# $\begin{array}{c} \textbf{Transient Simulation of a Sub- to Transcritical} \\ \textbf{C0}_2 \ \textbf{Refrigeration} \quad \textbf{Cycle} \end{array}$

by Michael Garces de Gois

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Supervisor: Mr Robert T. Dobson

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## **ABSTRACT**

The purpose of this project is to develop a numerical transient simulation model of the CO<sub>2</sub> refrigeration cycle containing a capillary tube as expansion device. A design procedure for CO<sub>2</sub> refrigerators is also developed; which makes use of a steady-state capillary tube model for acquiring the initial design of the capillary tube, and uses the transient simulation program to determine the low pressure side internal volume and validate the complete design of the refrigerator. Using this design procedure a CO<sub>2</sub> refrigerator was designed, built and then tested to validate the simulation model developed. The project was conducted at the Department of Mechanical and Mechatronic Engineering at the University of Stellenbosch.

A literature review on the history of refrigeration, the vapour-compression refrigeration cycle, the transcritical CO<sub>2</sub> refrigeration cycle, refrigerant properties, CO<sub>2</sub> properties, and a comparison of refrigerant performance was done as background to the use of CO<sub>2</sub> as refrigerant. Furthermore, literature review of an alternative expansion device, the vortex tube, was included, but found not practical for implementing with CO<sub>2</sub> which behaves more like a real gas and not an ideal gas. Lastly, theory on the development of the one-dimensional CFD finite volume method in terms of a general variable is shown. This provides background to the development of discretised conservation equations for the simulation model.

The transient model developed is capable of predicting transient operation from stand-still starting conditions through to steady-state conditions. The model makes use of well-known pipe friction and heat transfer correlations. Furthermore, it makes use of the real gas equation of state for CO<sub>2</sub> from Span and Wagner (1996). Moreover, the model determines whether the flow is single or two-phase and then calculates the appropriate properties. Lastly, it has the whole refrigerant circuit, from compressor outlet back to compressor inlet, as the simulation domain.

The simulation results for the pressure and temperature distributions show the transient behaviour at start-up. The transient and steady-state results also agree fairly well with the experimental results. The steady-state pressure graphs are as expected and the constant evaporation temperature is a confirmation that the model approximates real life operation quite well. In conclusion, the results show that the simulation model is a useful tool for designing and understanding capillary tube CO<sub>2</sub> refrigeration cycles. Future work involves developing a non-adiabatic compressor model and models for alternative expansion devices to be included in the current refrigerator simulation model.

## **OPSOMMING**

Die doel van hierdie projek is om 'n numeriese oorgangsfase-simulasie-model van 'n CO<sub>2</sub> verkoelingstelsel met 'n haarbuis as uitbreidingstoestel te ontwikkel. 'n Ontwerp prosedure vir CO<sub>2</sub> yskaste word ook ontwikkel; wat gebruik maak van 'n bestendige toestand haarbuis model vir die verkryging van die aanvanklike ontwerp van die haarbuis, en maak gebruik van die oorgangsfase-simulasie program om die lae druk kant se interne volume te bepaal en die geldigheid van die volledige ontwerp van die yskas te bevestig. Deur die toepassing van hierdie ontwerp prosedure is 'n CO<sub>2</sub> yskas ontwerp, gebou en dan getoets om die simulasie program wat ontwikkel is te valideer. Die projek is voltooi by die Departement van Meganiese en Megatroniese Ingenieurswese aan die Universiteit van Stellenbosch.

'n Literatuuroorsig oor die geskiedenis van verkoeling, die damp-samedrukkings verkoelingsiklus, die transkritiese CO<sub>2</sub> verkoelingsiklus, koelmiddel eienskappe, CO<sub>2</sub> eienskappe, en 'n vergelyking van koelmiddel prestasie is gedoen as agtergrond vir die gebruik van CO<sub>2</sub> as koelmiddel. Verder is 'n literatuuroorsig van 'n alternatiewe uitbreidingstoestel, die vortex buis, ingesluit, maar daar is gevind dat hierdie toestel nie praktiese is vir die implementering met CO<sub>2</sub> nie; omdat CO<sub>2</sub> eerder as 'n werklike en nie 'n ideale gas optree nie. Laastens word die teorie oor die ontwikkeling van die een-dimensionele numeriese vloeidinamika eindige volume metode in terme van 'n algemene veranderlike getoon. Dit bied agtergrond tot die ontwikkeling van die gediskritiseerde behoudsvergelykings vir die simulasie model.

Die ontwikkelde oorgangsfase-model is in staat om die oorgangsfase te voorspel van die rustende begintoestand tot by die bestendigetoestand. Die model maak gebruik van bekende pyp wrywing en hitte-oordrag korrelasies. Verder, maak dit gebruik van die werklike gas toestandsvergelyking vir CO<sub>2</sub> van Span en Wagner (1996). Nog verder, bepaal die model of die vloei enkel- of twee-fase is, en bereken dan die geskikte eienskappe. Laastens, dit het as die simulasie domein die hele koelmiddel kringloop vanaf die kompressor uitlaat terug na die kompressor inlaat.

Die simulasie resultate vir die druk- en temperatuurverspreidings wys die gedrag van die oorgangsfase vanaf begin toestand. Die oorgangsfase en bestendigetoestand resultate stem redelik goed ooreen met die eksperimentele resultate. Die bestendigetoestand drukgrafieke is soos verwag, en die konstante verdampingstemperatuur is 'n bevestiging dat die model werklike werking baie goed benader.

Ten slotte, die resultate toon dat die simulasie model 'n nuttige instrument is vir die ontwerp en begrip van haarbuis CO<sub>2</sub> verkoelingsiklusse. Toekomstige werk

behels die ontwikkeling van 'n nie-adiabatiese kompressor model en simulasie modelle vir alternatiewe uitbreidings toestelle wat in die huidige yskas-simulasie model geïmplementeer kan word.

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# **TABLE OF CONTENTS**

LIS	T OF	FIGURE	S	x
LIS	TOF	TABLES	<b>3</b>	xii
NO	MENC	LATUR	E	xiii
1.	INTR	ODUCT	ION	1
	1.1.	Objecti	ives	2
	1.2.	Motiva	tion	3
2.	LITE	RATURE	E REVIEW AND THEORY	4
	2.1.	The Hi	story of Refrigeration	4
	2.2.	Theore	etical Vapour-Compression Refrigeration Cycle	6
	2.3.	Carbor	n Dioxide (CO <sub>2</sub> ) Transcritical Refrigeration Cycle	7
	2.4.	Refrige	erant Properties	7
		2.4.1.	Ideal Properties of a Refrigerant	8
		2.4.2.	Properties of Carbon Dioxide	8
		2.4.3.	Refrigerant Comparison	9
	2.5.	The Vo	ortex Tube as an Alternative Expansion Device	11
		2.5.1.	Experimental Studies	11
		2.5.2.	Analytical and Numerical Studies	13
		2.5.3.	Geometrical Properties of the Vortex Tube	13
		2.5.4.	Thermo-Physical Parameters	17
	2.6.	The Fir	nite Volume Method	17
3.	DET	ERMININ	NG THE THERMODYNAMIC STATE	23
	3.1.	CO <sub>2</sub> Eo	quation of State from Span and Wagner	23
	3.2.	Satura	ted Property Determination	25
	3.3.	Determ	nining Single Phase and Two-Phase Properties	26
		3.3.1.	Determining Single Phase Properties	27
		3.3.2.	Determining Two-Phase Properties	28
		3.3.3.	Deciding whether the Fluid is Single Phase or Two-F	Phase. 31
4.	TRA	NSIENT	SIMULATION PROGRAM OF THE CO <sub>2</sub> REFRIGI	ERATION
CY	CLE			33

	4.1.	General Model Assumptions	33
	4.2.	Initialising the Simulation Domain	33
		4.2.1. Defining Geometric Properties of the Simulation Domain	33
		4.2.2. Initial Conditions for the Simulation Domain	35
	4.3.	Boundary Conditions for the Simulation Domain	36
	4.4.	Updating to the New Time-Step	38
	4.5.	Heat Transfer and Friction Definitions	38
	4.6.	Determining the Properties of Water	41
	4.7.	Discretisation of Equations of Change Applied to Control Volumes	42
		4.7.1. Discretisation of the Conservation of Mass	43
		4.7.2. Discretisation of the Conservation of Energy	44
		4.7.3. Discretisation of the Conservation of Momentum	45
	4.8.	Algorithm for Simulating a Refrigeration Cycle	46
5.	REF	RIGERATOR DESIGN	49
	5.1.	Compressor Selection	49
	5.2.	Internal Volume of High Pressure Side	49
	5.3.	Capillary Tube Design using a Steady-State Capillary Tube Simulat Model	
	5.4.	Internal Volume of Low Pressure Side	53
	5.5.	Heat Exchanger Designs	54
	5.6.	Final Design of Refrigerator	55
6.	EXPE	ERIMENTAL SETUP	56
	6.1.	Thermocouple Calibration	56
	6.2.	Experimental System Layout	57
	6.3.	Experimental Procedure	58
7.	SIMU	ILATION SETUP	60
	7.1.	Initial State of the Simulation Domain	60
	7.2.	Boundary Conditions and External Heat Exchangers	61
	7.3.	Grid Independence	61
	7.4.	Simulation Domain Geometry Properties	62
8.	SIMU	ILATION RESULTS	63
	Q 1	Transiant Simulation Posults	63

	8.2.	Steady-State Results
9.	EXPE	RIMENTAL VERSUS SIMULATION RESULTS 71
10.	OTHE	ER EXPERIMENTAL RESULTS76
11	DISC	USSION OF RESULTS77
12.	CONC	CLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK 79
13.	REFE	RENCES 81
API	PENDI	X A: SAMPLE CALCULATIONS84
	A1:	Sample Calculations for an Ideal CO <sub>2</sub> Refrigeration Cycle with an Ideal Work Recovering Expansion Device
API	PENDI	X B: Property Function Codes for CO <sub>2</sub> 87
	B1:	Function to Calculate the Single Phase Properties at a Given Density and Temperature
	B2:	Function to Calculate the Saturated Properties at a Given Temperature
	B3:	Function to Calculate the Single Phase Properties at a Given Density and Specific Internal Energy
	B4:	Derivatives Used in the Formulation of the Two-Phase Function 91
	B5:	Function to Calculate the Two-Phase Properties at a Given Density and Specific Internal Energy
	B6:	Function to Calculate the Thermal Conductivity
	B7:	Function to Calculate the Dynamic Viscosity
	B8:	Function to Calculate the Properties at a Given Density and Specific Internal Energy
API	PENDI	X C: TRANSIENT SIMULATION PROGRAM97
	C1:	Main Program Code of the Transient Simulation Model 97
	C2:	Program Code to Assign Initial Conditions of the Simulation Model . 98
	C3:	Program Code to Update Variables for the New Time-Step 106
	C4:	Program Code to Solve the Three Conservation Equations 106
API	PENDI	X D: COMPRESSOR PRODUCT DATA117
API	PENDI	X E: STEADY-STATE CAPILLARY TUBE SIMULATION MODEL 118
۸DI	DENIDI.	Y F: THERMOCOLIPLE CALIBRATION 121

APPEN	DIX G: EXPERIMENTAL APPARATUS	122
G1:	Embraco EK6210CD Compressor	122
G2:	Pressure Gauges	122
G3:	B.I.C.I.SA-5500 Water Pump	123
G4:	Hailea HS-28A Water Chiller	124
G5:	Agilent 34970A Data Acquisition/Data Logger Switch Unit	125
G6:	Efergy Energy Monitoring Socket	126

# **LIST OF FIGURES**

Figure 1: Vapour-compression refrigeration cycle	. 6
Figure 2: CO <sub>2</sub> refrigeration cycle	. 7
Figure 3: Ideal CO <sub>2</sub> refrigeration cycle operating at 258 K and 303 K	. 9
Figure 4: Counter-flow vortex tube	11
Figure 5: Tangential inlet nozzles	15
Figure 6: Control volume for tube fluid flow	18
Figure 7: Notation used in the control volume discretisation	19
Figure 8: Phase diagram for CO <sub>2</sub>	31
Figure 9: Program logic to determine the properties of CO <sub>2</sub> at a given dens and specific internal energy	
Figure 10: Basic refrigeration cycle for simulation	34
Figure 11: Tube-in-tube thermal resistance diagram	38
Figure 12: Control volume description	42
Figure 13: Density-based algorithm for solving compressible flow	48
Figure 14: Steady-state capillary tube model	51
Figure 15: Refrigerator final design	55
Figure 16: Thermocouple 1 - calibration curve	57
Figure 17: Experimental system	57
Figure 18: Compressor control unit (left) and measuring equipment (right)	58
Figure 19: Initial state of the simulation domain: (a) temperature, (b) pressure (c) density, (d) vapour quality	
Figure 20: Pressure distribution at 150 ms for grid independence study	61
Figure 21: Control volume length distribution	63
Figure 22: Transient pressure development	64
Figure 23: Transient temperature development	65
Figure 24: Transient velocity development	66
Figure 25: Transient mass flow rate development of: (a) simulation domain, (compressor	٠,
Figure 26: Transient development of: (a) evaporator heat absorption rate, (b) g cooler heat rejection rate	
Figure 27: Transient vapour quality development	68
Figure 28: Steady-state results for the distribution of: (a) pressure, (temperature, (c) velocity, (d) vapour quality	٠,

igure 29: Steady-state pressure drop for: (a) HP side, (b) capillary tube, (c) LF ide70
igure 30: Comparison of pressure development72
igure 31: Comparison of compressor inlet and outlet temperature
igure 32: Comparison of evaporator (a) inlet temperature, (b) cooling load 73
igure 33: Comparison of gas cooler cooling section (a) steady-state emperature distribution, (b) heat transfer rate
igure D1: EK6210CD product data117
igure G1: Embraco EK6210CD Compressor122
igure G2: Swagelok pressure gauges123
igure G3: B.I.C.I.SA-5500 water pump123
igure G4: Hailea HS-28A water chiller124
igure G5: Agilent 34970A Data Acquisition/Switch Unit
igure G6: Efergy energy monitoring socket

# **LIST OF TABLES**

Table 1:	Comparative refrigerant performance per kilowatt of refrigeration 10
Table 2:	Work recovering device versus normal throttling device 19
	Relations of the thermodynamic properties to the dimensionles tz function $\phi$
Table 4:	Tube details of the high pressure side
Table 5:	Tube details of the low pressure side
Table 6:	Details of the outer tubes of the heat exchangers
Table 7:	Comparison of experimental and simulation results
	Steady-state experimental results for different water inlet temperature
Table F1	: Thermocouple calibration equations12

