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# Digital Twin in Modelling Citronella Grass Essential Oil Distillation Process with Computational Fluid Dynamics Approach

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***Abstract.*** *This study aims to investigate distillation process of Citronella Grass (Cymbopogon nardus) essential oil and determine the effect of heating temperature on oil quality, which significantly influences the market value. The study procedures were carried out by developing a virtual model of distillation apparatus using Digital Twin (DT) approach, integrating Computational Fluid Dynamics (CFD) to stimulate fluid behavior as it transitioned from vapor to liquid during distillation. The core of DT is in the virtual model development and three-dimensional (3D) geometric representations of system. The methodology comprised creating 3D geometric model of distillation setup, followed by mesh generation as well as setting of boundary conditions and computational parameters. In addition, numerical iterations were used to refine the process, leading to the analysis of CFD visualizations. The convergent result showed that the developed model was accurate at 300 iterations. Observations confirmed the occurrence of vapor to liquid phase change in the spiral pipe, with vapor density below 1 kg/m$^3$ and liquid density between 800-1000 kg/ m$^3$. Temperature monitoring showed a reduction from 120◦C in distillation tank to 24-26◦C post-condenser, which was similar to the observed range of 25-30◦C. Further temperature exchange in the reservoir was stimulated and observed in 36-38◦C. The result also showed that DT model created using CFD was capable of reflecting the real conditions observed.*
**Keywords:** *Digital Twin; Computational Fluid Dynamics; Distillation; Essential Oil; Citronella Grass.*

**Type of the Paper:** Regular Article.

## 1. Introduction

Indonesia is known to possess various types of flower plant species, leading to the presence of different business potential, such as essential oil industry [1]. Essential oil also known as flower oil is a complex volatile chemical compound [2], which can easily evaporate [3] and is often obtained using certain techniques. Several studies have shown that the product is widely used across various industries, including food and beverages [4], fragrances [5], medicine [6], cosmetics, and skincare [7,8]. In this context, essential oil is often extracted from Citronella Grass (*Cymbopogon nardus*) using distillation process[9], where the product is obtained from plant cells by water vapor [10].

Essential oil distillation is a process of separating major components from the raw materials through heating and condensation with an apparatus. The main parts of the apparatus include boiler, furnace, condenser, and separator [1]. In essential oil industry, the quality of the product is very important due to the effect on the market value. Consequently, heating temperature [11] is



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one of the critical parameters that must be monitored during processing. Inappropriate or excessively high temperatures can cause essential oil to decompose or burn. This indicates that there is a need to develop a method for optimizing the pressure and heating temperatures to prevent the occurrence of adverse conditions.

A potential method with the ability to prevent adverse conditions is digital twin (DT) model, which has been proven to be an effective solution. DT is a virtual representation of a physical system [12,13] that combines a physical-based model with the virtual world [14]. Several reports have also reported that it is a concept with great potential in integrating the physical space with the virtual space. DT typically contains constructed virtual information that is integrated with the actual system [15] and considered the key to achieving a fusion between the physical and the virtual model. In addition, it allows close interaction between physical and virtual space, which creates a new opportunity in the use to improve monitoring, simulation, and control of process [16].

The application of Computational Fluid Dynamics (CFD) in DT is often used to simulate fluid flow in phase-changing from vapor to liquid phase during distillation process. The model is carried out by building the geometry of the physical system and collecting several related parameters. Due to the combination of DT model with CFD, fluid flow behavior can be depicted to provide predictions about system performance in various operational conditions.

According to previous studies, essential aspect in the use of DT is the virtual model development [17], which consists of three-dimensional (3D) geometric representations of systems [18]. The novelty in this current study is in the use of DT in Citronella Grass essential oil industry, with a focus on virtual space development. The model of essential oil distillation apparatus was discussed using CFD approach, which could also be referred to as DT because it was able to capture the characteristics and represent the existing physical system [19]. The correct solution to solve the existing problems in a short time is to use computer modeling to support effective calculations [20]. Therefore, this study aims to develop a concept of DT for modeling Citronella Grass essential oil production process using CFD to understand fluid behavior.

## 2. Materials and methods

### *2.1. Computational Fluid Dynamics (CFD)*

CFD was a computer-based system analysis that was enabled to solve problems through simulations of fluid flow, heat transfer, and chemical reaction phenomena [21]. This study used CFD as a tool to model fluid flow and transferred heat as temperature distribution in the system. The advantage of CFD was able to analyze fluid flow and temperature distribution without doing expensive physical testing.

