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Numerical Simulation of Ethanol Glycol –Air Two-Phase Flow Mixture Using COMSOL Multiphysics

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Index Terms

Two-phase flow, Mini channel, liquid-gas interface (Ethanol Glycol and Air), COMSOL Multiphysics 5.2.

Abstract

Two-phase flows involving volatile organic liquids such as ethanol glycol are utilized in combustion, fuel atomization, spray cooling, and chemical process engineering. Numerical investigations of the reaction between liquid ethanol glycol and air employed a two-phase flow interface to model interface dynamics, with phases simulated using COMSOL Multiphysics 5.2 software. These simulations included volume fraction of fluid (VOF) distributions, velocity fields, and temperature in Kelvin. With in the temperature range of 280 to 380 K, a minimal increase in heat capacity is observed, rising from 2300 J/K to around 2700 J/K at the same temperature, while the dynamic viscosity (eta(T)) diminishes from 0.65 Pa·s to around 0.05 Pa·s. The density approximates 1130 kg/m³ at lower thermal conditions and around 1060 kg/m³ under elevated thermal conditions. It additionally denotes specific heat capacity measured in (J/kg·K), which exhibits slight variation, and thermal conductivity quantified in (W/m·K) ranging from 0.244 to 0.262 W/m·K.The thermal conditions of the simulation were maintained within the interval of 280–380 K. It has been observed that prior to the manifestation of any intricate flow phenomena over time, the volumetric ratio converges towards the region occupied by liquid ethanol glycol at an approximate velocity of 1.7 m/s.

المحاكاة العددية لمزيج التدفق ثنائي الطور من الإيثانول جليكول والهواء باستخدام برنامج COMSOL Multiphysics

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الكلمات المفتاحية

تدفق ثنائي الطور، قناة صغيرة، واجهة سائل-غاز (إيثانول جلايكول وهواء)، COMSOL Multiphysics 5.2.

الملخص

أتستخدم التدفقات ثنائية الطور التي تحتوي على سوائل عضوية متطايرة، مثل الإيثانول جليكول في الاحتراق ورش الوقود وتبريد الرذاذ وهندسة العمليات الكيميائية. تمت الاستعانة بالدراسات العددية لتفاعل الإيثانول جليكول السائل مع الهواء من خلال واجهة تدفق ثنائية الطور لنمذجة ديناميكيات تلك الواجهة، حيث تم استخدام برنامج COMSOL Multiphysics 5.2 لمحاكاة الأطوار. شملت هذه المحاكاة توزيعات الكسر الحجمي للسوائل، وحقول السرعة، ودرجات الحرارة بالكيلفن. في مدى درجات الحرارة بين 280 و380 كيلفن، تم ملاحظة زيادة طفيفة في السعة الحرارية، حيث ارتفعت من 2300 جول/كيلفن إلى حوالي 2700 جول/كيلفن عند نفس درجة الحرارة، بينما انخفضت اللزوجة الديناميكية (η(T)) من 0.65 باسكال.ثانية إلى حوالي 0.05 باسكال.ثانية. الكثافة تبلغ حوالي 1130 كجم/م³ في الظروف الحرارية المنخفضة وحوالي 1060 كجم/م³ في الظروف الحرارية المرتفعة. يشير هذا أيضًا إلى السعة الحرارية النوعية المقيسة بوحدة (جول/كغم·كيلفن)، التي تظهر تباينًا خفيفًا، والتوصيل الحراري المُقاس بوحدة (واط/متر·كيلفن) والذي يتراوح بين 0.244 و0.262 واط/متر·كيلفن. تم الحفاظ على الظروف الحرارية للمحاكاة في نطاق 280-380 كيلفن. تمت ملاحظة أنه قبل حدوث أي ظواهر تدفق معقدة مع مرور الزمن، تتجه النسبة الحجمية نحو المنطقة التي يشغلها الإيثانول جليكول السائل بسرعة تقارب 1.7 متر/ثانية.