## **NOMENCLATURE**

A Cross-sectional area [m<sup>2</sup>]

Specific Helmholtz energy [kJ/kg]

 $A_{inlet}$  Inlet area of the first control volume [m<sup>2</sup>]

a Coefficient variable

 $C_f$  Skin friction factor

c Speed of sound [m/s]

 $c_P$  Specific heat capacity at constant pressure [kJ/(kg K)]

 $c_v$  Specific heat capacity at constant volume [kJ/(kg K)]

D Diameter [m]

D<sub>h</sub> Hydraulic diameter [m]

Di Inner diameter [m]

Do Outer diameter [m]

F Convection variable

f Function; Vector of function values; Length ratio variable

g Specific Gibbs energy [kJ/kg]

h Specific enthalpy [kJ/kg]

ht Heat transfer coefficient [W/(m² K)]

J Matrix of derivatives

k Loop variable for control volumes [-]

Conductivity [W/(m K)]

L Length [m]

m Mass [kg]

 $\dot{m}$  Mass flow rate [kg/s]

N Number of variables/control volumes [-]

Compressor speed [rpm]

Nu Nusselt number [-]

P Pressure [kPa]

*P<sub>s</sub>* Vapour/saturation pressure [kPa]

Pr Prandtl number [-]

 $\dot{Q}_{ht}$  Heat transfer rate [W]

R Specific gas constant [kJ/(kg K)]

R Thermal resistance [K/W]

Re Reynolds number [-]

r Radial direction/length [m]; Stretch ratio [-]

S Source term

 $S_C$  Constant part of source term

 $S_P$  Part of source term that depends on the variable value

s Entropy [kJ/(kg K)]

Temperature [K]

t Time [s]; Coefficient variable

u Specific internal energy [kJ/kg]

 $u_x$  Given specific internal energy [kJ/kg]

V Volume [m³]

 $V_{comp}$  Displacement volume of the compressor [m<sup>3</sup>]

 $V_{system}$  Volume of the system [m<sup>3</sup>]

Velocity [m/s] v Vector of unknowns x Axial direction/length [m] Greek Void fraction [-] α Relaxation factor for velocity [-]  $\alpha_v$ Pressure drop [kPa]  $\Delta P$ Time step size [s]  $\Delta t$  $\Delta V$ Infinitesimal volume [m<sup>3</sup>] Infinitesimal axial length [m]  $\Delta z$ Reduced density [-] δ Isentropic efficiency [-]  $\varepsilon_{isen}$ Volumetric efficiency [-]  $\varepsilon_v$ Fluid dynamic viscosity [Pa s] μ Perimeter [m] 80 General variable; Dimensionless Helmholtz energy [-] Density [kg/m<sup>3</sup>] Given density [kg/m<sup>3</sup>]  $\rho_{\chi}$ Inverse reduced temperature [-] τ Shear stress due to wall friction [Pa]  $au_{rz}$  $\theta$ -direction/angle [rad] Specific volume [m³/kg] υ

## **Subscripts**

CO<sub>2</sub> Carbon dioxide

Cu Copper

c Critical point value

comp Compressor

ct Capillary tube

 $ct_{in}$  Property at the capillary tube inlet

 $ct_{1ph}$  Single phase region of the capillary tube

 $ct_{2ph}$  Two-phase region of the capillary tube

comp\_gc Connecting tube between compressor and gas cooler

*Env* Environmental condition

e East face

ev Evaporator

ev\_IHX Connecting tube between evaporator and internal heat

exchanger

f Saturated liquid value

g Saturated vapour value

gc Gas cooler

gc\_IHX Connecting tube between gas cooler and internal heat

exchanger

IHX Internal heat exchanger

IHX\_comp Connecting tube between internal heat exchanger and

compressor

IHX\_ct Connecting tube between internal heat exchanger and

capillary tube

*i* i'th iteration; Inner tube/fluid

inlet Inlet condition of the simulation domain

 $in_{ev}$  Property at the inlet of the evaporator

*in\_comp* Inlet condition of the compressor

o Outer tube/fluid

outlet Outlet condition of the simulation domain

 $out_{ev}$  Property at the outlet of the evaporator

out\_comp\_isen Isentropic outlet condition of the compressor

P Node P; At constant pressure

tot Total

u Specific internal energy

w West face

z z-direction

 $\phi$  General variable

## **Superscripts**

n Exponent

o Old value; Ideal-gas part of dimensionless Helmholtz

energy

r Residual part of dimensionless Helmholtz energy

t Value at time t

 $\Delta t$  Time step

(over bar) Average value

\* Guess value

## Abbreviations/Acronyms

CFC Chlorofluorocarbon

CFD Computational fluid dynamics

COP Coefficient of performance

CO<sub>2</sub> Carbon dioxide

CV Control volume

E East node

GC Gas cooler

GWP Global warming potential

HP High pressure side

LP Low pressure side

ODP Ozone depletion potential

O<sub>2</sub> Oxygen

P Node P

TDMA Tri-diagonal matrix algorithm

W West node

1-D One-dimensional

## 1. INTRODUCTION

Refrigeration has become a highly essential part of modern day living; it is used to preserve food, cool drinks, maintain a comfortable environment through air conditioning, and to preserve organs for transplants in hospitals amongst other uses. Refrigeration comes in various forms, ranging from large to small refrigeration systems for use in supermarkets and households, respectively. According to Barthel and Götz (2012: 3) in 2012, an estimated 1.4 billion refrigerators and freezers were in use worldwide, with an average annual electricity consumption of 450 kWh each; this amounts to a staggering total annual consumption of 649 TWh.

The first refrigerators in the 1800's used refrigerants such as sulphur dioxide, ether, methyl chloride, carbon dioxide (CO<sub>2</sub>), as well as vinegar, wine, brandy, etc. (Briley, 2004). These systems were quite inefficient at first, but as time went on more knowledge of refrigerator construction methods and what properties the ideal refrigerant should exhibit became known. This led to the development of synthetic refrigerants such as Chlorofluorocarbons (CFC's). It was later discovered that these synthetic refrigerants cause ozone depletion and are partly responsible for global warming. Subsequently, their use was being phased out by the Montreal Protocol (1987), thus triggering renewed interest in designing refrigeration systems that work with safe alternative natural gases, such as CO<sub>2</sub>.

Improving refrigeration cycles has been the topic of many recent research papers, specifically CO<sub>2</sub> transcritical cycles (Sarkar, 2009). The cycle is called transcritical since it typically operates with the low pressure side at subcritical pressures and the high pressure side at supercritical pressures. pressure difference between these two sides causes a high irreversible friction loss when conventional expansion devices, such as capillary tube or expansion valve, are used. The urge to design and manufacture CO<sub>2</sub> refrigeration cycles with a higher COP has led to the development of simulation models to obtain a better understanding of the cycle's operating characteristics; to ascertain whether the high expansion loss through these expansion devices relates to the lower COP, and also to identify areas for improvement. The simulation models are also used to cut down on system design time and costs. It is of interest to see how the refrigeration cycle reaches steady state operation from standstill initial conditions. This has inspired the development of a transient simulation model of a system containing a capillary tube, capable of transient start-up from standstill subcritical conditions through to transcritical operation. The program uses a onedimensional computational fluid dynamics (1D-CFD) finite volume approach and has the whole refrigeration circuit, from compressor outlet back to compressor inlet, as the simulation domain.

This project presents an investigation into the literature of vapour-compression refrigeration cycles, CO<sub>2</sub> transcritical refrigeration cycles, and CO<sub>2</sub> properties; with the purpose of developing a transient simulation model of a CO<sub>2</sub> refrigerator and then constructing a CO<sub>2</sub> refrigerator capable of being used to validate the model. The project was proposed and supervised by Mr R.T. Dobson. This report discusses the objectives and motivation for the project, the literature review as background to the project, as well as literature on an alternative expansion device (the vortex tube) to investigate the possibility of increasing the COP of the refrigeration cycle. Also, it focuses on the use of the real gas equation of state from Span and Wagner (1996) to determine the thermodynamic properties of CO<sub>2</sub> for the control volume method. Furthermore, it discusses the development of the transient numerical simulation model capable of both single-and two-phase flow, the design and manufacture of a CO<sub>2</sub> refrigerator, the simulation and experimental results obtained, as well as a discussion of the results, conclusions and recommendations for future work.

## 1.1. Objectives

This project is aimed at developing a sub- to transcritical transient numerical simulation model of a CO<sub>2</sub> refrigeration cycle containing a capillary tube as expansion device. A literature review of refrigeration cycles and CO<sub>2</sub> properties was deemed necessary in providing the background to design and construct a CO<sub>2</sub> refrigeration system which can be used to experimentally validate the simulation's results. The objectives of the project are therefore:

- Perform a literature review of refrigeration cycles and CO<sub>2</sub> transcritical cycles.
- Investigate the properties of CO<sub>2</sub> in view of using it as refrigerant.
- Introduce literature of an alternative expansion device, the vortex tube, to investigate whether it can be used to increase the cycle's efficiency.
- Conduct a literature study on the control volume method, with the view to implementing it into the numerical simulation model.
- Describe the use of the real gas equation of state from Span and Wagner (1996) to determine the properties of CO<sub>2</sub> in a control volume, whether it's single - or two-phase.
- Develop discretised forms of the conservation equations and thus describe the development of the 1-D CFD finite volume transient simulation model of the refrigeration system.
- Construct a CO<sub>2</sub> refrigeration system with tube-in-tube external heat exchangers for the evaporator and gas-cooler. Water will be used in the outer tube since it allows for accurate measurement of heat addition or removal, also it allows for easier control of operating conditions for the refrigeration system.
- Perform experimental testing of the CO<sub>2</sub> refrigeration cycle built.

 Compare experimental and simulation results to validate the simulation model.

## 1.2. Motivation

Carbon dioxide, a by-product of all living breathing creatures, is part of the earth's natural atmospheric cycle. It is expelled by living creatures and by burning fossil fuels, absorbed by trees and plants during photosynthesis to again produce clean oxygen (O<sub>2</sub>). Carbon dioxide has a zero ozone depletion potential, a low global warming potential, is non-toxic, non-flammable, and along with other thermodynamic properties, such as high volumetric refrigerating capacity, greatly reduced compression ratio and high heat transfer properties, makes it a very attractive natural gas to use as refrigerant (Sarkar, 2010). The high pressures needed for heat rejection during operation has been the limiting factor in the past and hence its abandonment as a refrigerant. The higher pressure differential causes higher velocities in the expansion devices and thus higher irreversible friction losses through capillary tubes/expansion valves; thereby, leaving these CO<sub>2</sub> cycles with an inferior COP when compared to similar cycles using synthetic refrigerants.

A simulation model of the CO<sub>2</sub> refrigeration cycle may provide valuable information relating to its performance characteristics. Numerically simulating components of a refrigeration cycle, and then combining these single component results to have a complete solution for the refrigeration cycle, is what many researchers have done, such as Jensen (2008), Susort (2012), and Zhang et al. (2008). Most numerical models are steady-state models, and only few definitive transient models exist. A transient model will show how the system develops from start-up and how it reacts to a changing cooling load or operating conditions. Therefore, it was of interest to develop a fully transient numerical simulation model of the conventional vapour-compression CO2 refrigeration cycle, containing a capillary tube as expansion device. The program written allows transient start-up from resting initial conditions, i.e. from sub- to transcritical operation. It uses a 1-D CFD finite volume approach and has the whole refrigeration circuit, from compressor outlet back to compressor inlet, as the simulation domain. Furthermore, the program determines whether the flow is single - or two-phase. These features distinguish it from other simulation models This program provides a comprehensive design basis for CO<sub>2</sub> transcritical refrigeration systems, as it closely resembles real life operation of the refrigeration cycle without pre-assumptions made as to what type of flow is encountered in the different sections of the refrigeration cycle.

## 2. LITERATURE REVIEW AND THEORY

 ${\rm CO_2}$  refrigeration cycles operate at higher pressures than ordinary synthetic refrigerant refrigeration cycles, for example its critical temperature is 30.98 °C and critical pressure is 7.3773 MPa (Span & Wagner, 1996: 1520). Thus the cycle has to operate at supercritical pressures in order to achieve heat rejection to high ambient temperatures. The higher pressures needed to make the cycle operate is the major source of inefficiency in terms of higher compressor power consumption. The large pressure difference between high and low pressure side is normally accomplished by using a capillary tube or expansion valve between the gas cooler and the evaporator. These devices do not convert the energy associated with expansion into useful work, but rather waste the flow energy by dissipative resistance. Using a work recovering expansion device may improve the system's COP. This project's focus is developing a transient simulation model that can be used to describe and design  ${\rm CO_2}$  transcritical refrigeration systems; therefore it was deemed necessary to provide a literature review as background to the simulation model development.

## 2.1. The History of Refrigeration

The use of natural ice to provide cooling was one of the first forms of refrigeration. Stone Age cave men knew what ice was, but did not know it could be used to preserve food. There are references to the use of ice cellars as early as 1000 B.C. in an ancient Chinese collection of poems, called Shi Ching (Jordan & Priester, 1949: 3). They discovered that the use of ice in drinks improved its taste; consequently they cut ice in winter, insulated it with straw and chaff in ice cellars, and sold it during the summer. The Greeks and Romans had snow brought down from mountain tops and stored it in cone-shaped pits lined with straw and branches, and covered it with a thatched roof, earth or manure. The early Egyptians were the first to use evaporative cooling to cool water by placing it in porous jars on rooftops at sundown (Marsh & Olivo, 1979: 2). Another method used by the Indians, Egyptians, and Esthonians to cool water and even produce ice was by placing water in shallow, porous clay vessels, then leaving these overnight in holes in the ground. Evaporation of the water and heat radiation to the night sky accomplished the freezing. (Jordan & Priester, 1949: 3-4).

The use of ice and snow increased as people learned that it could be used to cool beverages and foods for enjoyment. In 1626 Francis Bacon attempted to preserve a chicken by stuffing it with snow. A Dutchman, called Anton van Leeuwenhoek, made a remarkable discovery in 1683 when he found millions of living organisms, now called microbes, in a clear water crystal with the microscope he invented. Scientists studied these microbes and found that they rapidly multiply in warm, moist conditions such as in food. This rapid

multiplication of microbes was recognized as the major source of food spoilage. It was found that these microbes do not multiply at temperatures below 50 °F (10 °C). Thus it now became apparent that food can be preserved by cooling. Since little was known at the time about how to create these low temperatures natural ice and snow were used. (Marsh & Olivo, 1979: 2).