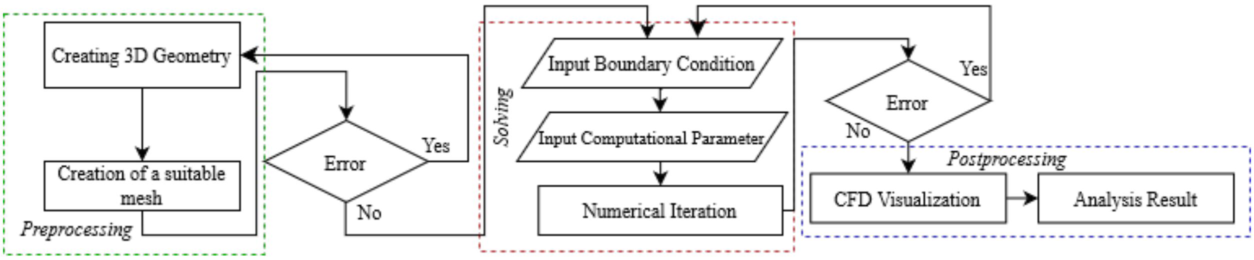



**Fig. 1.** CFD Flowchart

CFD modeling and simulation had several stages (Fig. 1), namely pre-processing, solving/processing, and post-processing. The initial stage in building CFD model analysis was pre-processing, and problem identification and determination were done in this stage. The determined case was then derived through Computer Aided Design (CAD) model. CFD analysis through CFD software needed to pay attention to CAD geometry and any of these mistakes must be avoided, such as missing surfaces or overlapping surfaces were common to happen. Grid or mesh determination was essential in addressing these geometry issues to ensure accurate CFD simulations [22,23]. Subsequently, the physical and chemical phenomena that needed to be modeled were selected. In this stage, the geometric model was done using Solidworks software, then the simulation was carried out using ANSYS software. The simulation in ANSYS software started by making the appropriate mesh and boundary type [24] based on the input and output of the problem to be simulated. The model was done based on the specifications of distillation equipment regulated in Indonesian national standards (SNI 8028-1:2014) which contained standards for distillation process, volume and dimensions of kettles ranging from small to large types, and material requirements for distillation equipment. Table 1 described the specifications of Citronella Grass essential oil distillation process with a capacity of 500 kg of citronella and a condenser length of 30 m.

**Table 1.** Specification of Citronella Grass Essential Oil Distillation Apparatus

| No | Description | Specification |
|---|---|---|
| 1 | Distillation cattle capacity | 500 kg (D 130 cm × T 160 cm) |
| 2 | Distillation cattle material | Mild steel plate |
| 3 | Plate thickness | 6.5 mm |
| 4 | Condenser | Pond, stainless steel pipe 30 m diameter |
| 5 | Water and oil separator | Stainless steel (D 38 cm × T 60 cm) |
| 6 | Distillation method | Distillation |
| 7 | Distillation time | 4-5 hours |
| 8 | The source of the raw material | Company-owned Citronella Grassland |
| 9 | The result of essential oil | 5 kg |
| 10 | Fuel | Firewood and citronella waste |

The next stage was solving or processing utilizing solvers, a complex numerical calculation programs to describe fluid and thermal flows in predetermined domains [25]. Solving stage began with solving the equation to obtain a numerical solution. However, the domain discretization, iteration, and convergence were done to generate a stable and accurate solution. The next step was handling the boundary conditions and parameter determination.

The last stage was post-processing stage, where in this stage the analysis and interpretation of the simulation results was carried out. The simulation results were the visualization in a graphical form and a picture of the behavior of fluid flow and heat distribution in distillation tank [21]. The results obtained were then analyzed to conclude decisions regarding design optimization.

Data processing was carried out using a numerical approach utilizing Computer Aided Design (CAD) and Computer Aided Engineering (CAE) software. Solidworks was a software to do 3D model [20] and was used to present 3D design of each component of essential oil distillation apparatus. ANSYS software was used to illustrate fluid flow and heat transfer of an object [26]. This software was capable of preparing and solving CFD problems by visualizing the results in post-processing stage [20,27].

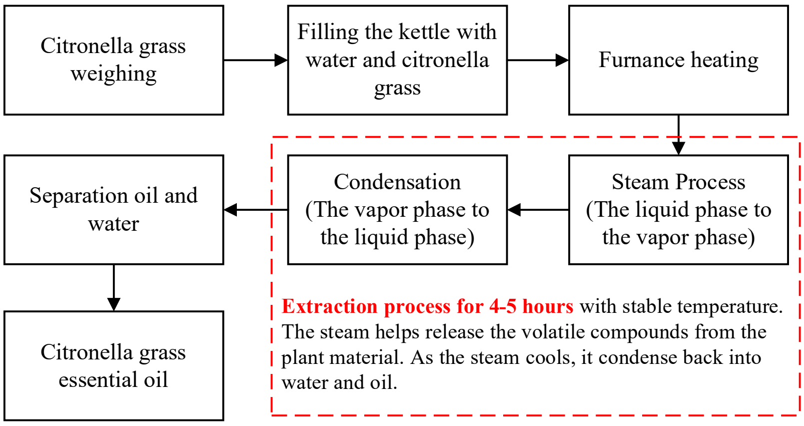



**Fig. 2.** Distillation Process

*2.2. Distillation Process*

Distillation process (Fig. 2) began by filling the kettle with 700-1000 liters of water. This type of distillation apparatus worked by boiling water, then the water vapor entered through the nest hole where Citronella was located. The company had 3 distillation units with a capacity of 500 kg and 1 distillation unit with a capacity of 300 kg and was carried out in 4-5 hours in the morning and afternoon. Unstable heat and overheating needed to be avoided because it greatly affected the quality of essential oil produced. The more water vapor formed, the more oil produced, but it did not mean that a big fire produced a lot of oil of good quality. However, the oil from the kettle was too hot and produced a burnt scent. Distilled steam from the boiler was streamed and cooled through the condenser, and this had a coil diameter of 90 cm and 30 m in length. The condenser pipe had a 3/8-inch exhaust hole made of stainless steel, and after going through the cooling process in the condenser, the water and oil were mixed and then streamed into the separator. The final step was to separate the oil from the water using a monyl cloth. The color of a good citronella essential oil was pale yellow to brownish yellow, and the yield was about 0.7-1%. Oil yields were usually influenced by several factors including climate, heating furnace temperature, and the fertility of Citronella leaves.