1. INTRODUCTION

Many engineering systems depend on two-phase flows, where liquids and gases interact such as the fine mist in spray devices, fuel bursts in injectors, or precise mixtures in microfluidic and chemical processing equipment. Grasping how these flows move and interact is essential for predicting the movement of the mixture, pressure changes, heat transfer, and overall system efficiency much like observing steam flowing from a hot pipe gives insight into what will happen next. Mixtures containing ethanol alcohols, especially those based on glycols, are now commonly used due to their versatile thermal properties, easy solubility, and wide range of cooling applications [1].

Ethanol glycol, in particular, has become popular among renewable energy producers because it burns cleanly, produces minimal soot and grey smoke, and can be sustainably produced over time. To improve combustion efficiency, lower emissions, and optimize fuel injection, it is important to understand how ethanol glycol and air behave as they separate, evaporate, and swirl into a fine mist during injection. However, because of the many interacting components and mixing phases, analyzing and precisely controlling the flow behavior remains challenging [2].

The high accuracy simulation of a two-phase flow of ethanol and air is complex, as temperature changes may distort the results. Ethanol glycol has thermophysical properties different from those of conventional hydrocarbons; it retains more heat after evaporation, and its vapor pressure.

The effect of temperature greatly influences the change. In the present research, there is a wide range of speeds and time values varying from 0.2 to 155 seconds. It is vital to use advanced techniques in order to simulate the process of interaction between distributed liquid droplets and the neighboring gas in conditions of propagation of a thermal pulse, molecules' movement, turbulent vortex formation, and chemical reaction initiation. Lately, the software COMSOL Multiphysics 5.2 proved that it is possible to employ the finite element method for studying. Using COMSOL Multiphysics 5.2 helps specialists investigate and visualize their models in numerous spheres of science such as electromagnetics, mechanical, fluid, acoustic, and chemical engineering processes occurring in real time. The software COMSOL Multiphysics 5.2 uses Euler-Lagrange spray models, VOF approaches, and multiphase mixing design in order to simulate two-phase flow and control the complex phenomena of multiphase processes, including interfacial tension, variations of viscosity and density, and segregation rate of ethanol glycol and air flowing inside the box.

This study focuses on the interaction between two-phase ethanol glycol streams and air, examining the key processes that underlie the movement and evaporation of droplets and how the mixture is formed. This framework focuses on the modelling of non-miscible or partially miscible ethanol glycols and air mixtures, given their prevalence in mechanical applications. It uses a multifluid approach with a separate set of equations for each phase and a mono-fluid approach with the transport equations for each component being interrelated. The first is closer to physical reality, as it separates the transport of the various components and follows the drag, weight, speed, pressure, viscosity, specific thermal capacity and thermal capacity temperature of the various stages, respectively 250 to 380 K.

The goal of analyzing these findings is to improve fuel injection and combustion systems that use ethanol glycol, either as a primary fuel or in combination with the strong smell of alcohol in lab air. In order to close modeling gaps, it is essential to compare two-component ethanol-glycol-air formulations. This is because there aren't many studies that fully describe interface and phase considerations. We plotted the ethanol-glycol-air boundary with a smooth, constant surface tension that was free of oscillations or ripples using the two-phase flow interface in COMSOL software. Next, we used the Navier-Stokes equations [3].

The motion of a two-phase ethanol-glycol-air combination is simulated and studied in this paper using COMSOL Multiphysics5.2 software. The goals of the study are to simulate interface behavior, investigate different flow regimes, and understand how mixture properties, including temperature, fluid velocity, density, and specific heat, influence flow patterns in real-world situations. The study's findings advance our knowledge of liquid-gas interactions in ethanol-glycol-air systems and open the door to better industrial processes that handle these mixes. This paper's benchmark simulation can be used as a benchmark for assessing COMSOL Multiphysics 5.2simulations in this domain.

2. METHODOLOGY

2.1 Comsol Simulation

calculations and analyses of the geometric and solid area of a mixture of air, ethanol, glycol (liquid)and air had used laminar flow, are first performed, with the dimensions have been of being 1.9 cm in length and 1 cm in width, at a time of range (0,0.2,150). The COMSOL Multiphysics 5.2 software is then used to process these equations, as shown below.