Increased natural ice demands created new business opportunities for the harvesting and transporting of ice to big cities. Frederic Tudor (called the "Ice King") exploited this opportunity. His first cargo of 130 tons of ice arrived in the harbour of St. Pierre, Martinique, in 1806 on the ship called Favourite. This first venture made a financial loss, since ice was yet unknown to this part of the country. He later build an icehouse at St. Pierre and by the use of pine sawdust as insulation during the transportation of his ice cargoes, Tudor turned his idea into an extremely profitable business. He contracted for the cutting of ice in ponds and rivers throughout New England and shipped it to other parts of the world; West Indies, South America, Persia, India and the East Indies. By 1849 his cargoes totalled 150 000 tons of ice; and by 1864 he was shipping to 53 ports around the world. Tudor's ice business was the first large-scale venture in refrigeration. In the 1880's artificial ice making slowly replaced the use of natural ice. (Jordan & Priester, 1949: 3).

Dr. William Cullen was the first to study the evaporation of liquids in a vacuum in 1720; and in 1748 he demonstrated the first known artificial refrigeration at the University of Glasgow by letting ethyl ether boil in a partial vacuum (History of Refrigeration, 2015). Michael Faraday invented the absorption refrigeration cycle in 1820 when he discovered that he could use silver chloride and ammonia in a closed test tube to provide cooling. Silver chloride has a special characteristic that it absorbs the ammonia gas, similar to water in modern absorption refrigerators. When the silver chloride (with absorbed ammonia gas) in the one end of the tube is subjected to heat the ammonia vapour is released. This ammonia vapour is then cooled at the other end of the tube in a chilling agent to form ammonia liquid. The liquefied ammonia end can now be used to provide cooling (by absorbing heat); and in the process boil the liquid back into gas which is again absorbed by the silver chloride; then the whole process can be repeated. (Marsh & Olivo, 1979: 10).

One of the earliest recorded patents for a refrigerator was issued in Great Britain to Jacob Perkins, in 1834, an American. This refrigerator had a hand-operated compressor, a water-cooled condenser with a weighted valve at the discharge, and an evaporator contained in a liquid cooler. In 1851 the first American patent for an ice machine, designed to use compressed air as refrigerant, was granted to Dr. John Gorrie of Florida. (Jordan & Priester, 1949: 4-5). Within the next fifty years ice-makers were produced in the United States, France and Germany. Nearly everyone favoured natural ice, believing that artificial ice was unhealthy.

This superstition was soon overcome and refrigeration has improved considerably since then. (Marsh & Olivo, 1979: 2).

## 2.2. Theoretical Vapour-Compression Refrigeration Cycle

The vapour-compression refrigeration cycle is the most frequently used refrigeration cycle (Cengel & Boles, 2007: 291). It consists of four main components, as seen in Figure 1: a compressor, a condenser (or gas cooler in the case of a CO2 cycle), an expansion device such as a capillary tube or expansion valve, and an evaporator. The working fluid used in a refrigerator is called the refrigerant. Synthetic refrigerants are mostly used since they are specifically made to have the desired properties of a refrigerant, such as a high critical temperature at a relatively low pressure, a high latent heat of vaporization, low viscosity etc. The cycle operates as follows: The refrigerant enters the compressor as a saturated vapour and is compressed to a higher pressure (condenser pressure), and thus higher temperature. The exiting superheated refrigerant vapour now flows through the condenser coils where it rejects heat to the outside environment and condenses to a saturated liquid. It now enters the capillary tube or expansion device where its temperature and pressure drop considerably due to the throttling effect. Finally the cold two-phase refrigerant now flows through the evaporator coils where it evaporates (boils) by absorbing heat from the refrigerated environment. The cycle is completed as the refrigerant leaves the evaporator and re-enters the compressor. (Cengel & Boles, 2007: 291-292).

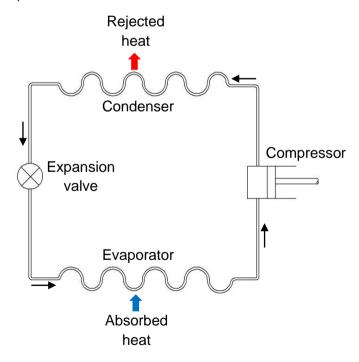


Figure 1: Vapour-compression refrigeration cycle

## 2.3. Carbon Dioxide (CO<sub>2</sub>) Transcritical Refrigeration Cycle

Figure 2 shows a basic CO<sub>2</sub> transcritical refrigeration cycle. It is similar to the conventional cycle discussed in section 2.2; the only difference is the replacement of the condenser with a gas cooler and the use of a different compressor suited for CO<sub>2</sub> refrigerant. It is called a gas cooler since it may, in certain circumstances, contain only supercritical gas as opposed to two-phase flow in a condenser. Furthermore, it operates at higher pressures due to CO<sub>2</sub>'s relatively higher pressure needed for the same temperature as compared to synthetic refrigerants, and hence it must be designed for this purpose. More information on the CO<sub>2</sub> transcritical cycle and modifications to the cycle can be seen in Sarkar (2010).

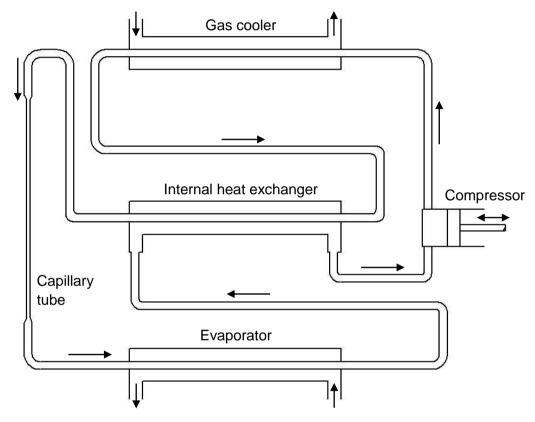


Figure 2: CO<sub>2</sub> refrigeration cycle

## 2.4. Refrigerant Properties

To select a refrigerant to use in a vapour-compression refrigeration cycle it is necessary to first identify the properties of the different refrigerants and to consider its application, whether for household refrigeration or large scale refrigeration. The desired properties of a refrigerant will be discussed, the properties of CO<sub>2</sub>, and finally a comparison is made between the different refrigerants.

## 2.4.1. Ideal Properties of a Refrigerant

A refrigerant is a substance that is able to easily absorb and reject a large quantity of heat usually through phase change. According to Trott and Welch (2000: 28) the ideal properties for a refrigerant are: a high latent heat of vaporization, high density suction gas, non-corrosive, non-flammable and non-toxic, a working range outside the triple point and critical temperature, compatibility with lubricating oil and component materials, reasonable working pressures that are not below atmospheric pressure nor too high, a high dielectric strength especially for hermetic compressors, low cost, environmentally friendly, and finally easy leak detection. Other properties include chemical stability at operating conditions, a high thermal conductivity and low viscosity (ASHRAE-Fundamentals, 2001: 19.1).

## 2.4.2. Properties of Carbon Dioxide

Carbon dioxide is a naturally occurring gas that is readily obtainable at low cost, non-toxic, non-flammable, has a low global warming potential (GWP), zero ozone depletion potential (ODP), and is compatible with most materials (Nellis & Klein, 2002). This has led to renewed interest in using CO<sub>2</sub> as a potential alternative to synthetic refrigerants. Carbon dioxide has a relatively low critical temperature of 30.98 °C. This low critical point allows for it to be used easily for carrying out technical processes within the transcritical or super critical region. In terms of thermodynamics, carbon dioxide serves as a well-known reference for a molecule with a strong quadruple moment and as a testing fluid for calibration purposes. (Span & Wagner, 1996). Carbon dioxide has a very high critical pressure of 7.3773 MPa, which makes it more challenging to use as a refrigerant, and also more inefficient in most circumstances due to higher expansion losses, through throttling expansion devices, than other refrigerants. The triple point temperature and pressure of carbon dioxide, is relatively easily obtainable. Due to the relative ease at which the triple point and critical point of CO<sub>2</sub> is reached, it is used frequently for scientific study of the processes that an element undergoes in these two extremes. Span & Wagner (1996) has done remarkable work at developing an equation of state for CO<sub>2</sub> that can be used from the triple-point temperature to 1100 K at pressures up to 800 MPa. This equation of state is in the form of a fundamental equation explicit in the Helmholtz free energy, which is a function of density and temperature only. It describes all necessary thermodynamic properties to within their experimental uncertainty, and a reasonable description even in the immediate vicinity of the critical region. The equation doesn't use any complex coupling to a scaled equation of state, thus making it very easily implementable within computer codes. (Span & Wagner,

1996). Therefore the equation of state from Span & Wagner (1996) was used to determine the properties of CO<sub>2</sub> in the refrigeration cycle simulation program written for this thesis.

## 2.4.3. Refrigerant Comparison

In order to choose the refrigerant for a particular application it is first necessary to compare the different refrigerant's performance per unit of refrigeration effect achieved. For this, an ideal refrigeration cycle is assumed that operates at the design temperatures of the study in hand. The use of an ideal cycle simplifies calculations and gives good initial insight into possible performance, but actual performance may be somewhat different. In most cases the assumptions are that the suction gas is saturated (1), the compression is adiabatic or at constant entropy (1-2), the heat rejection (2-3) and - absorption process (4-1) is isobaric with no pressure drop, the condenser fluid leaves as a saturated liquid (3), and the expansion process follows an isenthalpic throttling process (3-4). In this study the evaporator temperature is set at 258 K and condenser temperature is at 303 K. Figure 3 shows the ideal CO<sub>2</sub> cycle operating at these design temperatures.

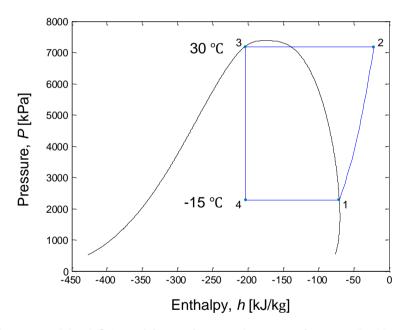


Figure 3: Ideal CO<sub>2</sub> refrigeration cycle operating at 258 K and 303 K

Table 1 shows the refrigerant performance per kilowatt of refrigeration for a few commercial refrigerants used as well as R-12 refrigerant. The data was calculated assuming the same ideal refrigeration cycle and design temperatures of 258 K ( $\approx$  -15 °C) for evaporation and 303 K ( $\approx$  30 °C) for condensation as described before.

Table 1: Comparative refrigerant performance per kilowatt of refrigeration

Refrigerant ASHRAE no.	Evapo- rator Pressure, MPa	Con- denser Pressure, MPa	Com- pression Ratio	Net- Refriger- ating Effect, kJ/kg	Refrig- erant Circu- lated, g/s	Specific Volume of Suction Gas, m <sup>3</sup> /kg	Com- pressor Displace- ment, L/s	Power Con- sump- tion, kW	Coefficient of Performance	Comp. Dis- charge Temp., K
R-744 (CO <sub>2</sub> )	2.281	7.189	3.15	133.25	7.50	0.0165	0.124	0.368	2.72	343
R-290	0.291	1.077	3.71	279.88	3.57	0.1542	0.551	0.211	4.74	320
R-410A	0.481	1.88	3.91	167.68	5.96	0.0542	0.318	0.227	4.41	324
R-12	0.183	0.745	4.07	116.58	8.58	0.0914	0.784	0.213	4.69	311
R-600a	0.089	0.407	4.60	262.84	3.80	0.4029	1.533	0.220	4.55	318
R-134a	0.164	0.770	4.69	149.95	6.66	0.1223	0.814	0.217	4.60	309
R-717 (Ammonia)	0.236	1.164	4.94	1102.23	0.91	0.5106	0.463	0.207	4.84	371

(Modified from ASHRAE-Fundamentals (2001: 19.8))

From the table above it is seen that the CO<sub>2</sub> cycle has a coefficient of performance that is somewhat lower than the rest for this operating case. However it has other advantageous characteristics such as the lowest compression ratio, the lowest specific volume of suction gas and also the lowest compressor displacement rate. The lower compressor displacement rate directly signifies that small compressors may be used. The use of small compressors simplifies design for such a high pressure operating environment. The COP of the system may be improved by exploiting the high pressure difference expansion process by using an alternative work recovering device such as a vortex tube or piston expander etc. For example, implementing an isentropic work recovering expansion device for the CO<sub>2</sub> cycle and using the recovered work to reduce compression power consumption it can be shown, ideally, that the COP may be improved to a value of 4.84 (sample calculations can be seen in Appendix A1). Table 2 illustrates how the cycle's performance would change in comparison to isenthalpic expansion with no work recovery.

Table 2: Work recovering device versus normal throttling device

Refrigerant ASHRAE no.	Evapo- rator Pressure, MPa	Con- denser Pressure, MPa	Com- pression Ratio	Net- Refriger- ating Effect, kJ/kg	Refrig- erant Circu- lated, g/s	Specific Volume of Suction Gas, m <sup>3</sup> /kg	Com- pressor Displace- ment, L/s	Power Con- sump- tion, kW	Coefficient of Performance	Comp. Dis- charge Temp., K
R-744 (CO <sub>2</sub> ) isenthalpic expansion	2.281	7.189	3.15	133.25	7.50	0.0165	0.124	0.368	2.72	343
R-744 (CO <sub>2</sub> ) isentropic expansion with work recovery	2.281	7.189	3.15	151.14	6.62	0.0165	0.109	0.207	4.84	343

The inclusion of a work recovering isentropic expansion device increases the net refrigerating effect; therefore, decreasing the mass flow rate and compressor displacement rate. The lower mass flow rate reduces the total compressor power consumption needed; furthermore the assumption that 100% of the work recovered is used by the compressor means that the compressor power is

drastically reduced. The lowered compressor power consumption translates to a significantly improved COP. The cycle's actual COP may be somewhat different; nonetheless, this serves as a good illustration of the potential for increasing the cycle's COP.

## 2.5. The Vortex Tube as an Alternative Expansion Device

It has been proposed by many that a vortex tube may be used as an alternative expansion device for refrigeration purposes (Sarkar, 2009 & 2010; Nellis & Klein, 2002; Mohiuddin & Elbel, 2014). The vortex tube, also called Ranque-Hilsch vortex tube, was first discovered by Ranque in 1933 and was later improved by Hilsch in 1947. It is a simple mechanical device with no moving parts that is capable of splitting a high pressure gas into two streams of lower pressure flows of different temperatures; one of higher total temperature than the inlet and one of lower total temperature than the inlet (Aljuwayhel et al., 2005). The vortex tube, as shown in Figure 4, consists of a long tube with tangential inlet nozzles near one end and a conical valve at the other end. Immediately to the left of the tangential inlet nozzles is a small hole called the cold orifice. The compressed gas enters the tangential inlet nozzles and is forced to produce a vortex or swirling motion to the inlet gas which spirals down the tube to the right of the inlet nozzles. The conical valve at the right end allows some of the outer annulus gas to exit and prevents the central portion from exiting. The central part of the gas flows in the reverse direction and exits through the left end cold orifice, creating a cold stream that's colder than the inlet gas stream. The outer annulus of gas that exits the right end, called the hot stream, is also considerably hotter than the inlet gas stream. (Singh et al., 2004). The physical method in which this so called "energy separation" occurs is still not completely understood, even after extensive research in this field.