Some data collected during distillation process were used as parameters in pre-processing phase. The parameters listed in Table 2 were essential for conducting CFD simulations. Each of these parameters played a critical role in modeling distillation process. Carefully setting these parameters enhanced the quality of the simulation outcomes.

**Table 2.** Main parameter for CFD model

| No | Parameters | Description |
|---|---|---|
| 1 | Furnace combustion temperature | 200 - 300ºC |
| 2 | Distillation tank temperature | 130ºC |
| 3 | Density of materials: | |
| | Water | 1 Gram/ml |
| | Essential oil | 0.850 – 0.892 Gram/ml |
| 4 | Materials of equipment | |
| | Tank | Mild steel plate |
| | Spiral condenser | Stainless steel |
| | Separator tube | Stainless steel |
| 5 | Oil yield | 0.7-1% |

### *2.3. Digital Twin (DT) Model*

The model presented included various integrated components and layers to connect physical and digital systems. Components in building DT generally consisted of physical space and virtual space, as shown in Fig. 3.

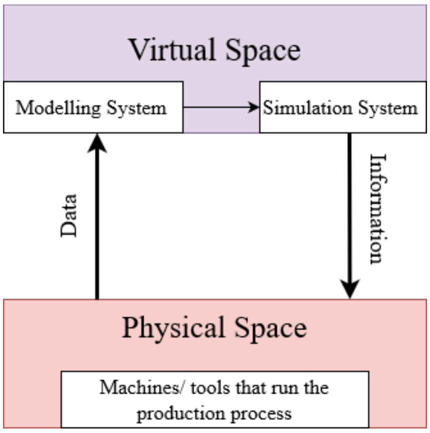


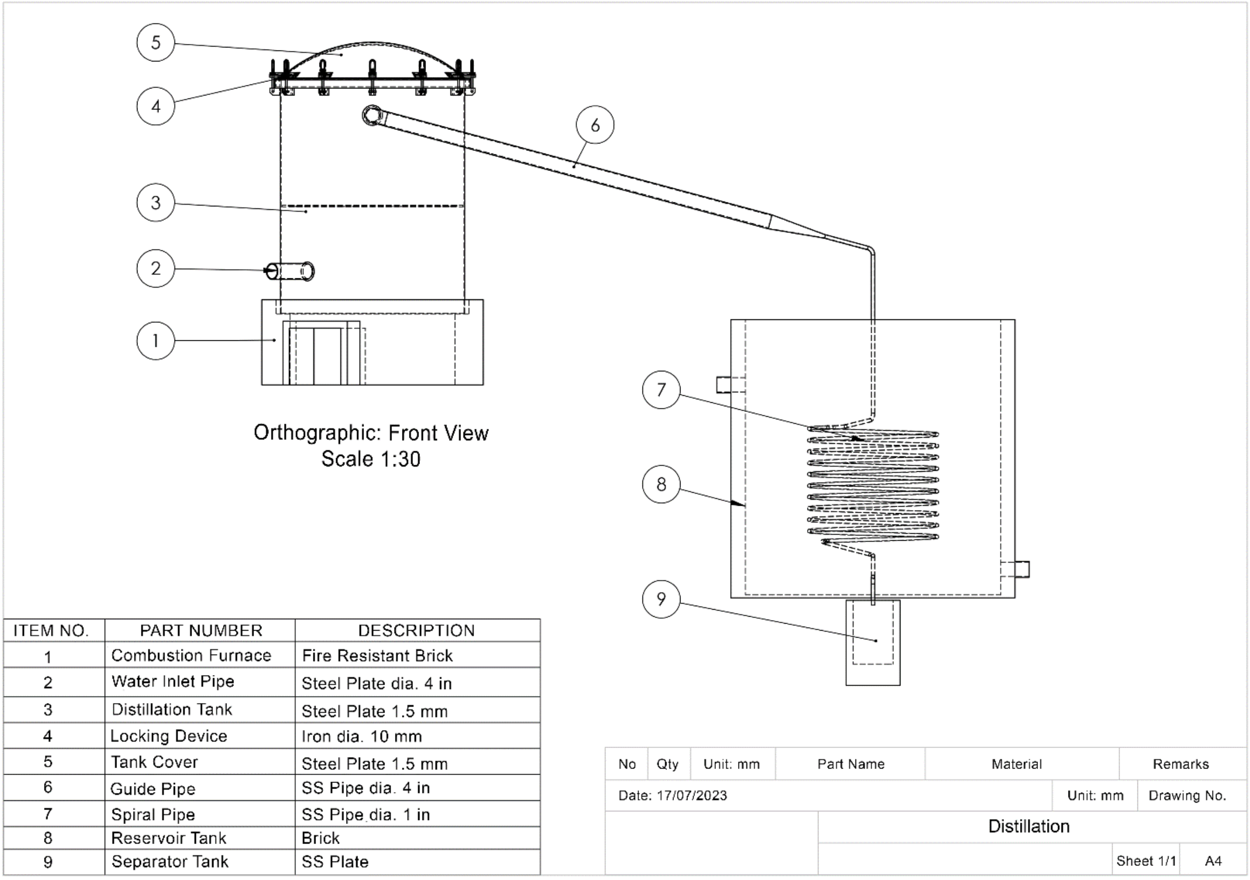

**Fig. 3.** DT model

Virtual Space was a digital representation of the physical system, namely DT of the device/system. This reflected the state of the physical system by building 3D model and simulating it according to the real situation. The geometry objects in this work were built with 3D modeling software SolidWorks [28]. DT concept that was discussed was related to the model development of the objects that had been studied. Building a good DT model opened the possibility of enhancing the high-precision digital representation of the physical components. This concept was the first step towards developing high-precision geometrics [18] as the core of DT concept. The use of CFD approach [17] in previous studies had proven the effectiveness of this approach, and some DT model were built using ANSYS software [19,29]. This software could help for an in-depth look at flow and temperature profiles

## 3. Results and Discussion

The application of CFD in DT model was used to simulate fluid flow in the process of phase-changing from vapor phase to liquid phase during distillation process. The model was done by building the geometry of the physical system and collecting several related parameters. As a result of DT model with CFD approach, fluid flow behavior could be depicted to provide predictions about system performance in various operational conditions.