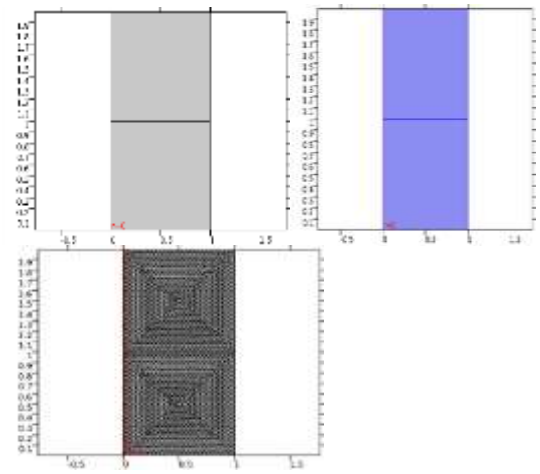


Figure 1. (a,b) 2D geometry of block
(c) Meshed block

3. MATERIAL PROPERTIES

TABLE I. FLUIDS PROPERTIES ENTRY TO THE COMSOL SIMULATED MODEL MEASURED FROM THE LABORATORY EXPERIMENTAL WORK.

Property	Ethanol glycol (Liquid)	Air (Gas)
Density	~789 kg/m³	~1.2 kg/m³
Viscosity	1.2×10^{-3} Pa·s	1.8×10^{-5} Pa·s
Surface tension (ethanol–air)	~0.022 N/m	—

In this study, the laminar two-phase flow physics has needed to provide the results with COMSOL 5.2 Multiphysics software.

3.1 Ethanol

The figure 2(a) below illustrates the hypothesis that temperature (in Kelvin) affects the viscosity of a liquid, while the following figure 2 (b) shows the effect of temperature on specific heat capacity. Viscosity decreases to between 0.0005 and 0.0018 Pa·s as the temperature increases from 250 to 380 K, indicating an inverse relationship. After this point, the figure 2(a) shows a plateau, meaning that viscosity changes slowly with increasing temperature. In contrast, viscosity rises sharply from 0.006 to 0.0018 Pa·s between 270 and 280 K. Specific heat capacity increases almost linearly with temperature between 275 and 380 K, reaching a minimum of 2300 J/kg·K and a maximum of 2900 J/kg·K. This means that specific heat capacity can also change, rather than simply increasing and decreasing, with temperature.

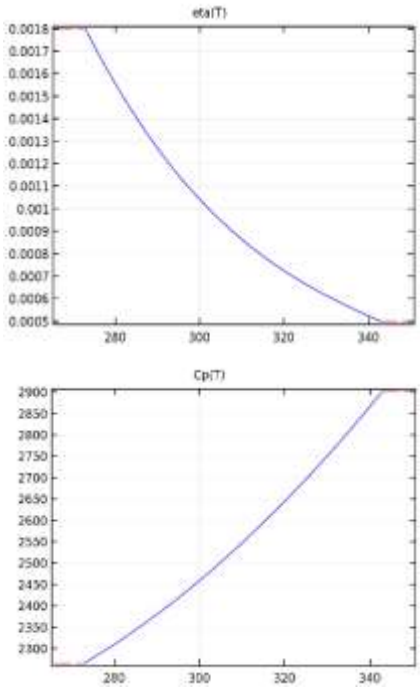


Figure 2. (a) Dynamic viscosity
(b) Heat capacity

3.2 Ethanol Glycol

Figure 2(a) has changed temperature influences the viscosity of ethanol glycol and its heat capacity. The temperature on the x-axis is measured in Kelvin and varies between 280 and 380 K. In Figure 3(b), the vertical plot represents the heat capacity (Cp) and viscosity of ethanolic glycol (eta(T)). With the increasing temperature, heat capacity also increases from about 2300 J to 2700 J/K. A second graph at the same temperature depicts. The value of the heat capacity of ethanol glycol rises with rising temperatures of the liquid. Simultaneously, the value of the dynamic viscosity (η(T)) falls from roughly 0.065 Pa to around 0.005 Pa. Heat capacity grows steadily with respect to temperature, and the formula is nearly homogeneous. In the graph, the heat capacity of ethanol glycol appears to be constant across this range of temperatures. Tapre, R. W. (2023) had stated Microfluidic mechanics is a field of study that focuses on the behavior of fluids at the microscopic level and its applications in various industries. Fluid flow characteristics are influenced by the properties of the materials.