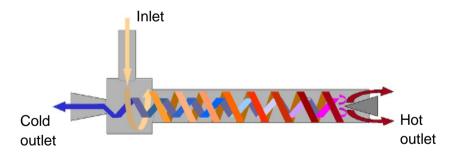


Figure 4: Counter-flow vortex tube (Vera, 2010)

## 2.5.1. Experimental Studies

Researchers have tried to explain what the physical reason is behind the temperature separation within the vortex tube since its existence in 1947. There is still no single encompassing theory that perfectly explains and predicts the

working principle of the vortex tube. Many have experimentally investigated the influence of the vortex tube's geometric properties on its performance. Eiamsa-ard and Promvonge (2007) provides a detailed review of the different researchers' results. The researchers did not all record the same or all the necessary variables, thus making it a nearly impossible task to compare their results. Geometric properties that were varied by researchers include tube diameter, inlet nozzle diameter, number of inlet nozzles, cold orifice diameter and hot outlet area. Other parameters that were also varied include inlet mass flow rate, inlet pressure, outlet pressure (most experiments were however done with the outlet being atmospheric pressure) and cold mass fraction (obtained by varying the hot outlet area).

Christensen *et al.* (2001) did an experimental study in using the vortex tube as an alternative expansion device in a  $CO_2$  transcritical refrigeration cycle. They found that the vortex tube produces an enthalpy separation, and therefore in an ideal gas resulted in a temperature separation. However, for the  $CO_2$  in the refrigeration cycle, which behaves more like a real gas, there is a small temperature split in certain circumstances and no split in temperature when the gas becomes two-phase during expansion. Their proof as to why this occurs is as follows:

Supposing that enthalpy h is a function of temperature T and pressure P, i.e. h=h(T,P), then the total differential of h is:

$$dh = \left(\frac{\partial h}{\partial T}\right) dT + \left(\frac{\partial h}{\partial P}\right) dP \tag{2.1}$$

Noting that  $\left(\frac{\partial h}{\partial T}\right)_P = c_P$  and using Maxwell's relations this can be written as:

$$dh = c_P dT + \left(v - T\left(\frac{\partial v}{\partial T}\right)\right) dP \tag{2.2}$$

For an ideal gas the last part is equal to zero (by substitution of ideal gas equation Pv = RT). i.e.:

$$v - T\left(\frac{\partial v}{\partial T}\right) = 0 \tag{2.3}$$

The remaining relation,  $dh = c_P dT$ , therefore means that a change in enthalpy directly signifies a change in temperature for an ideal gas. For a real gas this last part, equation (2.3), is not zero and therefore a change in enthalpy does not necessarily mean a change in temperature. Thus Christensen *et al.* (2001) concluded that the vortex tube would be of little use in a refrigeration cycle if

there is no means of separating the two phases and ensuring that the vortex tube remains in single phase operation.

## 2.5.2. Analytical and Numerical Studies

From the experiments many researchers have tried to develop a mathematical formula that would predict the outlet temperatures of the vortex tube, with very limited success. The formulas developed only worked for certain conditions such as outlet condition being atmospheric. Also the gas used in most instances is air. Furthermore, when the vortex tube geometry changed the formula no longer gave reasonable results, which leads to the belief that the working principle is not fully explained by the formula in question. Other attempts were to numerically simulate the vortex tube with CFD programs such as Fluent, StarCD etc. These programs do produce results that correlate well with the vortex tube's performance, however only if the gas which is used exhibits ideal gas behaviour; since most models used in CFD make use of an ideal gas relation for the state of the fluid.

## 2.5.3. Geometrical Properties of the Vortex Tube

Researchers have focused their efforts mainly on finding the optimal geometrical shape and properties of the vortex tube to give the required output which is either one of two: maximum temperature difference output or maximum cooling output. Uses for maximum temperature difference output include spot cooling and cryogenic cooling applications (Nellis & Klein, 2002) amongst others. Maximum cooling output is used mainly in refrigeration cycles, which is the topic of this project.

Through years of experimentation researchers have stipulated what they have found as the optimal design for a vortex tube. It is worth mentioning that all researchers haven't reached the exact same design parameters, some even contradicting each other's findings; thus it is very hard to choose which design advice one should follow. Another important consideration is that this vortex tube is intended to be used as an expansion device in a CO<sub>2</sub> refrigeration cycle in place of a capillary tube or expansion valve; which means that the vortex tube's input and output conditions vary according to the refrigeration cycle's operation. The CO<sub>2</sub> may be two-phase or close to saturation conditions which means that it behaves more like a real gas, in which case the vortex tube's efficiency improvement potential in the cycle is diminished. The refrigeration cycle's varying operating conditions might require a vortex tube with variable geometric capabilities within operation. A discussion of research results for the geometric properties of a vortex tube follows beneath. Note that these geometric properties were determined mostly by using air, which exhibits ideal gas behaviour, as working fluid.

## 2.5.3.1. Length to Tube Diameter Ratio

The length of tube has a significant influence on the performance of the vortex tube since it provides room for the swirling flow to develop and ultimately separate into two streams of flow, one being colder and one hotter than the inlet flow. Yilmaz et al. (2009) reported from their literature survey that the length of tube significantly influences its performance, the optimum L/D ratio is a function of other geometrical and operational parameters, and that L/D beyond 45 has no further effect or improvement on performance. Saidi and Valipour (2003) have experimented and found that the optimum range of L/D ratio is between 20 and 55.5. Singh et al. also found that the length of tube has no effect when it's increased beyond 45 diameters long (Singh et al., 2004). Eiamsa-ard and Promvonge (2007) found that L/D should be around 20 for optimum performance. Others still have suggested that L/D higher than 10 is sufficient.

Behera *et al.* (2005) stipulated that maximum temperature separation is obtained by lengthening the tube up to where the stagnation point is furthest from the inlet nozzle and just within the length of the tube. Thus from all the research it is evident that depending on what inlet pressures the vortex tube is subjected to the length needed would be different. Also Promvonge and Eiamsa-ard (2005) show that an insulated vortex tube gives higher efficiency and temperature separation; therefore a shorter tube may be used. Considering all above, a length of 20D or more would be a good design criterion for a vortex tube, it would in most cases mean that the stagnation point lies within the vortex tube and thus maximum swirl is used to allow higher energy separation to be achieved.

#### 2.5.3.2. Inlet Nozzle Diameter/Area

The inlet nozzle is a crucial component of the vortex tube. It creates the vortex flow (swirling flow) within the vortex tube which causes the energy separation. In order to achieve the best performance of the vortex tube, the Mach number at the exhaust of the inlet nozzle should be as high as possible, the pressure loss over the inlet nozzle should be as low as possible, and the momentum flow at the exhaust should be as large as possible (Yilmaz et al., 2009). The nozzle outlet diameter should be not too small otherwise it would cause a higher pressure drop over it, but it should also not be too large, in which case it would fail to produce a high velocity flow and hence not a strong enough vortex. Both these extremes would cause a low diffusion of kinetic energy and thus a low temperature separation. The inlet nozzle should be located as close as possible to the cold outlet orifice to yield high tangential velocities near the orifice and hence high temperature separation (Eiamsa-ard & Promvonge, 2007).

#### 2.5.3.3. Vortex Tube Diameter

The diameter of the vortex tube is an important parameter in the design since it is the tube's inner wall which ultimately causes the swirling motion of the incoming tangential flow. Past researchers have experimented with vortex tube diameters as low as 4.4 mm and as high as 800 mm (Eiamsa-ard & Promvonge, 2007). Larger diameter vortex tubes are generally used for gas liquefication and separation (Yilmaz *et al.*, 2009).

According to a CFD simulation of a vortex tube done by Aljuwayhel et al. (2005), reducing the diameter from 2 cm to 1.5 cm led to an increase in cold temperature drop by 1.2 K, and increasing the diameter from 2 cm to 3 cm decreases the cold temperature drop by 6.5 K. These simulations were run with the same inlet pressure and conditions, thus it is evident that the larger the diameter of the tube, the lower the angular velocity of the flow is, and thus the less energy separation occurs. Depending on the inlet pressure, the smaller the diameter of the vortex tube is the higher the energy separation is up to a certain diameter. If the diameter is made too small it would produce considerably higher back pressure due to the high density of gas in the tube, and therefore, the tangential velocities between the periphery and the core would not differ much while high axial velocities are encountered in the core region as the gas tries to escape. The low tangential velocities cause low diffusion of kinetic energy which also means low temperature separation. With that said, a very large tube diameter would also result in lower overall tangential velocities both in the periphery and in the core, and hence lower temperature separation. (Aljuwayhel et al., 2005).

Researchers have focused their attention more on the L/D ratio rather than the diameter of the tube. The diameter of the tube depends on the inlet pressure. It is seen that tangential velocity (or swirl) causes the energy separation. The vortex tube diameter should be chosen within the two extremes mentioned in the previous paragraph. However, it is seen that designs lean towards smaller tubes for better temperature separation.

#### 2.5.3.4. Number of Inlet Nozzles



Figure 5: Tangential inlet nozzles

Saidi and Vailpour (2003) have found through their experiments that three inlet nozzles are more efficient than four inlet nozzles. The reason being that four intake nozzles produce more turbulent flow in the tube which results in more

mixing between the cold and hot layers of flow, and thus less energy separation, hence lower cold temperature difference and lower efficiency. Promvonge and Eiamsa-ard (2005) have experimented with 1, 2 and 4 inlet nozzles and found that 4 nozzles gave better temperature separation and efficiency. Their conclusion reached was that increasing the number of nozzles helped to speed up the flow, to increase the mass flow rate and to generate stronger swirl flow in the vortex tube.

Hamdan *et al.* (2013) states that there is an optimum number of nozzles for a vortex tube of specific geometry and operating conditions and found that 4 inlet nozzles produced the best energy separation. Furthermore, they found that the inlet nozzles should be tangential to the vortex tube periphery.

## 2.5.3.5. Cold Orifice Diameter

The cold orifice diameter is one of the most important parameters in the design of a vortex tube, since this component is integral to the temperature separation effect of the vortex tube. If the orifice is too large relative to the tube's diameter, inlet gas from the inlet nozzles would escape directly into the cold outlet stream instead of creating the necessary vortex flow in the vortex tube. This would result in poor temperature separation due to lack of vortex flow near the cold orifice and also due to mixing of the inlet gas and the cold outlet stream. However, if the cold orifice is too small there is a high pressure drop over the cold orifice, therefore a high back pressure inside the vortex tube and hence a smaller pressure drop across the inlet nozzles. This would cause insufficient vortex flow in the tube and thus lower temperature separation. (Yilmaz et al., 2009).

Saidi and Valipour (2003), as well as Promvonge and Eiamsa-ard (2007) found that the optimum cold orifice diameter to vortex tube diameter should be 0.5. A review done by Yilmaz *et al.* (2009) suggests that the optimum cold orifice diameter should be between 0.4D and 0.6D.

## 2.5.3.6. Hot Outlet Area or Cold Mass Fraction

The hot outlet area is described as the area between the hot valve (conical control valve, shown on the right in Figure 4) and vortex tube wall. The hot outlet area is normally variable by adjusting the hot valve's axial position. The hot outlet area is closely related to the cold mass fraction. A change in position of the control valve alters the hot outlet area and hence causes a difference in back pressure by the hot valve and thus changes the fraction of gas allowed to escape through the hot end; therefore the cold fraction changes too.

It is claimed by many research experimental articles that the cold mass fraction is the only factor that needs to be controlled in order for the vortex tube to achieve maximum temperature separation or maximum cooling efficiency. Gupta *et al.* (2012) state that a cold mass fraction of 0.4 gives the maximum temperature drop and maximum cooling effect is seen between 0.35 and 0.65. The cooling effect is a function of the temperature drop and the mass flow rate of cold gas. Nimbalkar and Muller (2009) claims that a cold fraction of 0.6 gives the maximum energy separation or cooling effect.

## 2.5.4. Thermo-Physical Parameters

The performance of the vortex tube is affected by the thermo-physical properties of the gas used, such as inlet flow temperature and pressure, moisture content and specific heat ratio etc. (Saidi & Valipour, 2003). Increasing the inlet pressure increases the temperature separation up to a certain point. As the pressure is increased the flow inlet velocity increases up to the point where it becomes choked. A further increase in pressure only causes a slowly increasing temperature difference. The efficiency also increases up to the point that the flow becomes choked and then decreases as the energy separation decreases. Efficiency and cold temperature difference decreases with increasing moisture content of the inlet gas. Gases with higher specific heat capacity ratio attain higher temperature difference. (Saidi & Valipour, 2003).

#### 2.6. The Finite Volume Method

The finite volume method provides for a definitive method of expressing the conservation equations of fluid flow in a discretised form that can easily be implemented within a computer code. The flow field is divided into a finite number of control volumes (CV), hence the name finite volume method. The intention of this project is to model fluid flow in small diameter refrigerator tubes, therefore a one-dimensional (1-D) model would suffice. A simple derivation of the necessary discretised equations is to follow; for a more detailed discussion refer to Patankar (1980), and Versteeg and Malalasekera (2007). The three equations of change that governs 1-D fluid flow and heat transfer of a compressible fluid are (as derived from Versteeg and Malalasekera (2007:24)):

conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho v_z) = 0 \tag{2.4a}$$

conservation of momentum:

$$\frac{\partial(\rho v_z)}{\partial t} + \frac{\partial}{\partial z}(\rho v_z v_z) = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{rz}}{\partial r}$$
(2.4b)

and conservation of energy:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial z}(\rho u v_z) = -P \frac{\partial v_z}{\partial z} + \bar{\tau}_{rz} \frac{\partial(v_z)}{\partial r} + S_u$$
 (2.4c)

where  $\rho$  is the density, t is time, z is axial direction, r is radial direction,  $v_z$  is the velocity, P is the pressure,  $\tau_{rz}$  is the shear stress on the fluid due to friction on the tube walls, u is the specific internal energy,  $\bar{\tau}_{rz}$  is the average friction shear stress, and finally the source term  $S_u$  is used to incorporate external radial heat transfer.

