Numerical Analysis of Supercritical Fluids in 2D Chamber

Rathan Babu Athota[1](✉), Sai Puravardhan Korani[1], Polaiah Bojja[2], Surya Hevanth Nimmala[1], and Prem Kumar Bet[1]

[1] Department of Aeronautical Engineering, Institute of Aeronautical Engineering, Dundigal, Hyderabad, Telangana 500043, India
`{a.rathanbabu,20951A2164,20951A2192,20951a2152}@iare.ac.in`
[2] Department of Computer Science and Information Technology, Institute of Aeronautical Engineering, Dundigal, Hyderabad, Telangana 500043, India

Abstract. Supercritical fluids have been recognized as a working media to improve thermal efficiencies in power cycles and for energy conversion, and have been used or selected as the working fluids in engineering fields, and so on. To better understand the interesting characteristic or abnormal behavior's of supercritical fluids, most valuable research works (including experimental results and numerical studies) have been performed and documented. The main purpose of this project is interaction of two supercritical fluids in a chamber. It focuses on research in which, two supercritical fluids are mixed and observed and CFD analysis is performed which focuses on particle traces and mixture analysis. The following processes, (a) Model development Schemes and calculations, (b) CFD Analysis, have been carried out. The two Supercritical Fluids used for the process are Supercritical Carbon dioxide (SCO2) and Supercritical Methane (SCH4). Here, we study the interaction of these two supercritical fluids by mixing them in a tank, for which the Volume of Fluids (VOF) method, under the Multiphase model, was used and results were obtained, in the ANSYS Fluent software. The simulations have shown the interaction of the fluids.

Keywords: Supercritical fluids · Mixing · Interaction · CFD · Multiphase · VOF · Carbon-di-oxide · Methane

1 Introduction

1.1 Supercritical Fluids

Any substance at a temperature and pressure higher than its Critical point is referred to as a supercritical fluid. Example: The supercritical fluids sCO_2 and sH_2O are commonly employed. A substance's liquid and vapour phases become indistinguishable at a specific temperature and pressure, which is known as CRITICAL CONDITION. SUPERCRITICAL FLUIDS (SCF) are substances that are above the critical point [1]. At 31.1 °C, the critical point for CO_2 is 7.38 MPa. Water has a critical point of 22.06 MPa at 373.95 °C [2].

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Table 1: Comparison of gases, supercritical fluids and liquids.

	D***ensity(kg/m2)***	V***iscosity (µṖạ.ṡ)***	Diffusivity(mm^2/s)
Gases	1	10	1–10
Critical fluids	100–1000	50–100	0.01–0.1
liquids	1000	500–1000	0.001

Table 2: Critical properties of various solvents (Reid et al., 1987)

S***olvent***	Molecular weight ***g/mol***	Critical Temperature ***k***	Critical pressure ***MPa(atm)***	Critical density ***g/cm3***
Carbon di oxide (CO_2)	44.01	304.1	7.38(72.8)	0.469
Water (H_2O)	18.015	647.096	22.064(217.775)	0.322
Methane (CH_4)	16.04	190.4	4.60(45.4)	0.162

Many features of a supercritical fluid can be “fine-tuned” by small changes in pressure or temperature near the critical point, resulting in significant variations in density. Supercritical fluids can be found in the atmospheres’ other gas giants Jupiter and Saturn, as well as the terrestrial planet Venus and, most likely, Uranus and Neptune. On Earth, supercritical water can be found in black smokers, which are a form of underwater hydrothermal vent [3]. In the laboratory we use organic solvents by taking common supercritical fluids CO_2 and water as a supercritical-fluids and they are often used as in the process of decaffeination, power generation and extraction methods (Table 1).

In the recent years, researchers have lot more focused on the Supercritical Fluid (SCF) technology, due to the superior inherent properties such as higher diffusivity, lower viscosity, etc., than that of a liquid, and much stronger solvent power, and so on, than that of a gas, that they exhibit. Now a days, we can see that SCFs are being involved in many industrial applications such as extraction of oils, regenerative cooling in engines, decaffeination, dry cleaning, mass transfer processing and food processing, etc. (Table 2).

1.2 Properties of Supercritical Fulids

SCFs have physical and thermal properties that fall somewhere between that of a pure liquid and that of a gas, hence they’re also known as ‘compressible liquids’ or ‘dense gases’.