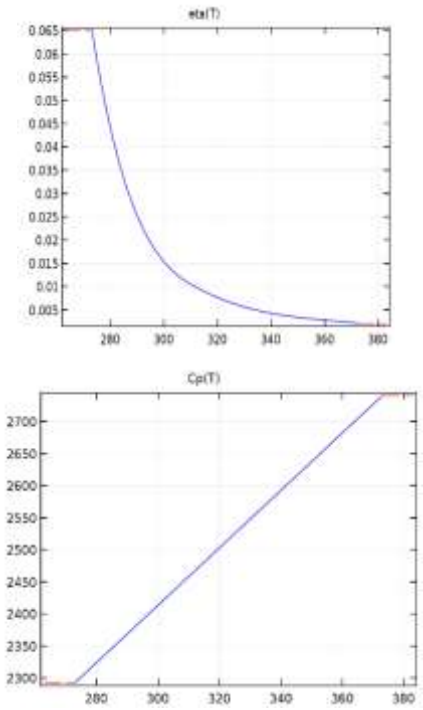


Figure.3 (a) Dynamic viscosity
(b) Heat capacity

4. LAMINAR TWO-PHASE FLOW, LEVEL SET

The method known as separation was initially created by Usher and Serbian in a research project by [4]. Separation is an essential tool in both theory and application. The fundamental concept of this approach involves isolating fluids, like ethanol, from the atmosphere. The figure 3 demonstrates a configuration for a COMSOL Multiphysics 5.2 simulation, possibly using software such as COMSOL Multiphasic, for a laminar two-phase flow problem using a level-group approach. The diagram has been interpreted as follows: Computational domain: The image shows a defined two-dimensional rectangular modeling area with values ranging approximately from -0.5 to 1.5cm on the x-axis, and from 0.1 to 1.9cm on the y-axis. Liquid phases: The area occupied by one or both of the immiscible liquids (ethanol glycol liquid and air) have represented by the blue-shaded region. In order to describe processes like droplet formation, capillary action, or free surface flows, the setup shows that Navier-Stokes equations for laminar flow solved concurrently with the level set equation to track the interface motion over time. The main use of the schematic is for geometric considerations.

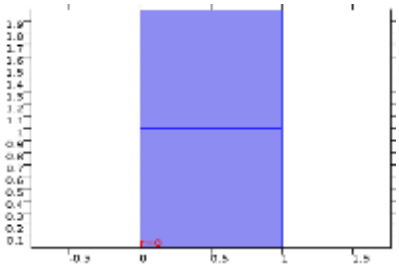


Figure 4. laminar two-phase flow

5. LAMINAR FLOW EQUATIONS SIMULATION

The COMSOL Multiphysics 5.2 software was employed for the numerical implementation, involving the solution of the Navier-Stokes equations in conjunction with a level-set function. The level-set function, represented as follow.

5.1 Fluid Properties 1 Equations

In our research paper, we examine some equations that have used the numerical model for simulating the two-phase flow of ethanol glycol, and air in COMSOL Multiphysics 5.2. where u present the mixture velocity of 1.7 m/s., ρ present density1130 kg/m³ at lower thermal conditions and around 1060 kg/m³, and μ present viscosity rises sharply from 0.006 to 0.0018 Pa·s, g presents the gravity and the surface tension force is present at ~0.022 N/m by F_{st}. The Mini channel **below** study [5].

$$\rho\frac{\partial u}{\partial t}+\rho(u.\nabla)u=\nabla.[-\rho I+\mu(\nabla u+(\nabla u)T)]+\rho g+Fst+F \quad (1)$$

The hydrodynamic behavior and velocity field of the immiscible two-phase system are governed by the incompressible Navier-Stokes equation [6].

$$\nabla.\mathrm{U}=0 \quad (2)$$

laminar or low-Reynolds flow to avoid turbulence modeling, no-slip boundaries, and isothermal conditions unless heat transfer is specified; for two-phase mixtures like ethanol glycol (liquid) and air (gas), constant surface tension and negligible mass transfer are often applied [7].