It can be seen that the three conservation equations all have a similar form and can therefore be written for a general variable,  $\phi$ , as:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial z}(\rho\phi v_z) = S_{\phi} \tag{2.5}$$

where  $\phi = 1$ ,  $\phi = v_z$  and  $\phi = u$  for the three conservation equations respectively. This equation is referred to as the transport equation for property  $\phi$ .

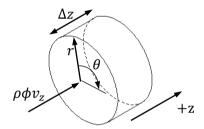


Figure 6: Control volume for tube fluid flow

Figure 6 shows the control volume used in the control volume method for the transportation of the general variable  $\phi$ . The finite volume method involves the integration of the conservation equations over a control volume. This leads to:

$$\int_{CV} \frac{\partial (\rho \phi)}{\partial t} dV + \int_{CV} \frac{\partial}{\partial z} (\rho \phi v_z) dV = \int_{CV} s_{\phi} dV$$
 (2.6)

Using Gauss's divergence theorem the second integral can be represented by a surface integral as:

$$\int_{CV} \frac{\partial}{\partial z} (\rho \phi v_z) \, dV = \int_{A} (\rho \phi v_z) \, dA \tag{2.7}$$

This states that the volume integral is equal to the surface integral over the entire bounding surface of the control volume. The direction of  $\rho\phi v_z$  is normal to the surface which bounds the control volume integrated, this is the application of Gauss's divergence theorem. In this case only flow in the z direction is

encountered therefore the area over which this integral is calculated would be the inlet and outlet control volume cross-sectional areas.

Since a transient time-dependent simulation model is developed, it is first necessary to decide which temporal discretisation scheme to use. There are three well known schemes that exist, namely; fully explicit, Crank-Nicolson, and fully implicit. The fully explicit scheme uses only old time step values to calculate the new time step value. This allows for easy computation; however there is a stringent limitation to time step size due to the Scarborough criterion which states that all coefficients of the discretised equation must be of the same sign, normally all positive, to ensure bounded and physically realistic results (Versteeg & Malalasekera, 2007: 247). The fully explicit scheme also possesses no intrinsic means for correcting or ensuring that the conservation equations remain conserved as time progresses. In the fully implicit scheme the old time value is treated as a source term and new time values are used to calculate the new values. This scheme is therefore iterative in nature; also it is unconditionally stable for any time step size since all discretisation equation coefficients are positive. However since the accuracy of the scheme is first-order in time, small time steps are needed to ensure the accuracy of the results (Versteeg & Malalasekera, 2007: 249). The Crank-Nicolson scheme uses a weighting of half the new - and half the old time step values to compute the new values. This method is more robust than the fully explicit method, in that it has a less restrictive time step size limit. Other schemes with a different weighting between new – and old time step values also exist but are of no interest to this study.

The robustness and unconditional stability of the fully implicit scheme are the reasons for it being the method of choice for transient simulation purposes. Furthermore the iterative nature of this scheme ensures that the conservation equations remain conserved as time progresses. Therefore, all subsequent derivations will focus on the implementation of the fully implicit scheme.

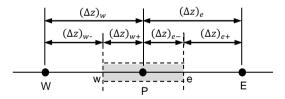


Figure 7: Notation used in the control volume discretisation

Integration of a conservation equation over a control volume, as shown in Figure 7, yields a discretised equation at the node, P, of the control volume (usually at its center). The discretised equation contains neighbouring node values depending on the discretisation scheme used to represent face values of the current control volume. To illustrate how a differential conservation equation is transformed into a usable discretised equation, the discretised form of the

general transport equation (2.5) for  $\phi$  will be developed. The method also applies to the transformation of the different conservation equations (2.4a-c).

Rewriting integral equation (2.6) using equation (2.7) and integrating yields the discretised equation (2.9) in its most elementary form:

$$\frac{\partial}{\partial t} \left( \int_{CV} \rho \phi \, dV \right) + \int_{A} (\rho \phi v_z) \, dA = \int_{CV} s_\phi \, dV \tag{2.8}$$

$$[(\rho\phi)_{P} - (\rho\phi)_{P}^{o}] \frac{\Delta V}{\Delta t} + [\rho v_{z}A]_{e}\phi_{e} - [\rho v_{z}A]_{w}\phi_{w} = \bar{S}_{\phi}\Delta V$$
 (2.9)

The values with superscript,  $^{\circ}$ , refers to the previous time step's values, and the values without superscript refers to the new time step's values.  $\Delta V$  is the volume,  $\Delta t$  is the time step size, A is the cross-sectional area of the control volume face, and  $\bar{S}_{\phi}$  is the average value of the source term,  $S_{\phi}$ , over the control volume. The source term,  $S_{\phi}$ , may be a function of the dependent variable  $\phi$ ; in such cases Patankar (1980: 48) suggests that the source term be approximated by a linearised form:

$$\bar{S}_{\phi}\Delta V = S_C + S_P \phi_P \tag{2.10}$$

where  $S_P$  has a negative value to ensure that the Scarborough criterion is satisfied and  $S_C$  is a constant source.

A variable is defined to more compactly represent the convective mass flux at control volume faces, as:

$$F = \rho v_z A \tag{2.11}$$

Thus the face convective mass fluxes are:

$$F_{\rho} = (\rho v_z A)_{\rho}$$
 and  $F_w = (\rho v_z A)_w$  (2.12)

Substitution of the above gives:

$$[(\rho\phi)_{P} - (\rho\phi)_{P}^{o}] \frac{\Delta V}{\Delta t} + F_{e}\phi_{e} - F_{w}\phi_{w} = (S_{C} + S_{P}\phi_{P})$$
(2.13)

To derive useful forms of the discretised equation it is necessary to find appropriate representation of the face values of the control volume in terms of the surrounding/neighbouring nodal values. All scalar quantities such as  $\rho$ , P, u, and  $\phi$  are defined at control volume nodes and not at the faces; therefore a suitable

interpolation or other consistent discretisation scheme has to be used to represent face values in terms of the nodal values.

For example for face values of  $\phi$  linear interpolation (also called central differencing), with reference to Figure 7, yields the following:

$$\phi_e = f_e \phi_P + (1 - f_e) \phi_E \text{ and } \phi_W = f_W \phi_P + (1 - f_W) \phi_W$$

$$\text{where } f_e = \frac{(\Delta z)_{e+}}{(\Delta z)_e} \text{ and } f_W = \frac{(\Delta z)_{W-}}{(\Delta z)_W}$$

$$(2.14)$$

According to Patankar (1980: 34) it is not necessary to use the same discretisation scheme for every variable; the discretisation scheme chosen for a variable depends on how well it describes the physical behaviour of that variable. Versteeg and Malalasekera (2007: 141) state that the most fundamental properties that a discretisation method requires are conservativeness, boundedness and transportiveness. Conservativeness entails using a consistent expression for the flux of a property  $\phi$  through a common face in adjacent control volumes. This means that  $\phi$  leaving one control volume through a face must enter the adjacent control volume through the same face, thus ensuring conservation of  $\phi$  through the whole simulation domain. Boundedness ensures that the results are physically realistic in the sense that the values of internal nodes are bounded by its boundary values in the absence of internal sources. For the boundedness requirement all coefficients of the nodal values in the discretised equation must satisfy the Scarborough condition in that they are all of the same sign (usually all positive). This ensures that an increase in  $\phi$  at one node would result in an increase in  $\phi$  in the neighbouring nodes. Transportiveness in a discretisation scheme ensures that the flow direction is taken into account by ensuring that the value of node P is predominantly influenced by the upstream neighbouring node, as is physically occurring, and not the downstream neighbour.

The central differencing scheme requires small control volumes, hence a large number of control volumes, and does not recognize the direction of flow, i.e. does not possess the transportiveness property. The simulation model developed will make use of the minimum amount of control volumes possible, to keep computation time to a minimum, therefore it was decided to use the upwind differencing scheme. This scheme is relatively robust in the sense that it can produce physically realistic results with the minimum amount of control volumes and it possesses all three fundamental properties of a discretisation scheme.

A development of the discretised equation of the general variable  $\phi$  using the upwind differencing scheme is to follow.

If the flow is in the positive direction  $(v_z)_e > 0$ ,  $(v_z)_w > 0$   $(F_e > 0, F_w > 0)$ :

$$\phi_e = \phi_P \text{ and } \phi_W = \phi_W \tag{2.15}$$

Substitution of the upwind differencing values into the discretised equation yields:

$$[(\rho\phi)_{P} - (\rho\phi)_{P}^{o}] \frac{\Delta V}{\Delta t} + F_{e}\phi_{P} - F_{w}\phi_{W} = (S_{C} + S_{P}\phi_{P})$$
(2.16)

Rearranging gives:

$$\left[\rho_P \frac{\Delta V}{\Delta t} + F_e - S_P\right] \phi_P = F_W \phi_W + 0.\phi_E + \left[\rho_P^o \frac{\Delta V}{\Delta t}\right] \phi_P^o + S_C$$
 (2.17)

If the flow is in the negative direction  $(v_z)_e < 0$ ,  $(v_z)_w < 0$   $(F_e < 0, F_w < 0)$ :

$$\phi_e = \phi_E \text{ and } \phi_w = \phi_P \tag{2.18}$$

Substitution of the upwind differencing values into the discretised equation yields:

$$[(\rho\phi)_{P} - (\rho\phi)_{P}^{o}] \frac{\Delta V}{\Delta t} + F_{e}\phi_{E} - F_{w}\phi_{P} = (S_{C} + S_{P}\phi_{P})$$
(2.19)

Rearranging gives:

$$\left[\rho_P \frac{\Delta V}{\Delta t} - F_W - S_P\right] \phi_P = 0. \phi_W - F_e \phi_E + \left[\rho_P^o \frac{\Delta V}{\Delta t}\right] \phi_P^o + S_C$$
 (2.20)

Identifying the coefficients of  $\phi_P$ ,  $\phi_W$ , and  $\phi_E$  as  $a_P$ ,  $a_W$ , and  $a_E$  respectively, equations (2.17) and (2.20) can be written in general form as:

$$a_P \phi_P = a_W \phi_W + a_E \phi_E + a_P^0 \phi_P^0 + S_C \tag{2.21}$$

where:

$$a_P = a_W + a_E + (F_e - F_w) + (a_P^o) \frac{\rho_P}{\rho_P^o} - S_P$$

$$a_W = \max(F_w, 0) \qquad a_E = \max(0, -F_e)$$

$$a_P^o = \rho_P^o \frac{\Delta V}{\Delta t}$$

Discretised equations of the form (2.21) must be set up at each node in the simulation domain. The discretised equation is modified for boundary control volumes to incorporate boundary conditions.

The equations are now written in the form:

$$-a_W \phi_W + a_P \phi_P - a_E \phi_E = a_P^{\ o} \phi_P^{\ o} + S_C \tag{2.22}$$

where  $\phi_P$  is the variable being solved.

The set of equations for the simulation nodes are all written in a matrix starting with the first node's equation in the first row and continuing till the last node's equation in the last row. The resulting matrix has a tri-diagonal form and can then be solved by forward elimination and back-substitution. This algorithm, called the tri-diagonal matrix algorithm (TDMA), can be implemented in a for-loop and is less computationally expensive than direct methods. It requires a number of computations in the order of  $\approx 2N$  versus  $\approx N^2$  for direct methods, where N is the number of variables being solved. A detailed description of the TDMA algorithm can be obtained in Versteeg and Malalasekera (2007: 213).

#### 3. DETERMINING THE THERMODYNAMIC STATE

Simulation of a CO<sub>2</sub> refrigeration cycle would necessitate an equation of state that is not only accurate, but also computationally inexpensive. The accurate equation of state from Span and Wagner (1996) involves no complex coupling to a scaled equation and thus makes it less computationally expensive and easier to program.

## 3.1. CO<sub>2</sub> Equation of State from Span and Wagner

The equation of state from Span and Wagner (1996) is used in the simulation program of the refrigeration cycle to determine the thermodynamic properties of  $CO_2$ . This equation is in the form of a fundamental equation explicit in the Helmholtz energy, A, which is a function of density  $\rho$  and temperature T. The equation is structured to use the dimensionless Helmholtz energy  $\phi = A/(RT)$  which is split into a part depending on the ideal-gas behaviour  $\phi^o$  and a part to take into account the residual fluid behaviour  $\phi^r$ , namely:

$$\phi(\delta, \tau) = \phi^{o}(\delta, \tau) + \phi^{r}(\delta, \tau) \tag{3.1}$$

where  $\tau = T_c/T$  is the inverse reduced temperature and  $\delta = \rho/\rho_c$  is the reduced density. Both the temperature T and the density  $\rho$  are reduced with their critical values,  $T_c = 304.1282$  K and  $\rho_c = 467.6$  kg/m³, respectively.

All thermodynamic properties of a pure substance can be obtained by combining derivatives of eq. (3.1), because the Helmholtz energy as a function of density and temperature is one form of a fundamental equation. Table 3 in Span and Wagner (1996: 1517) gives the thermodynamic property relations to the reduced Helmholtz energy  $\phi$  and its derivatives. In the context of having a detailed

discussion of how the equation of state is solved with other variables such as density and specific internal energy, it was decided to have the thermodynamic property relations as a reference in the table below.