The virtual model development was a critical thing [17], and it had 3D geometric representations of systems [18]. This study discussed the model of essential oil distillation apparatus using CFD approach, which could be called DT because it could capture the characteristics and represent the existing physical system [18]. The correct solution to solve the existing problems in a short time was to use computer modeling to support effective calculations and problem-solving in an effective way [20].




| ITEM NO. | PART NUMBER | DESCRIPTION |
|---|---|---|
| 1 | Combustion Furnace | Fire Resistant Brick |
| 2 | Water Inlet Pipe | Steel Plate dia. 4 in |
| 3 | Distillation Tank | Steel Plate 1.5 mm |
| 4 | Locking Device | Iron dia. 10 mm |
| 5 | Tank Cover | Steel Plate 1.5 mm |
| 6 | Guide Pipe | SS Pipe dia. 4 in |
| 7 | Spiral Pipe | SS Pipe dia. 1 in |
| 8 | Reservoir Tank | Brick |
| 9 | Separator Tank | SS Plate |

**Fig. 4.** Distillation Apparatus Component in 2D

Distillation Apparatus Component presented in Fig. 4 provided an orthographic perspective of distillation system, and this was made from 5 mm thick steel plates. The condenser featured a 1-inch hole and extended 30 cm into a reservoir measuring 1 × 1 m. The pipes of distillation apparatus were made of stainless steel, and the modeling of Citronella Grass essential oil distillation apparatus was made by utilizing SolidWorks software.

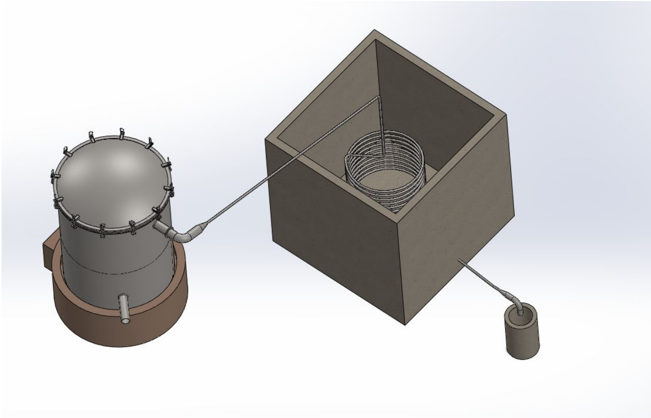


**Fig. 5.** 3D geometry of essential oil distillation apparatus

### *3.1. Pre-processing*

The 3D modeling results of essential oil distillation apparatus in Fig. 5 were exported to the STEP format. Furthermore, an analysis was conducted utilizing ANSYS software, and simulation using ANSYS helped to find solutions for a complex case. This allowed designers to identify and addressed problems in the early stages of product development to save time and costs before doing physical experiments. The analysis that was carried out in CFD simulation started from releasing the water vapor to become condensate when it passed through the condenser or could also be done in the phase change from vapor phase to liquid phase.