The following are the changes in attributes for a SCF:

As we study the properties and the behaviour of SCF we can observe it has a Good solvating power, Surface tension reduction whereas it can also shows Low viscosity (10–100 times less than liquid) and Compressibility qualities similar to that of a gas.

As the Densities that are similar to liquids (100–1000 times greater than gases) they have Higher diffusivities than liquids as a result, they have a lot of penetrating power [6].

1.3 Applications of Supercritical Fluids

The SCF's are widely used in Industries and in Chemical reactions Impregnation and colouring Nano and micro particle production Supercritical fluid extraction These are also helpful for Supercritical fluid decomposition Dry-cleaning.

Some other applications are for Supercritical fluid chromatography, Biodiesel production Enhanced oil recovery, carbon capture and storage Enhanced geothermal system. Refrigeration Supercritical fluid in power generation is mostly used in the Industrial sectors. In aircraft, supercritical fluids are used for cooling, power generation, nuclear engineering, and many more applications [7].

2 Literature Survey & Problem Identification

A detailed experimental procedure adopted in this investigation is presented in this chapter.

Supercritical fluids (SCF) are presently used in a variety of industrial processes and offer a wide range of possible new uses. Dry powder coating, aerogel manufacture, nanotechnology, pharmaceutical crystallization and particle formation, and many more powdered goods are examples of applications relating to product design and formulation of high-quality materials.

The use of SCF fluid as an extracting solvent or mobile phase aids species in the separation and extraction of chemical components of interest from samples or products such as coffee. Baron Cagnior made the first sighting in 1892 and Green coffee was decaffeinated with CO_2 in 1970.

The SEDSTM process considers two possible precipitation mechanisms: drop dispersion followed by mass transfer between the droplet and SCF, and micromixing with SCF. The main mechanism is determined by the miscibility of SCF and the solvent. Mixing on different sizes, dispersion in multiphase systems, mixing and production of super-saturation, followed by quick nucleation and growth stages, are all part of the anti-solvent precipitation process. Mixing becomes difficult due to the rapidity of nucleation [11].

The solubilities of benzoic acid in supercritical CO2 were tested using pure co-solvents, ethyl acetate or ethanol, and combination co-solvents, ethyl acetate + ethanol, at a co-solvent concentration of 2 mol percent (molar ratio 1:1). The experiments were carried out at three distinct temperatures: 308.15, 318.15, and 328.15 K, with pressures ranging from 8.0 to 23.0 MPa (In the experimental procedures done by York and Hanna, 1996). The crossover stress of the blended co-solvent machine was originally predicted to be 14.5 MPa. The improvement in combined cosolubility solvent is less than that of ethanol, yet it is still significant [12].

Reynolds number and math of the miniature channel chooses the development of vortex. Thus, the rectangular furrows were utilized for this reason [13].

Athulya A.S, Miji Cherian R, India have done major instigations on “CFD Modelling of Multi phase flow T junction”.

The SEDS (result enhanced dissipation by supercritical fluids) fashion is distinguished by three most important features (York and Hanna, 1996). They also stated that the material present in multiphase flow is often identified as belonging to the primary or secondary phases. The primary phase is defined as the phase that is continuous or enveloping the secondary phase. The secondary phase is the material that is distributed throughout the primary phase [14].

Jerzy Bałdyga, Dominik Kubicki, Boris Y. Shekunov, Keith B. Smith have performed investigations on “Mixing effects on particle formation in supercritical fluid”. In this paper, the writer stated that supercritical liquids applied either as solvents or enemies of solvents offer benefits that permit a control of molecule size dissemination and morphology. Actual properties of SCF, for example, thickness and solvency can be effortlessly tuned inside a large number of handling conditions by shifting both tension and temperature [15].

3 Scope and Objective

We can conduct different experiments with various no. of supercritical fluids to know their change in properties and how can we use those and make applications with them. The supercritical fluids we are using are Supercritical Carbon Dioxide and Supercritical Methane. We have used the two different solvers to analyse the properties they exhibit when they interact and mix with one other. With this we can learn their change in properties.

4 Methodology

In this Section, the methodology is presented. Firstly, the Geometry and Meshing are discussed. We also the briefed about the grid or mesh generation in this section.

4.1 Geometry and Meshing Process

The geometry and the meshing were created using the software ANSYS 19.2R. In this we used fluent solver to find the CFD analysis of mixing and interaction of supercritical fluid. Since we have to do multiphase flow of two different fluids which are above the critical state (supercritical state), we need to make the geometry with two inlets into the chamber, so that the interaction and mixing of fluids can be done We have made the geometry by considering the different research papers and textbook. We made sure that the geometrical Design of the chamber should not affect the action between the fluids [16].