Table 3: Relations of the thermodynamic properties to the dimensionless Helmholtz function  $\phi$ 

Property and common thermodynamic definition	Relation to the dimensionless Helmholtz energy and its derivatives <sup>a</sup>
Pressure: $P(\rho,T) = -(\partial A/\partial v)_T$	$\frac{P(\delta,\tau)}{\rho RT} = 1 + \delta \phi^r_{\delta}$
Entropy: $s(\rho, T) = -(\partial A/\partial T)_v$	$\frac{s(\delta,\tau)}{R} = \tau(\phi^o_{\tau} + \phi^r_{\tau}) - \phi^o - \phi^r$
Internal energy: $u(\rho,T) = A - T(\partial A/\partial T)_v$	$\frac{u(\delta,\tau)}{RT} = \tau(\phi^o_{\tau} + \phi^r_{\tau})$
Enthalpy: $h(\rho,T) = A - T(\partial A/\partial T)_v - v(\partial A/\partial v)_T$	$\frac{h(\delta,\tau)}{RT} = 1 + \tau(\phi^o_{\tau} + \phi^r_{\tau}) + \delta\phi^r_{\delta}$
Isochoric heat capacity: $c_v(\rho,T) = (\partial u/\partial T)_v$	$\frac{c_v(\delta,\tau)}{R} = -\tau^2(\phi^o_{\tau\tau} + \phi^r_{\tau\tau})$
Isobaric heat capacity: $c_P(\rho,T)=(\partial h/\partial T)_P$	$\frac{c_P(\delta, \tau)}{R} = -\tau^2 (\phi^o_{\tau\tau} + \phi^r_{\tau\tau}) + \frac{(1 + \delta\phi^r_{\delta} - \delta\tau\phi^r_{\delta\tau})^2}{1 + 2\delta\phi^r_{\delta} + \delta^2\phi^r_{\delta\delta}}$
Speed of sound: $c(\rho,T) = \sqrt{(\partial P/\partial \rho)_s}$	$\frac{c^{2}(\delta,\tau)}{RT} = 1 + 2\delta\phi^{r}_{\delta} + \delta^{2}\phi^{r}_{\delta\delta} - \frac{(1 + \delta\phi^{r}_{\delta} - \delta\tau\phi^{r}_{\delta\tau})^{2}}{\tau^{2}(\phi^{o}_{\tau\tau} + \phi^{r}_{\tau\tau})}$
$^{a} \phi_{\delta} = \left[\frac{\partial \phi}{\partial \delta}\right]_{\tau},  \phi_{\delta\delta} = \left[\frac{\partial^2 \phi}{\partial \delta^2}\right]_{\tau},  \phi_{\tau} = \left[\frac{\partial^2 \phi}{\partial \delta}\right]_{\tau},  \phi_{\tau} = \left[\frac{\partial^2 \phi}{\partial \delta}\right]_{\tau} = \left[\frac{\partial^2 \phi}{\partial \delta}\right]_{\tau},  \phi_{\tau} = \left[\frac{\partial^2 \phi}{\partial \delta}\right]_{\tau} = \left[\partial$	$= \left[\frac{\partial \phi}{\partial \tau}\right]_{\delta}, \ \phi_{\tau\tau} = \left[\frac{\partial^2 \phi}{\partial \tau^2}\right]_{\delta}, \ \text{and} \ \phi_{\delta\tau} = \left[\frac{\partial^2 \phi}{\partial \delta \partial \tau}\right].$

Relations and the coefficients used for the ideal-gas part of the dimensionless Helmholtz function  $\phi^o$  and its derivatives can be obtained from Table 28 and 27, respectively, of Span and Wagner (1996: 1540-1541). Relations and the coefficients used for the residual part of the dimensionless Helmholtz function  $\phi^r$  and its derivatives can be obtained in Table 32 and 31, respectively, of Span and Wagner (1996: 1544-1545).

The MATLAB script file, CO2\_Property.m, written to calculate the thermodynamic properties, as shown in Table 3, from a given density  $\rho$  and temperature T using Span and Wagner's equation can be seen in Appendix B1. All coefficients of Span and Wagner's equation are stored in .mat format and called when needed.

### 3.2. Saturated Property Determination

The vapour pressure  $P_s$  and densities of saturated vapour  $\rho_g$  and saturated liquid  $\rho_f$  can be determined by solving the following equations simultaneously. These equations correspond to the equality of temperature, pressure and specific Gibbs energy (Maxwell criterion) in the coexisting phases (Span and Wagner, 1996: 1516).

$$\frac{P_s}{\rho_f RT} = 1 + \delta_f \phi^r_{\delta} (\delta_f, \tau)$$
 (3.2a)

$$\frac{P_s}{\rho_g RT} = 1 + \delta_g \phi^r_{\delta} (\delta_g, \tau)$$
(3.2b)

$$\frac{P_s}{RT} \left( \frac{1}{\rho_g} - \frac{1}{\rho_f} \right) - \ln \left( \frac{\rho_f}{\rho_g} \right) = \phi^r (\delta_f, \tau) - \phi^r (\delta_g, \tau)$$
(3.2c)

Span and Wagner (1996: 1524-1525) give simple correlations, based on temperature, for the vapour pressure, saturated vapour density and saturated liquid density, which can be used as a very good initial guess in a program to solve the above equation set. The correlations are:

$$ln\left(\frac{P_S}{P_C}\right) = \frac{T_C}{T} \left[ \sum_{i=1}^4 a_i \left(1 - \frac{T}{T_C}\right)^{t_i} \right]$$
(3.3)

for the vapour pressure, where  $a_1 = -7.0602087$ ,  $a_2 = 1.9391218$ ,  $a_3 = -1.6463597$ ,  $a_4 = -3.2995634$ ,  $t_1 = 1.0$ ,  $t_2 = 1.5$ ,  $t_3 = 2.0$  and  $t_4 = 4.0$ .

$$ln\left(\frac{\rho_f}{\rho_c}\right) = \sum_{i=1}^4 a_i \left(1 - \frac{T}{T_c}\right)^{t_i} \tag{3.4}$$

for the saturated liquid density, where  $a_1=1.9245108$ ,  $a_2=-0.62385555$ ,  $a_3=-0.32731127$ ,  $a_4=0.39245142$ ,  $t_1=0.34$ ,  $t_2=\frac{1}{2}$ ,  $t_3=\frac{10}{6}$  and  $t_4=\frac{11}{6}$ .

and finally

$$ln\left(\frac{\rho_g}{\rho_c}\right) = \sum_{i=1}^5 a_i \left(1 - \frac{T}{T_c}\right)^{t_i} \tag{3.5}$$

for the saturated vapour density, where  $a_1=-1.7074879,\ a_2=-0.82274670,\ a_3=-4.6008549,\ a_4=-10.111178,\ a_5=-29.742252\ t_1=0.340,\ t_2=\frac{1}{2},\ t_3=1,\ t_4=\frac{7}{3}$  and  $t_5=\frac{14}{3}$ .

Since the thermodynamic properties of  $CO_2$  are functions, as shown in Table 3, its derivatives will in themselves be functions as well. Therefore the Newton-Raphson method (Chapra, 2008: 144) can be applied to simultaneously solve equations such as equation set (3.2). Once these equations are solved for a specific temperature, the calculated saturated density and temperature can be used to calculate all other saturated properties using the function script file CO2\_Property.m. The MATLAB script, CO2\_Sat\_Prop\_at\_T.m in Appendix B2, calculates saturated properties using equations (3.3-3.5) as initial guesses for  $P_s$ ,  $\rho_f$ , and  $\rho_g$  and then equations (3.2a-c) are solved using the Newton-Raphson method. Solving equations (3.2a-c) simultaneously for temperatures from the triple point up to the critical point in a loop a vector of points can be generated for any saturated properties, which can then be used to draw saturated property graphs. The MATLAB script file, CO2\_Sat\_Prop\_at\_T\_Iteration.m (can be seen in the project file), is used to create these vectors and plot the graphs.

## 3.3. Determining Single Phase and Two-Phase Properties

Simulating fluid flow using the control volume approach, one would split up the flow domain in control volumes of finite size and then simultaneously solve the three conservation equations namely mass, momentum and energy. The nonlinear nature of the momentum equation makes it very difficult to solve these three equations simultaneously using direct methods and therefore an iterative method such as commonly used in CFD would be adapted. Solving these three equations simultaneously the density  $\rho$  and specific internal energy u of each control volume are obtained and then the equation of state is used to determine the pressure, temperature and all other properties; thus linking the mass and energy equation to the momentum equation.

Since the equation of Span and Wagner uses  $\rho$  and T, but only  $\rho$  and u are known; it would be necessary to guess a temperature and use an appropriate iteration method to find the correct temperature, and consequently all other properties that satisfy  $\rho$  and u. The following two sections explain how the properties are obtained for the single phase and the two-phase regions. The third section discusses the logical process of determining whether the fluid is single - or two-phase, and then selecting the appropriate functions to calculate the thermodynamic properties, as well as the viscosity and thermal conductivity.

#### 3.3.1. Determining Single Phase Properties

The single phase program is easier to implement and understand, thus its derivation will be explained first. Since one of the variables in Span and Wagner's equation is already given, namely the density, it is only required to find the correct temperature that satisfies the given specific internal energy i.e. u may be treated as a function of T only at this fixed density. Therefore it is required that the specific internal energy  $u(\rho_x, T)$  calculated from the guessed temperature, or iteratively improved temperature, be equal to the given specific internal energy  $u_x$ . Writing the difference between these two in function form gives:

$$f(\rho_x, T) = -u_x + u(\rho_x, T) \tag{3.6}$$

This has now reduced to a root finding problem which the Newton-Raphson method (Chapra, 2008: 144) is well suited for, especially if a good initial guess for *T* is available. The error is defined as the absolute value of *f*.

The new value of *T* is defined by the Newton-Raphson formula as:

$$T_{i+1} = T - \frac{f(\rho_x, T)}{\frac{\partial f}{\partial T}(\rho_x, T)}$$
(3.7)

where

$$\frac{\partial f}{\partial T}(\rho_x, T) = \frac{\partial}{\partial T}(-u_x + u(\rho_x, T)) = \frac{\partial}{\partial T}(u(\rho_x, T)) = c_v(\rho_x, T)$$
(3.8)

Note that  $u_x$  is the given specific internal energy and therefore is treated as a constant in the derivation. The value for  $u(\rho_x,T)$  and  $c_v(\rho_x,T)$  are determined from the equations in Table 3 in a script file called u\_and\_cv\_script.m. This script file is a shortened version of CO2\_Property.m, written only for determining u and  $c_v$ . This shortened version allows time saving in the iteration process as opposed to using the whole CO2\_Property.m script.

The updated temperature is again used to determine new properties and the whole procedure is repeated until the error reaches a prescribed level. Finally when the error level is reached all thermodynamic properties are updated using CO2\_Property.m. The script file, CO2\_1Ph\_Prop\_at\_rho\_and\_u.m, written to determine the single phase thermodynamic properties can be viewed in Appendix B3.

#### 3.3.2. Determining Two-Phase Properties

Assuming a homogeneous mixture for the two-phase fluid a set of four unknowns emerge. Determining the state from a given density,  $\rho_x$ , and specific internal energy,  $u_x$ , the four unknowns are temperature T, saturated vapour density  $\rho_g$ , saturated liquid density  $\rho_f$ , and volume fraction  $\alpha$ . The temperature and volume fraction at the old time level or previous iteration can be taken as a good initial guess. Equations (3.4-3.5) are used to obtain good guesses for  $\rho_f$  and  $\rho_g$  based on the guessed temperature. Four equations are needed to determine the four unknowns. These equations are given below.

The two-phase internal energy per volume is represented by:

$$\rho_x u_x = \alpha \rho_g u_g + (1 - \alpha) \rho_f u_f \tag{3.9a}$$

The two-phase flow homogeneous density is represented by:

$$\rho_x = \alpha \rho_q + (1 - \alpha)\rho_f \tag{3.9b}$$

The vapour and liquid are in equilibrium thus the pressure is equal for both:

$$P_{q}(\rho_{q},T) = P_{f}(\rho_{f},T) \tag{3.9c}$$

Also equilibrium between vapour and liquid means that the specific Gibbs energy g is the same for both phases:

$$g_g(\rho_g, T) = g_f(\rho_f, T) \tag{3.9d}$$

The specific Gibbs energy is defined as:

$$g = h - Ts (3.10)$$

where h is the specific enthalpy, T is the temperature, and s is the specific entropy.

Simultaneously solving the four equations (3.9a-d) necessitates an efficient method and hence the Newton-Raphson method is again implemented (Chapra, 2008: 272-276). First the four equations are written in difference form i.e. reduced to a root finding problem.

$$f_1(T, \rho_g, \rho_f, \alpha) = -\rho_x u_x + \alpha \rho_g u_g + (1 - \alpha)\rho_f u_f$$
(3.11a)

$$f_2(\rho_q, \rho_f, \alpha) = -\rho_x + \alpha \rho_q + (1 - \alpha)\rho_f \tag{3.11b}$$

$$f_3(T, \rho_g, \rho_f) = P_g(\rho_g, T) - P_f(\rho_f, T)$$
(3. 11c)

$$f_4(T, \rho_g, \rho_f) = g_g(\rho_g, T) - g_f(\rho_f, T)$$
 (3. 11d)

Derivatives of these four functions are now developed. Note that  $\rho_x$  and  $u_x$  are the given density and specific internal energy; therefore they are treated as constants in deriving derivatives of the above functions. Appendix B4 contains the other derivatives used in the following derivations.

$$\frac{\partial f_1}{\partial T} = \alpha \rho_g \frac{\partial u_g}{\partial T} + (1 - \alpha) \rho_f \frac{\partial u_f}{\partial T} = \alpha \rho_g (c_v)_g + (1 - \alpha) \rho_f (c_v)_f$$
(3.12a)

$$\frac{\partial f_1}{\partial \rho_g} = \alpha u_g + \alpha \rho_g \frac{\partial u_g}{\partial \rho_g} = \alpha u_g + \alpha \rho_g \frac{T_c R}{\rho_c} \left[ \left( \phi^o_{\delta \tau} \right)_g + \left( \phi^r_{\delta \tau} \right)_g \right]$$
(3.12b)

$$\frac{\partial f_1}{\partial \rho_f} = (1 - \alpha)u_f + (1 - \alpha)\rho_f \frac{T_c R}{\rho_c} \left[ \left( \phi^o_{\delta \tau} \right)_f + \left( \phi^r_{\delta \tau} \right)_f \right]$$
 (3.12c)

$$\frac{\partial f_1}{\partial \alpha} = \rho_g u_g - \rho_f u_f \tag{3.12d}$$

$$\frac{\partial f_2}{\partial T} = 0, \qquad \frac{\partial f_2}{\partial \rho_g} = \alpha, \qquad \frac{\partial f_2}{\partial \rho_f} = 1 - \alpha, \qquad \frac{\partial f_2}{\partial \alpha} = \rho_g - \rho_f$$
 (3.13)

$$\frac{\partial f_3}{\partial T} = \frac{\partial}{\partial T} (P_g - P_f) 
= \left(\frac{P_g}{T} - \rho_g R \tau \delta_g (\phi^r_{\delta \tau})_g\right) - \left(\frac{P_f}{T} - \rho_f R \tau \delta_f (\phi^r_{\delta \tau})_f\right)$$
(3.14a)

$$\frac{\partial f_3}{\partial \rho_g} = \frac{\partial}{\partial \rho_g} (P_g - P_f) = \frac{\partial}{\partial \rho_g} (P_g) 
= \frac{P_g}{\rho_g} + \delta_g RT \left[ (\phi^r_{\delta})_g + \delta_g (\phi^r_{\delta\delta})_g \right]$$
(3.14b)

$$\frac{\partial f_3}{\partial \rho_f} = \frac{\partial}{\partial \rho_f} (P_g - P_f) = \frac{\partial}{\partial \rho_f} (-P_f)$$

$$= -\frac{P_f}{\rho_f} - \delta_f RT \left[ (\phi^r_{\delta})_f + \delta_f (\phi^r_{\delta\delta})_f \right]$$
(3.14c)

$$\frac{\partial f_3}{\partial \alpha} = 0 \tag{3.14d}$$

$$\frac{\partial f_4}{\partial T} = \frac{\partial}{\partial T} (g_g - g_f) 
= \left[ R \left( 1 + \delta_g (\phi^r_{\delta})_g - \delta_g \tau (\phi^r_{\delta \tau})_g \right) - s_g \right] 
- \left[ R \left( 1 + \delta_f (\phi^r_{\delta})_f - \delta_f \tau (\phi^r_{\delta \tau})_f \right) - s_f \right]$$
(3.15a)

$$\frac{\partial f_4}{\partial \rho_g} = \frac{\partial}{\partial \rho_g} (g_g - g_f) = \frac{RT}{\rho_c} \left( 2(\phi^r_{\delta})_g + (\phi^o_{\delta})_g + \delta_g(\phi^r_{\delta\delta})_g \right)$$
(3.15b)

$$\frac{\partial f_4}{\partial \rho_f} = \frac{\partial}{\partial \rho_f} (g_g - g_f) = -\frac{RT}{\rho_c} \left( 2(\phi^r_{\delta})_f + (\phi^o_{\delta})_f + \delta_g(\phi^r_{\delta\delta})_f \right)$$
(3.15c)

$$\frac{\partial f_4}{\partial \alpha} = \frac{\partial}{\partial \alpha} (g_g - g_f) = 0 \tag{3.15d}$$

The Newton-Raphson method is now applied to simultaneously solve the set of equations (3.15a-d). To use the Newton-Raphson method for a set of equations it is necessary to write the equations in matrix form. The formula remains the same as for solving a single equation in one variable; the only difference is that the derivative is now replaced by a matrix of derivatives.

