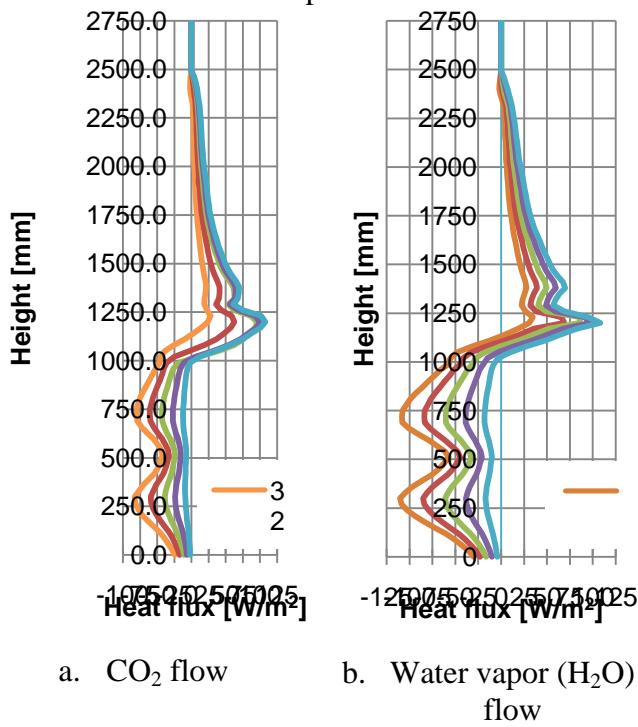


Figure 10. Comparison wall heat flux in different temperature on outer glass wall

Future work

- Determine approaches for the gas mixtures model into a new solver based on euler-euler or euler-lagrange continued by developing codes that are able to solve the phase change problem due to heat transfer.
- Tested another models of turbulences for better accuracy on numerical simulations.

Acknowledgements

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