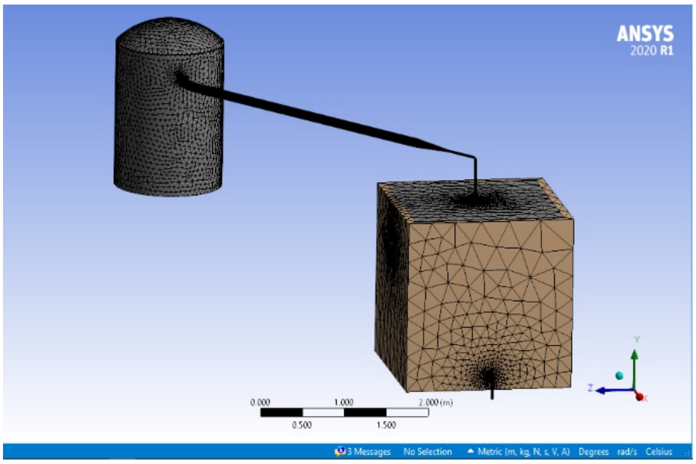



**Fig. 6.** Mesh component of distillation apparatus

The meshing process using the tetrahedron mesh type produced 1040608 elements and 264646 nodes. Mesh quality was determined by skewness and orthogonal quality metrics, and were recommended by ANSYS Inc. from CFD software package as benchmarks for assessing mesh quality. Skewness value in the range of 0.25 to 0.50 and orthogonal quality value from 0.20 to 0.69 were considered good [19]. From the above result, meshing process produced skewness value of 0.35952 and orthogonal quality result of 0.63962, and it could be concluded that the mesh had good quality. Fig. 6 was the result of meshing that was done before moving on to solving stage.

The materials observed in this simulation were the condensate of Citronella Grass oil and water. The material properties needed for solving stage were Citronella Grass oil (Table 3), water (Table 4), and stainless steel (Table 5).

**Table 3.** Material properties of Citronella Grass oil

| **Material properties** | **Units** | **Method** | **Value** |
|---|---|---|---|
| Density | $kg/m^3$ | Constant | 892 |
| Cp (Specific Heat) | j/kg-k | Constant | 2250 |
| Thermal Conductivity | w/m-k | Constant | 0.136 |
| Viscosity | kg/m-s | Constant | 0.17 |
| Molecular weight | kg/kmol | Constant | 31.626 |
| Standard State Enthalpy | j/kgmol | Constant | -2,548e+08 |
| Temperature Reference | °C | Constant | 25 |
| Thermal Expansion Coefficient | 1/k | Constant | 0 |
| Sound Speed | m/s | Constant | #f |

Boundary conditions were the domain boundaries of fluid flow during the simulation process. These boundary conditions played a role in defining how fluids behaved in the system. The determination of boundary conditions was based on inlet and outlet boundaries [25]. Inlet Boundary Conditions involved the specification distribution of flow variables in the inlet boundary. Inlet used in this study was a pressure inlet, where the initial process that occurred was the combustion that led to vapor pressure. Outlet used was a default atmosphere pressure, and this specified the distribution of flow variables at the exit boundary

**Table 4.** Material properties of water

| **Material properties** | **Units** | **Method** | **Value** |
|---|---|---|---|
| Density | $kg/m^3$ | Constant | 998.2 |
| Cp (Spesific Heat) | j/kg-k | Constant | 4182 |
| Thermal Conductivity | w/m-k | Constant | 0.6 |
| Viscosity | kg/m-s | Constant | 0,001003 |
| Molecular weight | kg/kmol | Constant | 18.0152 |
| Standard State Enthalpy | j/kgmol | Constant | -2,548e+08 |
| Temperature Reference | °C | Constant | 25 |
| Thermal Expansion Coefficient | 1/k | Constant | 0 |
| Sound Speed | m/s | Constant | #f |

### *3.2. Solving/Processing*

Solving stage was the process of carrying out numerical calculations involving basic fluid equations which were solved through a computational process. Physical parameters/material properties and boundary conditions that had been determined at the pre-processing stage were used as the input to calculate fluid behavior. This was needed to obtain the velocity, pressure, as well as temperature of the conducted simulation [25]. Calculation at this stage was done and continued until it reached a convergent value, which meant that the result obtained had the smallest error value. Convergence in CFD simulations indicated that fluid flow equations were nearing an accurate solution, verified by monitoring progressively smaller residues in each iteration to reach a stability point [30]. By achieving a good convergence, the stability of the process could be ensured from various simulation conditions.

**Table 5.** Material Properties of Stainless Steel

| Material properties | Units | Method | Value |
|---|---|---|---|
| Density | kg/m$^3$ | Constant | 8000 |
| Cp (Specific Heat) | j/kg-k | Constant | 502 |
| Thermal Conductivity | w/m-k | Constant | 16.2 |