$$\frac{\partial\phi}{\partial t}+u.\nabla\phi=\gamma\nabla.\left(\epsilon\mathrm{Is}\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right),\phi=phils \quad (3)$$

Where: ϕ is the phase arena dimensionless changeable, γ movement, the mixture properties such as viscosity and density are the function of volume fraction ∇ (volume fraction = 1). The air and ethanol glycol volume fraction are ∇ = (1 + ϕ)/2 and V0 = (1- ϕ)/2 respectively. Over the interface viscosity and density are computed for the two-phase model [8,9,10].

$$n.u = 0 \quad (4)$$

$$-\nabla.\mathrm{N}\phi = 0 \quad (5)$$

$$\sigma(\mathrm{n} - n_{int}\cos(\theta\mathrm{w}))\eth = -F_{fr} = \frac{\mu}{\beta}u \quad (6)$$

Driving Force Surface Tension and Contact Angle. Surface Tension σ The force per unit length at the liquid-gas interface. Deviation from Equilibrium The term. Calculates the difference between the actual interface orientation and the static equilibrium defined by the young equation.

Driving Stress: This "uncompensated" force acts at the contact line to drive the fluid motion until it reaches its equilibrium contact angle.

5.2 Level Set Equations

Equations in level phase function as listed below [7].

$$\frac{\partial\phi}{\partial t} + u.\nabla\phi = \gamma\nabla.\left(\epsilon\mathrm{Is}\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right), \phi = \mathrm{phils2} \quad (7)$$

6. RESULTS

6.1 Study 1/Solution 1

This dataset, meant for testing the revolution 2D and other two- and three-dimensional parts, is discussed in sections. Some essential considerations were made in each case to determine the distinctions between the lengths of the simulations ranging from 0 to 2cm during the periods of (0, 0.2, and 150) with relative tolerance of 0.2. Two-phase flows can be discussed using ethanol glycol and air in COMSOL Multiphysics 5.2. It has now been possible to conduct this calculation in COMSOL Multiphase 5.2, thus providing data on two-phase flows with ethanol glycol and air. This work solves the fluid flow, heat transfer, and diffusion equations, as well as the actual kinetic equations and the analysis that makes them one. To account for surface tension in multiphase flows, the Navier-Stokes equations—used for the flow of incompressible viscous fluids—were specially modified. The first equation of the laminar flow simulation equations provides an example of its use in finding the mole fraction [11].

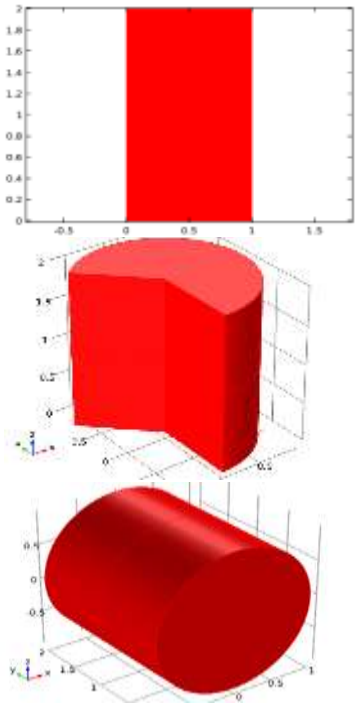


Figure .5 (a) Data set: Study 1/Solution 1
(b) Data set: Revolution 2D 1
(c) Data set: Revolution 2D 2

Visualizing internal variables hidden within two- and three-dimensional geometry is key. This is crucial for understanding phenomena like fluid interfaces and velocity profiles in COMSOL Multiphasic 5.2 and two-phase flow simulations.

Figure 6 shows plane sections of the cross-section (1, 2). A two-dimensional, orthogonal, and three-dimensional coordinate system is used, which is useful in complex fluid dynamics where internal events influence the simulation results. In two-phase flow, the contact surface between ethanol, glycol, and air is often represented by planes or a phase-domain function. This reveals the fluid flow velocity through the cross-section. The distribution on the plane is shown, and the scale labels on the axes (0.5, 0, -0.5, etc.) represent the model's coordinates and dimensions.