A. Boundary Conditions

In which the pressure of the chamber was set as 80 atm which is higher than the critical pressures of both the Carbon dioxide and Methane, therefore they exhibit supercritical nature in such conditions. The temperature was set at 310K which is greater than the critical temperature value of both these fluids. The Boundary conditions were provided for both the fluids. The inlet velocity (v) was given as 2 m/s i.e., it is the velocity at which both these fluids enter the chamber via the inlet. The volume of fluids (VOF) is taken in multiphase flow. Hence the fraction is in mixture phase which in volumetric fraction is given as 1 in the same phase and given 0 in opposite fluid selected. n this way, the necessary inputs, in terms of boundary conditions and operating were provided to run the simulation.

B. Meshing

With the settings of the surface mesh grid adjusted to appropriate values and the first structured mesh could be generated. Later, an unstructured mesh is obtained for the geometry, basing at the inlets and edge proximities. Sizing and edge refinement was done as part of obtaining a finer mesh, which helps in obtaining a more converging and better solution. As we can observe Fig. 1. The meshing of the chamber and shown in Table 3.

Results and Discussions

Table 3. Details of Mesh

Mesh Method	Hybrid
Element Size	5mm (Face Sizing)
Proximity	Face and Edge enabled
Nodes	48450
Elements	47853

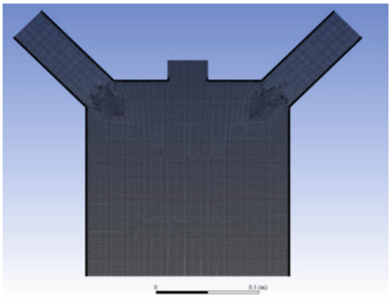

Fig. 1. Mesh

Upon the undertaking of this project, the study of the mixing and interaction between the supercritical fluids was carried out to investigate and obtain the results of doing the research which will help in understanding the behavior of the fluids. As discussed earlier, the fluids used as part of this research are carbon dioxide (CO_2) and methane (CH_4). We have understood until now that both these fluids i.e., CO_2 and CH_4 exhibit various properties when they are dealt separately and are therefore used for various purposes, due to the numerous advantages they offer. But the focus of this study was more or less towards understanding whether the advantages these fluids offer remain the same, or will there be any changes that can be observed in them, when these fluids are subjected to high pressures and temperatures, which are above the critical values of the pressures and temperatures of these fluids, and after the mixture and interaction in between both of them. Also, the focus was also more on the particle traces that can be observed while mixing. In this section, the changes that have occurred in the properties of the fluids after mixing in supercritical states can be observed and also the particle traces in terms of the fluid's respective phases and volume fractions can be seen.

4.2 Phases

See Figs. 2, 3 and 4.

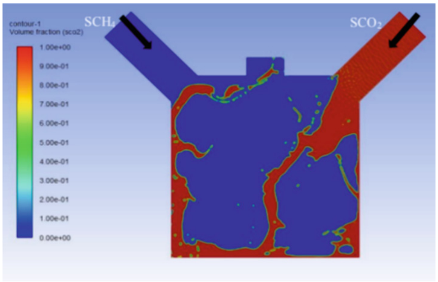

Fig. 2. Phase Contour of SCO_2 and SCH_4 Mixture

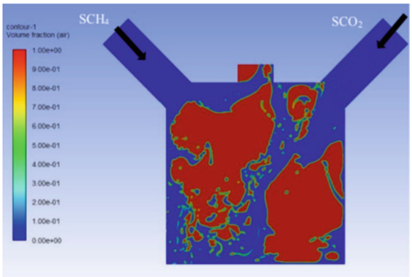

Fig. 3. Volume Fraction of SCH4

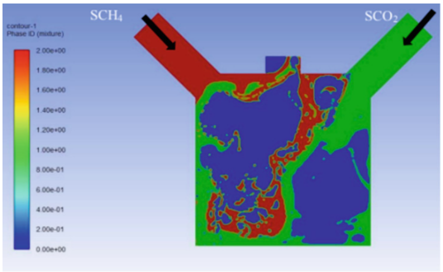

Fig. 4. Volume Fraction Contour of SCO_2

4.3 Pressure and Velocity

The total pressure contour of the mixture phase can be hereby observed at Fig. 5. With the help following contour figure. It can be noticed that there is a variation in the values of the total pressure that can be observed in the contour. The maximum value of the pressure reached is observed to be as close as 1.6e + 06 Pa. For the most of the part of the contour, the value of the total pressure is observed to be as close to as 8.02e + 05Pa.