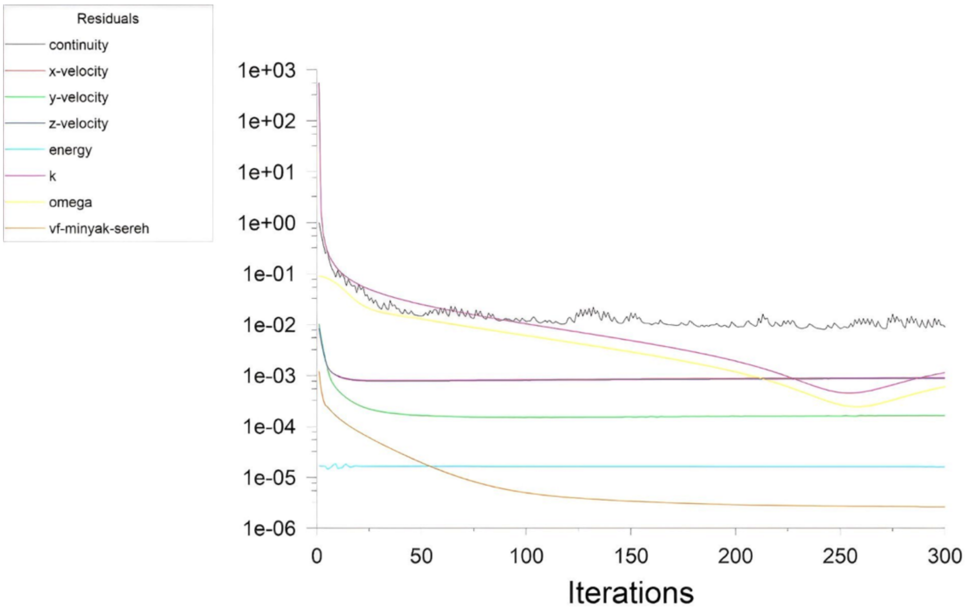



**Fig. 7.** Residual Graph

Residual graph was a visualization of how residual values changed as the iterations in CFD process. Dips in graphics could be drastic, but it slowed down as the convergence approached the steady state. Residual results in Fig. 7 were convergent at 300 iterations as it was shown that the convergence process tended to go down and towards the number 0 until it reached a stable point. Assiddiqie and Bunga [31] in their study discussing distillation of patchouli oil, required 423 iterations to achieve convergence. This showed how varying parameters could influence the iterations needed to achieve stability of the process.

**Table 6.** Comparison of the Simulation Result and the Observation

| Parameter | Observation | Simulation result |
|---|---|---|
| Temperature of distillation tank | 130°C | 125 - 150°C |
| Condensate temperature | 24 – 26°C | 25 - 30°C |
| Water temperature in the reservoir | 36 – 38°C | < 56°C |

Table 6 compared actual observations with simulation results for temperature parameters in distillation system. Site observations indicated that temperature of distillation tank was around 130°C, while temperature ranged for the simulation was set at 125-150°C. Temperatures of the condensate show ranged close to the observations and there was a discrepancy between the observed water temperature in the reservoir. Therefore, it could be seen that the simulation results closely approximate reflected the real conditions observed.

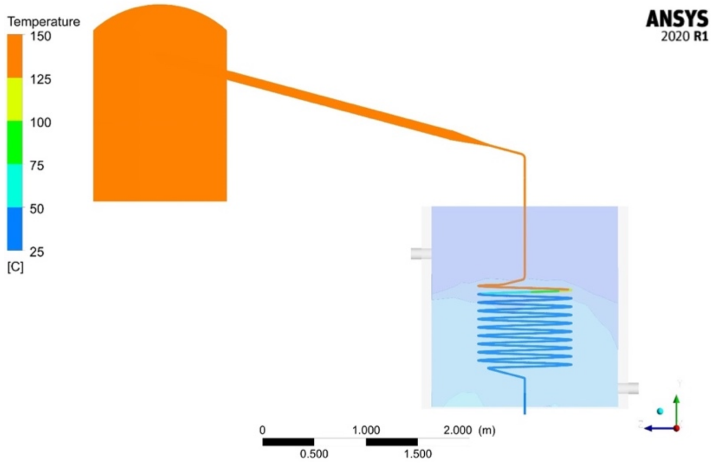



**Fig. 8.** Temperature Contour

### *3.3. Post-Processing*

Fig. 8 showed the results of temperature contour that described temperature distribution during distillation process. Fluid temperature decreased as the phase change occurred from vapor phase into liquid phase. This was shown as the steam moved through the spiral pipe which touched the cooling water. In distillation tank, temperature contour was orange and gradually changed to dark blue. A rapid temperature change occurred as the water vapor entered the condenser. Temperature in the tank during distillation process was in the range of 120-130$^o$C and decreased as it entered the reservoir. The condensate that came out through the spiral pipe in the simulation results was in temperature range of 25-30$^o$C. This result corresponded with the observations made at distillation site where the condensate temperature from distillation process was around 23-24$^o$C. The study by Turmizi and Hamdani [32], which focused on heat transfer during distillation process of patchouli oil, in the simulations, also discovered that temperature of patchouli oil distillate exiting through the condenser was approximately 25°C.