The vector of unknowns x and the vector of function values f (calculated from equations (3.15a-d)) are:

$$x = \begin{bmatrix} T \\ \rho_g \\ \rho_f \\ \alpha \end{bmatrix}, \qquad f = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

The matrix of derivatives is:

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial T} & \frac{\partial f_1}{\partial \rho_g} & \frac{\partial f_1}{\partial \rho_f} & \frac{\partial f_1}{\partial \alpha} \\ \frac{\partial f_2}{\partial T} & \frac{\partial f_2}{\partial \rho_g} & \frac{\partial f_2}{\partial \rho_f} & \frac{\partial f_2}{\partial \alpha} \\ \frac{\partial f_3}{\partial T} & \frac{\partial f_3}{\partial \rho_g} & \frac{\partial f_3}{\partial \rho_f} & \frac{\partial f_3}{\partial \alpha} \\ \frac{\partial f_4}{\partial T} & \frac{\partial f_4}{\partial \rho_g} & \frac{\partial f_4}{\partial \rho_f} & \frac{\partial f_4}{\partial \alpha} \end{bmatrix}$$

The Newton-Raphson formula for updating the vector x is:

$$x_{i+1} = x_i + J^{-1}f (3.16)$$

where  $J^{-1}$  is the inverse of J.

All derivatives and function values needed in the Newton-Raphson formula are obtained by use of the property calculating script CO2\_Property.m.

The error is defined as the maximum absolute value of *f*. The updated temperature and densities are used again to determine new properties and the whole procedure is repeated until the error reaches a prescribed level. Finally when the error level is reached the vapour fraction is calculated and all homogeneous thermodynamic properties are calculated. The void fraction obtained is later used to calculate the homogeneous viscosity and thermal conductivity. The script file written to determine the two-phase thermodynamic properties, CO2\_2Ph\_Prop\_at\_rho\_and\_u.m, can be viewed in Appendix B5.

#### 3.3.3. Deciding whether the Fluid is Single Phase or Two-Phase

To determine the state of each control volume based on  $\rho$  and u it is first necessary to determine whether it is two-phase or single phase. The fluid phase is determined with the help of a phase diagram as shown in Figure 8. If a point  $(\rho, u)$  lies within the polygon it is two-phase else it is single phase. The vectors used to plot the graph in Figure 8 are saturated density and saturated specific internal energy. These vectors were generated by the script file, CO2\_Sat\_Prop\_at\_T\_Iteration.m as explained in section 3.2.

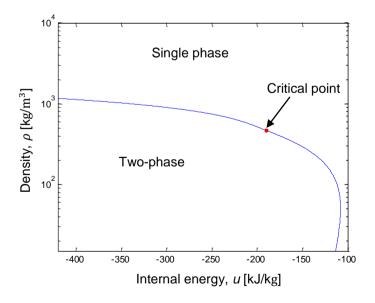


Figure 8: Phase diagram for CO<sub>2</sub>

Figure 9 shows the program logic to decide whether the fluid is single phase or two-phase. Once determined if the fluid is single - or two-phase the appropriate script file is called to calculate the thermodynamic properties. The single phase thermodynamic properties are calculated with CO2 1Ph Prop at rho and u.m. as explained in section 3.3.1., and the two-phase thermodynamic properties are calculated with CO2 2Ph Prop at rho and u.m as explained in section 3.3.2. The thermal conductivity is calculated by the script file CO2\_Conductivity.m, shown in Appendix B6, which uses the equation developed by Scalabrin, Marchi, Finezzo and Span (2006). The dynamic viscosity is calculated by the script file Viscosity\_CO2.m, shown in Appendix B7, which uses the equation developed by Fenghour, Wakeham and Vesovic (1998). Both the conductivity and dynamic viscosity equations are a function of density and temperature. The two-phase thermal conductivity and dynamic viscosity are calculated based on the homogeneous flow model with the use of the volume fraction. The MATLAB script file, CO2 Prop at rho and u.m, written to calculate all properties following the logic set out in Figure 9 can be viewed in Appendix B8.

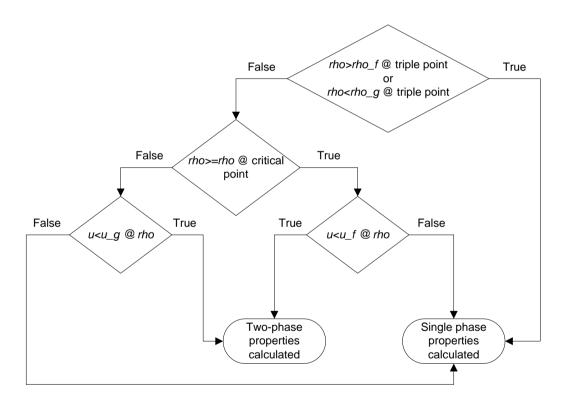


Figure 9: Program logic to determine the properties of CO<sub>2</sub> at a given density and specific internal energy

# 4. TRANSIENT SIMULATION PROGRAM OF THE CO<sub>2</sub> REFRIGERATION CYCLE

A transient simulation program for the basic  $CO_2$  refrigeration cycle, containing a capillary tube as expansion device, is written and will be explained in this chapter. The one-dimensional finite volume method, as explained in section 2.6, is used to write the simulation program. The simulation program code may be viewed in Appendix C. The main program can be viewed in Appendix C1.

## 4.1. General Model Assumptions

The simulation model is developed under the following assumptions:

- The refrigerant is pure CO<sub>2</sub> with no oil entrained.
- A homogeneous model is used for two-phase flow. This simple model is easily implemented within a finite volume formulation, and gives results that are reasonably accurate. It is assumed well suited for the simulation since the flow is confined to small tubes, thus separated flow is not readily expected.
- No gravity effects are incorporated in the simulation equations since its
  effects are assumed negligible for such a small household refrigeration
  system. Also the homogenous flow model used ignores gravity effects.
- The compressor operates in a continuous manner with no pauses between suction and expulsion i.e. it sucks and expels gas at the same instant in time. This allows simplification in programming the simulation model.
- The refrigeration system starts from resting conditions, where the gas in the system is at equilibrium with the surrounding environmental temperature and there is no flow.

## 4.2. Initialising the Simulation Domain

The simulation domain is initialised/created by first defining its geometric properties (section 4.2.1) and then defining initial conditions for the fluid in the simulation domain (section 4.2.2). The program code to initialise the simulation domain can be viewed in Appendix C2.

### 4.2.1. Defining Geometric Properties of the Simulation Domain

The refrigerator layout being simulated is shown in Figure 10. The whole refrigerant circuit, from compressor outlet back to compressor inlet forms part of the simulation domain. External counter-flow water-cooled heat exchangers are incorporated within the simulation to calculate the heat transferred during

operation. The compressor's effect on the simulation domain is incorporated through boundary conditions applied to the simulation domain as will be explained in section 4.3.

The simulation domain is split into a number of control volumes of differing lengths; closer to inlets and changes in tube diameters the control volumes are made shorter to enable the simulation to capture the fine changes occurring in these regions. Stretching of the control volume lengths allows saving on computing power necessary for the simulation. A stretch ratio is applied to define the control volume lengths as:

$$\Delta z_{i+1} = r \Delta z_i \tag{4.1}$$

where  $\Delta z_{i+1}$  is the next control volume length, and r is the stretch ratio. A stretch ratio close to one is however used in order to have a good aspect ratio between control volume lengths.

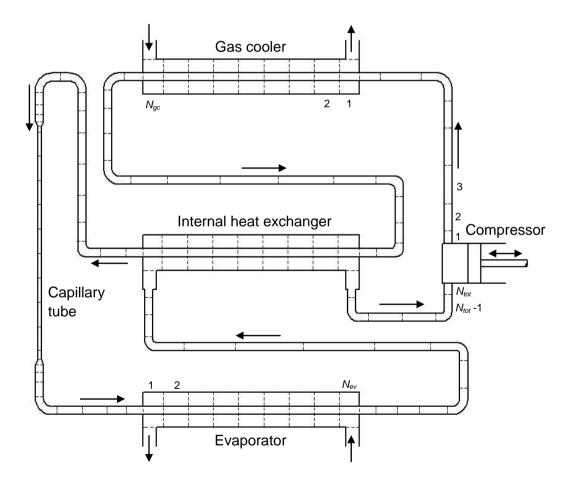


Figure 10: Basic refrigeration cycle for simulation

Control volume numbering of the  $CO_2$  refrigerant (simulation domain) starts with k=1 at the compressor outlet and ends with  $k=N_{tot}$  at the compressor inlet. The gas cooler and evaporator outer tubes contain water which is flowing in the opposite direction of the  $CO_2$  refrigerant in the inner tube. The numbering of the outer tubes' control volumes are as indicated in the figure above. It was chosen to be numbered in this particular order to facilitate programming of the heat exchange between the water and  $CO_2$  control volumes. The number of control volumes used for the gas cooler, internal heat exchanger, capillary tube and evaporator are 400, 120, 230 and 300 respectively. For other details such as the number of control volumes for connecting tubes and transition pieces (for connection fittings between tubes) refer to the initialise script file in Appendix C2.

#### 4.2.2. Initial Conditions for the Simulation Domain

To start the simulation the initial conditions for each control volume are assigned. The initial temperature of the water in the outer tubes of the gas cooler and evaporator is at ambient temperature of 25 °C. The initial conditions for the  $CO_2$  refrigerant were calculated assuming the system is in equilibrium with its outside environment. The temperature of the  $CO_2$  in the system is thus at environmental temperature:

$$T = T_{Env} = 25 \,^{\circ}\text{C} = 298.15 \,^{\circ}\text{K}$$
 (4.2)

The mass of CO<sub>2</sub> charged in the system is:

$$m_{CO2} = 0.435 \text{ kg}$$
 (4.3)

The volume of the system is calculated by measuring the length and using the specified inner diameters of the tubes. The properties of the CO2 can now be calculated based on  $\rho = m_{CO2}/Vol_{System}$  and T. The properties are calculated by a script file called CO2\_Prop\_at\_rho\_and\_T.m, which can be viewed in the project file. This function can calculate single phase and two-phase properties. It is determined that the system fluid is two-phase at the initial conditions. To provide starting conditions for the simulation model it was decided to have all the saturated fluid in the last control volumes of the high pressure side and saturated vapour in the rest of the control volumes, including the low pressure side. This is a fair assumption noting that: i) the highest mass of CO2 and hence fluid would end up in the high pressure side during and after operation, ii) the refrigerator design is such that there is a large enough length/volume of tube on the high pressure side which is lower to the ground than the other tubes, thus enabling gravity to keep the liquid in the high pressure side. The tubing is laid out in this manner to avoid liquid from entering the compressor inlet. iii) Furthermore, the temperature of the low pressure side (with less fluid in it) will go back to the higher environmental temperature when operation stops; thus the fluid inside

would end up being saturated vapour at the environmental temperature once equilibrium is reached.

### 4.3. Boundary Conditions for the Simulation Domain

The inlet water temperature for the outer tubes of the external heat exchangers (gas cooler and evaporator) is 25 °C. The inlet and outlet boundaries of the simulation domain of the CO<sub>2</sub> refrigerant circuit are dependent on the compressor's operating characteristics. Data of the compressor efficiency and speed was not available; hence, some reasonable assumptions are made in this section to develop the simulation model. The boundary conditions are continually updated at the start of each iteration (as needed by the fully implicit temporal scheme used). A continuous compressing model is adopted for the compressor, in which the compressor sucks and expels gas at the same instant in time.

The outlet of the simulation domain is the inlet to the compressor. Therefore:

$$\rho_{in\_comp} = \rho(N_{tot}) \tag{4.4a}$$

$$h_{in\_comp} = h(N_{tot}) (4.4b)$$

$$s_{in\_comp} = s(N_{tot}) (4.4c)$$

The mass flow rate through the compressor is determined by:

$$\dot{m}_{comp} = \rho_{in\_comp} Vol_{comp} \frac{N}{60} \varepsilon_{\nu} \tag{4.5}$$

where  $Vol_{comp}=1.75x10^{-6}~\mathrm{m}^3$  is the given compressor displacement volume, N=2400 is the assumed speed of the compressor in rpm, and  $\varepsilon_v$  is the compressor volumetric efficiency. For the compressor used a value of  $\varepsilon_v=0.954$  is calculated to ensure that equation (4.5) satisfies the compressor rated mass flow rate as determined in section 5.3. Also for the simulation model it is assumed that the compressor reaches full speed instantly, at t=0 s.

Since a transient model for the compressor efficiency is not available, it is decided to use a constant efficiency as determined from a steady-state test point. There were however no power usage rated by the compressor manufacturer data; therefore, the compressor efficiency could not be calculated. An isentropic efficiency of  $\varepsilon_{isen}=0.716$  is thus assumed and validated later during experimentation.