It can be noticed that there is a variation in the values of the velocity that can be observed in the contour. The maximum value of the velocity reached is observed to be as close as 37.8 m/s. For the most of the part of the contour, the value of the velocity is observed to be as close to as 8 m/s. These observations can lead us to the understanding

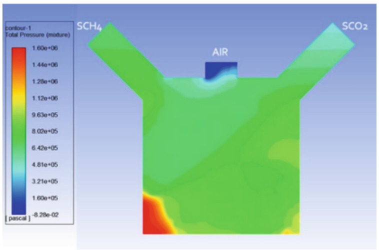

Fig. 5. Total Pressure Contour of mixture

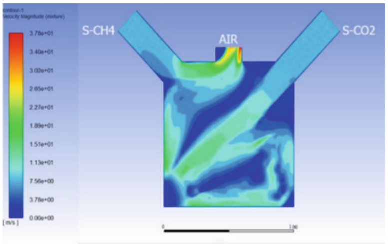

Fig. 6. Velocity Contour of mixture

of the behavior of these supercritical fluids and the variation in the advantages or disadvantages that these fluids can offer when in mixture phase to that of their own phases which is given above in Fig. 6.

4.4 Thermal Conductivity

The Thermal conductivity contours of the mixture phase, SCO_2 phase and SCH_4 phase can be hereby observed. The variation in the Thermal conductivity of the fluids in each phase is clearly seen. We can observe that there is a difference in the maximum possible Thermal conductivity obtained for both the fluids in separate phases vs when in the mixture phase. As we can see in Fig. 7 the contour of mixture differences.

The maximum Thermal conductivity of SCO_2 in Fig. 9 its own phase can be observed to be as close as 1.45e-02 w/m-k, the maximum Thermal conductivity of SCH_4 can be observed in Fig. 8 to be as close as 3.32e-02 w/m-k, whereas the value of the maximum Thermal conductivity of the mixture phase can be observed to be as close as 3.32e-02

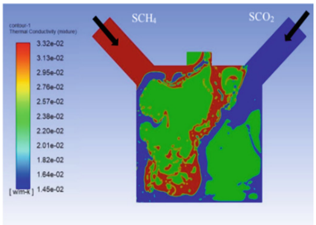

Fig. 7. Thermal Conductivity Contour of mixture

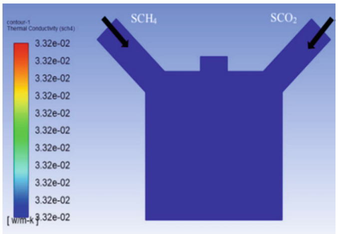

Fig. 8. Thermal Conductivity Contour of SCH4

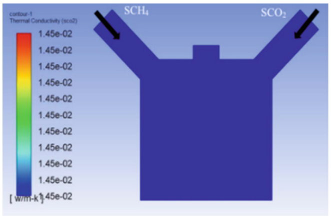

Fig. 9. Thermal Conductivity Contour of SCO_2

w/m-k. From the above observations, it can be noticed that there is a variation in the values of the Thermal conductivity of the fluids when in separate phases vs when in mixture phase.

5 Conclusion & Future Work

The purpose of this project is to investigate the supercritical fluids mixing in a chamber and to identify the change of effects in the fluid properties. For this experiment the best suited numerical simulation that can be used is Volume of fluid approach. Using the VOF approach the interaction and mixing of supercritical fluid is captured such as for velocity, pressure, thermal conductivity. And we have examined the results of all the simulations and approached to this conclusion. We can see that the velocity, thermal conductivity had taken a rise in the mixture phase when compared against its own individual values. With this, we have come to the conclusion that the properties experience a change while they are in the mixture phase and these properties of the mixture phase supercritical fluids can be taken help of and be used for wide range of applications, by performing further research and experimentation in this very domain. As we are trying to learn about mixing chamber at different pressures and results can be shown in future work and we can give better explanation about subcritical dropping of pressure.

Study on molecular viscosity, specific heat compressibility factor and density will be done in future work, as we are trying to approach this analysis by using OPENFOAM source in future analysis.

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