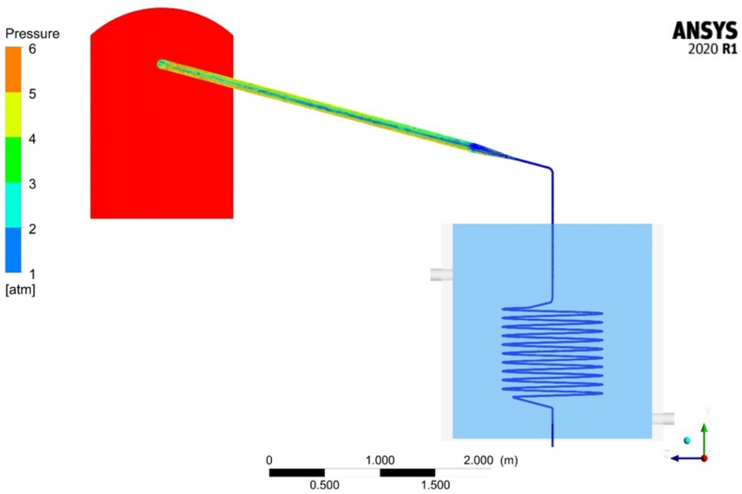



**Fig. 9.** Pressure Contour

There was a decrease in fluid pressure when it approached the spiral pipe which indicated the occurrence of a condensation process, and the higher temperature, the higher the pressure. The change of pressure in Fig. 9 was depicted in orange, which meant that the pressure in distillation furnace was considered high, reaching ≥ 6 atm. The pressure flowing towards the spiral pipe was decreased, and this could be seen from the color change in the lead pipe to the condenser or spiral pipe. The color changed into blue, which meant that the pressure continued to decrease and reached 1 atm. This was following the results of Turmizi and Hamdani [32], which identified a direct correlation between increases in temperature and pressure. The simulation results further revealed that as hot vapor passed through the condenser, heat was absorbed by the cooling medium.

Fluid flowed to the condenser as depicted in Fig. 10 showing the orange line, which described that the water was heated above 100°C and thus turned into water vapor. The evaporation process mixed with oil in Citronella Grass and brought it to flow towards the lead pipe. The orange color then changed into blue, which meant that vapor phase had changed into liquid phase. Cooling water in the reservoir was in a fixed position and did not flow, this was necessary to help the phase changes that occurred in the condenser. Spiral pipes enhanced cooling efficiency due to the larger surface area and extended contact time with fluid, facilitating improved heat transfer. The coiled shape also supported effective turbulent flow and optimizes space utilization. This study was similar to Simbolon and Setia [33] which also founded that pressure tended to decrease as the pipe length increased, which meant that there could be a reduction in both temperature and pressure when passing through the condenser. According to Rubianto et al. [34], heat transfer simulation process experienced temperature drop when passing through the condenser. This indicated that the spiral condenser was considered effective in supporting efficient steam condensation.

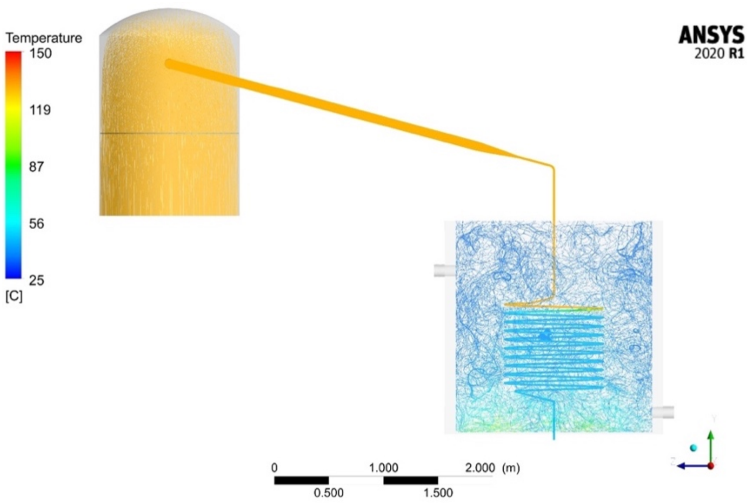



**Fig. 10.** Fluid Flow to the Condenser

Fig. 10 also showed random movement in the reservoir tank as a sign that there was heat absorption process from the spiral pipe which caused temperature increase in the water tank. This was following the observations made in the production site, where the water temperature in the reservoir was around 36-38◦C during distillation process.