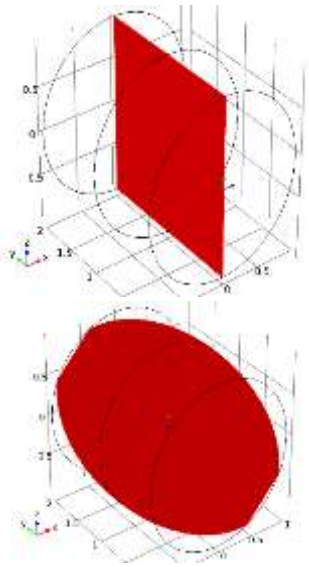


Figure 6. (a) Cut Plane 1
(b) Cut Plane 2

6.2 Volume Fraction (Tpf)

Figure 7 has shown a simulation from COMSOL Multiphysics 5.2 illustrating the volume ratio of a liquid in a two-phase flow model. the interface between two immiscible liquids. A value (the green area in the image) indicates that the cell is fully formed, while a value of 0 indicates that it is entirely composed of ethanol glycol. The interface between the two liquids (along the horizontal line in the image) ranges between 0 and 1.

this refers to the physical model or simulation interface used to track the interface between the two liquids over time. The green area (volume fraction = 1) after applying its equivalent indicates the location of the ethanol glycol liquid. The air and ethanol glycol volume fraction are $\nabla = (1 + \phi)/2$ and $V0 = (1- \phi)/2$ respectively. Over the interface viscosity and density are computed for the two-phase model have used equation 3 [7].

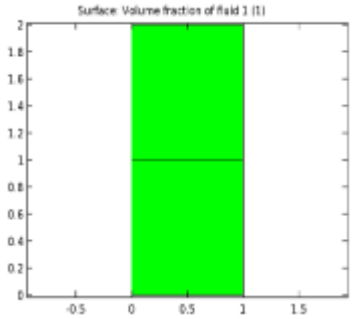


Figure 7. Surface: Volume fraction of fluid 1

6.3 Velocity (Tpf)

The velocity (m/s) has shown in Figure 8 involving the solution of the Navier-Stokes equations in conjunction with a level-set function. That velocity set as initial conditions are independent of the fluid flow dynamics within the system. The ethanol glycol velocity in (m/s) has represented by the color on this surface graph. The major area is completely covered in a consistent green hue, which corresponds to a speed of about 1.7 m/s. Before any complex flow phenomena such as turbulence, separation, or mixing occur, the ethanol is likely to proceed through the main channel at a constant, predetermined inlet velocity, as indicated by the uniformity of color. The volume percentage of ethanol glycol is visually represented by a crisp horizontal line. Across the center of the green region, marking a boundary between two regions.

This line likely represents the boundary at which the volume fraction of ethanol glycol transitions from 1 (air1) to 0 (ethanol glycol 2). This setup is typical of the initial conditions in multiphase flow simulations using methods such as the level group method or the phase field method to define the boundaries of ethanol glycol. The figure 8 has shown a system at the beginning of the simulation where a liquid moves at a constant speed, and two distinct phases (ethanol and air) meet at a sharp horizontal boundary; results are close to those obtained by Nouri, W. (2020).

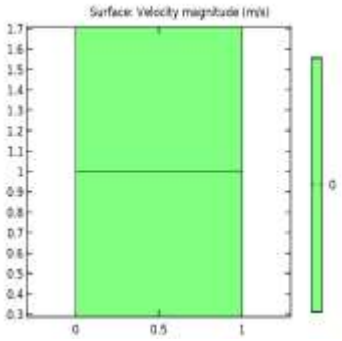


Figure 8. Surface: Velocity magnitude (m/s) Contour: Volume fraction of fluid

6.4 2D Plot Group two-dimensional

A two-dimensional thermal diagram depicting a "surface: level set variable (1)"in (Fig .9) is displayed in the picture. This kind of visual depiction is frequently used to show the geographical distribution of ethanol glycol over a certain area in scientific and engineering simulations, frequently within the COMSOL Multiphysics 5.2 program. The colors in this two-dimensional visual representation show the value of the "level set variable" at various spatial locations, which are