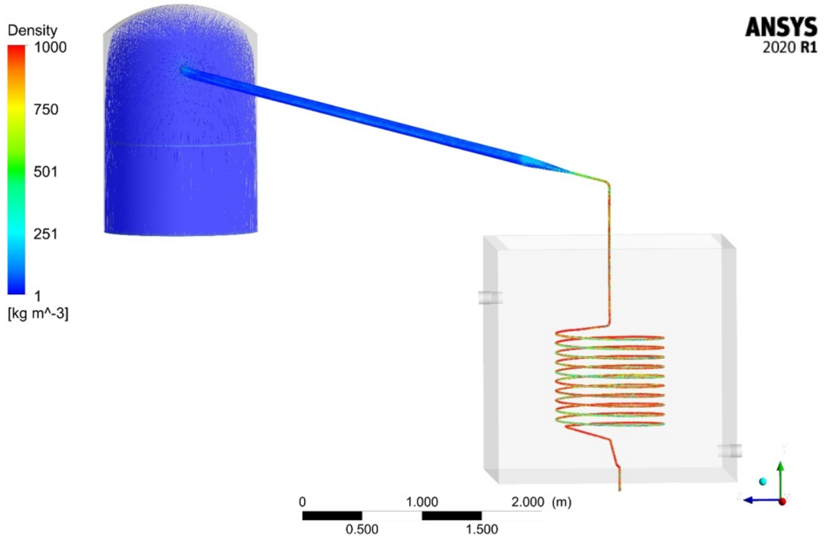



**Fig. 11.** Fluid Flow Density

Vapor phase density of Citronella oil/water was low and could fall below 1 kg/m$^3$. While in liquid phase, it had a density of 800-1000 kg/m$^3$. The results in Fig. 11 showed the phase change from vapor phase to liquid phase when passing through a cooled spiral pipe and showed fluid flow velocity that was shown in yellow on the tank and turned blue when it passed through the condenser. Condensation was the phase transition process from gas to liquid, during which heat energy was released, resulting in a decrease in temperature. Based on the results [31] that related to heat transfer analysis, the same simulation results were obtained where water as a coolant, gradually reduced temperature of patchouli vapor and also changed vapor phase to liquid. Fig. 12 showed the decrease in temperature that occurred during condensation reduced the velocity of gas molecules, thereby causing a deceleration in fluid flow rate.

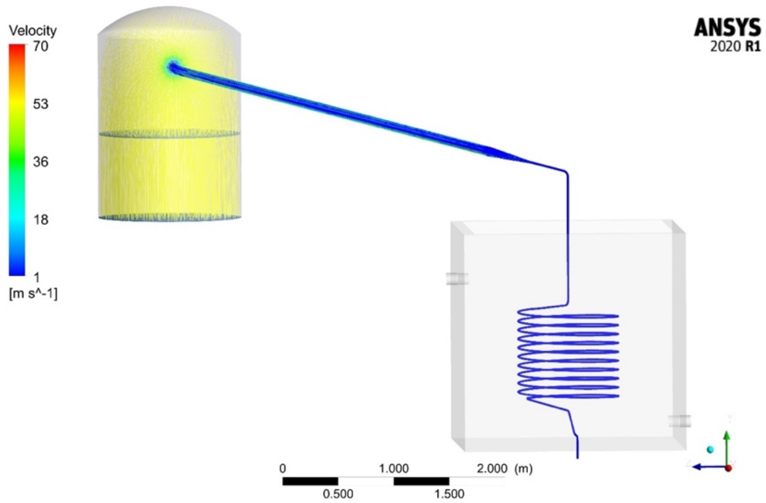



**Fig. 12.** Fluid Flow Velocity

In conclusion, the speed of fluid flow was influenced by several key factors, including the pressure in the system, fluid temperature, and the physical characteristics such as the shape of the pipes and tanks involved. These elements interacted in complex ways to dictate how quickly fluids moved through a system, underscoring the importance of considering each factor during design and operation to optimize fluid dynamics and system efficiency.

## 4. Conclusions

In conclusion, this study was focused on building a virtual space in the form of modeling essential oil distillation apparatus according to the specifications and conditions based on Indonesian national standards (SNI 8028-1:2014) for further simulation and analysis.

Residual graph showed convergent results at 300 iterations. This meant that the result of the model was close to an accurate solution. Temperature in distillation tank at the observation site was ±120$^{o}$C. Observations at the refinery site showed the change from vapor phase into liquid phase when passing through the spiral pipe. Following the simulation results, it could be that vapor phase of Citronella oil/water had a low density (below 1 kg/m$^3$) while in liquid phase, the density could reach 800-1000 kg/m$^3$. This meant that there was a change in vapor phase into liquid phase as it passed through the spiral pipe. Temperature leaving the condenser and heading to the separator tube was 24-26$^{o}$C. The simulation result was close to the observation result, which fell in temperature range of 25-30$^{o}$C. Temperature exchange also occurred in the reservoir where temperature changed to the range of 36-38$^{o}$C. The simulation results were close to the observed results, where temperature ranged ≤ 56$^{o}$C. Based on residual graph and simulation results, it could be seen that the model could reflect the real conditions observed in distillation process.

This study only focused on the modeling of existing digital model, and this was 3D geometric representation of the system. This model was the first step in building DT model and the core of DT itself. The development of a virtual model could be referred to as DT. Suggestions for future reports were to build DT in distillation process as a whole part by utilizing sensors and the Internet of Things (IoT) to provide real-time data and actual information from the system. The changes were recorded by sensors on the physical objects and reflected in digital objects. Using ANSYS Twin Builder software in building DT could also be considered.

## Abbreviations

| | |
|---|---|
| DT | Digital Twin |
| CFD | Computational Fluid Dynamics |
| CAD | Computer Aided Design |
| SNI | Standar Nasional Indonesia (Indonesian National Standards) |

## Data availability statement

Data will be shared upon request from the readers.

## CRediT authorship contribution statement

Arifia Noor Riwanti: Writing - Original Draft, Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data Curation, Visualization. Budi Hermana: Conceptualization, Methodology, Supervision, Resources, Writing - Review & Editing.

## Declaration of Competing Interest

The authors declare no competing financial interests or personal relationships that could have appeared to influence the work reported in this study.

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