indicated by the x and y axes. From blue (low values for the ethanol glycol -air mixture, close to 0) to red (high values for ethanol, close to 1), the color bar on the right connects numerical values to particular hues. "Level set variable" describes a numerical technique for depicting the borders or interfaces between several ethanol glycol -air interaction regions or phases. Whereas the blue areas show locations where the variable's value is near to 0, the red areas show areas where the variable's value is close to 1. A barrier or contact that the simulation tracks is shown by the abrupt changes between the two phases, ethanol glycol (liquid) and air (gas), which are shown in red and blue correspondingly, as this study simulates. Figure 9 illustrates Grzybowski and Mosdorf's simulation of bubble generation under comparable conditions [12].

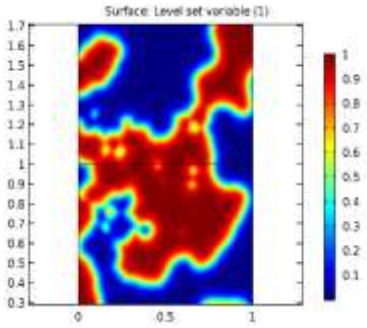


Figure 9. Surface: Level set variable

6.5 3D Plot Group three dimensional

The distribution of the level set variable for the ethanol glycol–air two-phase flow inside the cylindrical region is shown in Figure 10. The ethanol glycol phase is represented by the red region, while the air phase is represented by the blue region. The liquid-gas interface tracked by the level set approach is identified by the narrow transition region between the two phases. The outcomes show successful interface capturing and a distinct phase separation. Numerical stability and successful application of the Level Set formulation in COMSOL Multiphysics are indicated by the smooth interface profile. Simulation: A pioneering study of the explaining three-dimensional dimensionality reduction plots has been carried out Coimbra, D. B., Martins [13].

The boundary follows the curve where the value of φ reaches 0.5, marking the boundary between the two media. Instead of appearing in a sudden jump, the boundary forms a thin transition layer where the values of φ blend seamlessly. In simulations, the calculations are kept stable, and real-world changes are simulated, with properties fading gradually rather than changing abruptly. Contour lines centered at approximately 0.1 to 0.9 in φ define the transition zone, revealing how the ethanol glycol concentration changes across the cylinder curve. These images allow you to observe the change in motion using level array variables.

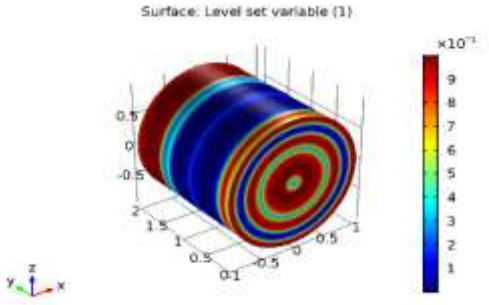


Figure 10. Surface: Level set variable

7. CONCLUSION

This study aimed to simulate the operation of a two-phase system (ethanol glycol and air) using COMSOL5.2 software. A two- and three-dimensional model was developed using phase separation in a liquid-gas mixture, and the model was validated through experimental measurements.

The temperature range of 280–380 K. On the other hand, the dynamic viscosity (eta(T)) decreases from approximately 0.065 Pa·s to approximately 0.005 Pa·s, while the heat capacity appears to increase slightly from approximately 2300 J/ K to approximately 2700 J/ K at the same temperature. Density is represented, which begins at roughly 1130 kg/m³ at low temperatures and drops to roughly 1060 kg/m³ at high temperatures, and also displays the thermal conductivity in watts per kilometer (W/m•K), with values ranging from roughly 0.244 to 0.262 W/m•K.

Ethanol glycol may become more effective at transferring heat as it warms, according to the rise in thermal conductivity with temperature. Since ethanol glycol's capacity to conduct heat increases with temperature, this property is crucial in heat transfer applications where it is utilized as a coolant or heat transfer fluid.

The simulation showed a temperature range of 280–380 K. It indicated that the volumetric fraction is concentrated at the ethanol glycol liquid position, corresponding to a velocity of approximately 1.7 m/s, before any complex flow phenomena appear over time.

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