The outlet of the compressor is taken to be at the pressure of the first control volume in the simulation domain i.e.:

$$P_{out\_comp} = P(1) (4.6)$$

To determine the state of the  $CO_2$  expelled by the compressor, it is first necessary to calculate the state following an isentropic process. Then an isentropic efficiency is applied to determine the actual state. The state is calculated as follows: For isentropic compression the enthalpy at exit,  $h_{out\_comp\_isen}$ , can be determined by the two independent variables at exit already known i.e. from  $P = P_{out\_comp}$  and  $s = s_{in\_comp}$ . The exit state would be single phase, thus the script file  $CO2\_1Ph\_Prop\_at\_P\_and\_s.m$  (included in the project file) is used to determine properties from a given pressure and specific entropy.

The actual enthalpy at the outlet of the compressor can be calculated as:

$$h_{out\_comp} = h_{in\_comp} + \frac{h_{out\_comp\_isen} - h_{in\_comp}}{\varepsilon_{isen}}$$
(4.7)

All properties at the outlet of the compressor can now be calculated from the pressure and enthalpy, i.e.  $P_{out\_comp}$  and  $h_{out\_comp}$ , with the script file CO2\_1Ph\_Prop\_at\_P\_and\_h.m (included in the project file).

The compressor discharge specific internal energy is treated as a source term in the boundary control volume of the energy equation (which is written in the form of specific internal energy) as shown in section 4.7.2. i.e.:

$$S_u = \dot{m}_{comp} u_{out\ comp} \tag{4.8}$$

where  $S_u$  is a source of internal energy.

The compressor discharge density is used to calculate the velocity which is treated as an inlet boundary velocity in the momentum equation as shown in section 4.7.3. i.e.:

$$v_z(1) = \frac{\dot{m}_{comp}}{\rho_{out\_comp} A_{inlet}} \tag{4.9}$$

where  $A_{inlet}$  is the inlet area of the first control volume.

The outlet boundary velocity of the simulation domain is also defined by the compressor mass flow rate as:

$$v_z(N_{tot} + 1) = \frac{\dot{m}_{comp}}{\rho_{in\_comp} A_{outlet}}$$
(4.10)

where  $A_{outlet}$  is the outlet area of the last control volume.

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To develop relations for the thermal resistances in Figure 11, it is necessary to first state some common variable definitions, such as Prandtl number and Reynolds number.

The Prandtl number of the fluid is defined as:

$$Pr = \frac{\mu \cdot c_P}{k} \tag{4.12}$$

where  $\mu$  is the dynamic viscosity,  $c_P$  is the isobaric specific heat and k is the thermal conductivity.

The Reynolds number for the flow is:

$$Re = \frac{\rho \cdot abs(\bar{v}_z) \cdot D_h}{\mu} \tag{4.13}$$

where  $\rho$  is the density,  $abs(\bar{v}_z)$  is the absolute value of the average velocity over the section considered and  $D_h$  is the hydraulic diameter of the flow.

The thermal resistance for the inner tube fluid is defined by:

$$R_i = \frac{1}{ht_i \cdot \pi \cdot Di_i \cdot \Delta z} \tag{4.14}$$

where  $Di_i$  is the inner diameter of the inner tube,  $\Delta z$  the length of tube being considered, and the heat transfer coefficient is

$$ht_i = \frac{Nu \cdot k}{D_h} \tag{4.15}$$

The Nusselt number is

$$Nu = 0.023 \cdot Re^{0.8} \cdot Pr^n \tag{4.16}$$

The exponent n is 0.3 when the fluid is expected to be cooled and is 0.4 when it's expected to be heated.  $D_h = Di_i$  is the hydraulic diameter of the flow.

The inner copper tube thermal resistance is defined as:

$$R_{Cu} = \frac{ln\left(\frac{Do_i}{D\dot{i}_i}\right)}{2 \cdot \pi \cdot k_{Cu} \cdot \Delta z} \tag{4.17}$$

where  $Do_i$  and  $Di_i$  is the inner tube outer and inner diameters, respectively.  $k_{Cu}$  is the thermal conductivity of copper, and  $\Delta z$  is the length of tube being considered.

The thermal resistance for the annulus fluid on the outer side of the inner tube is defined as:

$$R_o = \frac{1}{ht_o \cdot \pi \cdot Do_i \cdot \Delta z} \tag{4.18}$$

where  $Do_i$  is the outer diameter of the inner tube,  $\Delta z$  is the length of tube being considered and the heat transfer coefficient is

$$ht_o = \frac{Nu \cdot k_{fluid}}{D_h} \tag{4.19}$$

and

$$Nu = 0.023 \cdot Re_{flow}^{0.8} \cdot Pr^n \tag{4.20}$$

The exponent n is 0.4 when the fluid is expected to be heated and is 0.3 when it's expected to be cooled.  $D_h = Di_o - Do_i$  is the hydraulic diameter of the flow, where  $Di_o$  is the inner diameter of the outer tube and  $Do_i$  is the outer diameter of the inner tube.

The total thermal resistance is:

$$R_{tot} = R_i + R_{Cu} + R_o (4.21)$$

The heat transfer rate can now be calculated as:

$$\dot{Q}_{ht} = \frac{T_o - T_i}{R_{tot}} \tag{4.22}$$

The shear stress due to friction is calculated as follows:

The Reynolds number is calculated using equation (4.13) and the appropriate hydraulic diameter for the flow.

The skin friction factor  $C_f$  is calculated based on the flow type encountered:

if Re > 2300 (Flow is assumed turbulent)

$$C_f = 0.078 \cdot Re^{-0.25} \tag{4.23}$$

elseif  $Re \le 1e - 200$  (If Reynolds number is zero or close to zero, assume no friction)

$$C_f = 0 ag{4.24}$$

or else (Flow is assumed laminar)

$$C_f = \frac{16}{Re} \tag{4.25}$$

The average shear stress due to friction is now defined as:

$$\bar{\tau}_{rz} = 0.5 \cdot C_f \cdot \rho \cdot abs(\bar{v}_z) \cdot \bar{v}_z \tag{4.26}$$

## 4.6. Determining the Properties of Water

It was assumed that the use of saturated liquid properties for the water in the outer tubes of the heat-exchangers would provide results that are reasonably accurate, especially since the operating conditions for the water would be close to ambient temperature and pressure; furthermore, it would also require less computational effort in the simulation model.

The thermodynamic properties of water are calculated using the saturated liquid property equations given by Wagner and Pruß (2002). The conductivity, viscosity and isobaric heat capacity are calculated using the equations for saturated liquid water given by Kröger (1998: A.9).

The water side of the heat exchanger tubes are simulated as incompressible fluid and at a constant mass flow rate; therefore, in this simple model only the energy equation is used in the form:

$$u = u^{o} + \Delta t \left( \dot{m} \cdot h_{in} - \dot{m} \cdot h_{out} - \dot{Q}_{ht} \right) / m_{CV}$$
(4.27)

where u is specific internal energy,  $u^o$  is old time level's specific internal energy,  $\Delta t$  is time-step size,  $\dot{m}$  is mass flow rate,  $h_{in}$  is enthalpy flowing in from upstream neighbouring CV,  $h_{out}$  is enthalpy flowing out of the current CV,  $\dot{Q}_{ht}$  is heat loss from the CV, and  $m_{CV}$  is the mass of water in the current CV.

The properties of water are then calculated based on this assumed saturated liquid specific internal energy. The Secant method (Chapra, 2008: 150) is applied to iteratively find the corresponding temperature and then all other

properties are calculated. The water property functions used in the simulation program can be seen in the project file.

## 4.7. Discretisation of Equations of Change Applied to Control Volumes

Time-dependent equations of change used in the model, as stipulated in section 2.6, are:

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho v_z) = 0 \tag{4.28}$$

Conservation of energy:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial z}(\rho u v_z) = -P \frac{\partial v_z}{\partial z} + \bar{\tau}_{rz} \frac{\partial(v_z)}{\partial r} + S_u$$
(4.29)

Conservation of momentum:

$$\frac{\partial(\rho v_z)}{\partial t} + \frac{\partial}{\partial z}(\rho v_z v_z) = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{rz}}{\partial r}$$
(4.30)

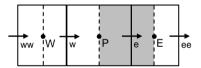


Figure 12: Control volume description

Figure 12 shows the control volumes used in the discretisation of the above three equations. The dots represent the nodes where all scalar quantities are calculated and the arrows represent the velocity nodes.

The mass and energy equations are solved on the node centered scalar control volumes i.e. the control volumes surrounding the nodes with capital letter designation. The momentum equation is solved on a staggered grid relative to the scalar control volumes, such as the shaded control volume in the figure. This arrangement is selected since it prevents the checkerboard pressure field problem encountered in CFD for non-staggered momentum control volumes. Also with this arrangement the calculated pressures are located at the faces of the momentum control volumes; and the calculated velocities can be taken to be at the cell faces of the scalar control volumes. This simplifies the discretisation of these three equations.

The three conservation equations are now developed into a discretised form that is easily capable of being solved by a computer program. A fully implicit temporal discretisation scheme is used. The fully implicit discretisation scheme is unconditionally stable, thus larger time-step sizes, than for explicit methods, can be used. A small time-step size is however used to ensure physically realistic results. The fully implicit scheme uses new values only, thus it requires iteration and in most cases under-relaxation is necessary.

The discretisation of the three conservation equations are to follow in the particular order in which it was implemented within the simulation model; as can be seen in the iteration script file, Itterate\_UD\_density\_based.m, in Appendix C4.

#### 4.7.1. Discretisation of the Conservation of Mass

The conservation of mass equation (4.28) is discretised to give an equation to solve for the new densities based on a velocity or guessed velocity field.

Conservation of mass, repeated here for convenience:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho v_z) = 0$$

The conservation of mass is first integrated over a control volume and written in terms of finite differences:

$$(\rho_P - \rho_P^{o}) \frac{\Delta V}{\Delta t} + [\rho v_z A]_e - [\rho v_z A]_w = 0$$
(4.31)

This expression is now formulated into a form to solve the density field based on a given (or guessed) velocity field:

$$(\rho_P - \rho_P^0) \frac{\Delta V}{\Delta t} + [v_z A]_e \rho_e - [v_z A]_w \rho_w = 0$$
(4.32)

Define convection values (provides a shortened method of writing the equations) as:

$$F_w = [v_z A]_w \text{ and } F_e = [v_z A]_e$$
 (4.33)

where  $[v_z A]_w$  is the product of velocity  $v_z$  and area A at the western face of the control volume and  $[v_z A]_e$  is the product - at the eastern face. Substitution gives:

$$(\rho_P - \rho_P^o) \frac{\Delta V}{\Delta t} + F_e \rho_e - F_w \rho_w = 0 \tag{4.34}$$

An upwind differencing scheme is selected for the face values of density, due to its robustness when using a small number of control volumes. The development of the final form of the discretised equation for the density follows the same procedure as explained in section 2.6 for any general variable  $\phi$ .

The final form is therefore:

$$a_{P}\rho_{P} = a_{W}\rho_{W} + a_{E}\rho_{E} + a_{P}^{o}\rho_{P}^{o} + S_{C}$$
(4.35)

where:

$$a_P = a_W + a_E + (F_e - F_w) + a_P^o - S_P$$

$$a_W = \max(F_w, 0) \qquad a_E = \max(0, -F_e) \qquad a_P^o = \frac{\Delta V}{\Delta t}$$

$$S_C = 0 \qquad S_P = 0$$

#### 4.7.2. Discretisation of the Conservation of Energy

The conservation of energy equation (4.29) is discretised to give an equation to solve for the new specific internal energy field based on the velocity field already used above and the newly obtained density field.

Conservation of energy, repeated here for convenience:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial z}(\rho u v_z) = -P \frac{\partial v_z}{\partial z} + \bar{\tau}_{rz} \frac{\partial(v_z)}{\partial r} + S_u$$

The conservation of energy is first integrated over a control volume and written in terms of finite differences:

$$[(\rho u)_{P} - (\rho u)_{P}^{o}] \frac{\Delta V}{\Delta t} + [\rho v_{z} A]_{e} u_{e} - [\rho v_{z} A]_{w} u_{w}$$

$$= -P_{P}[(A v_{z})_{e} - (A v_{z})_{w}] + \bar{\tau}_{rz} \delta \rho \Delta z \bar{v}_{z} + \bar{S}_{u} \Delta V$$
(4.36)

Define convection values as:

$$F_{w} = [\rho v_{z} A]_{w} \text{ and } F_{\rho} = [\rho v_{z} A]_{\rho}$$

$$(4.37)$$

Substitution and rewriting yields:

$$\left[\rho_{P} \frac{\Delta V}{\Delta t}\right] u_{P} + F_{e} u_{e} - F_{w} u_{w} 
= \left[\rho_{P}^{o} \frac{\Delta V}{\Delta t}\right] u_{P}^{o} - P_{P}[(Av_{z})_{e} - (Av_{z})_{w}] + \bar{\tau}_{rz} \wp \Delta z \bar{v}_{z} 
+ \bar{S}_{u} \Delta V$$
(4.38)

The source term  $\bar{S}_u \Delta V$  is used to incorporate the heat transferred  $\dot{Q}_{ht}$  through the tube walls and axial conduction in the gas. Also to accommodate programming the pressure and shear stress components are included in the source term. Any suitable discretisation method can now be used to represent the face values of specific internal energy. Once again upwind differencing is selected for its robustness and fundamental properties as discussed in section 2.6. Following the procedure as outlined in section 2.6 gives:

$$a_P u_P = a_W u_W + a_E u_E + a_P^0 u_P^0 + S_C (4.39)$$

where:

$$a_P = a_W + a_E + (F_e - F_W) + a_P^o \frac{\rho_P}{\rho_P^o} - S_P$$

$$a_W = \max(F_W, 0) \qquad a_E = \max(0, -F_e) \qquad a_P^o = \rho_P^o \frac{\Delta V}{\Delta t}$$

$$S_C = -P_P[(Av_z)_e - (Av_z)_w] + \bar{\tau}_{rz} \wp \Delta z \bar{v}_z + \dot{Q}_{ht}$$

$$S_P = 0$$

#### 4.7.3. Discretisation of the Conservation of Momentum

Before the momentum equation is discretised, the equation of state is used to obtain updated values of all properties, including pressure, based on the newly obtained density - and specific internal energy field.

The conservation of momentum equation (4.30) is discretised to give an equation to solve for the new velocities based on the newly obtained density field and properties (especially the pressure field).

Conservation of momentum, repeated here for convenience:

$$\frac{\partial(\rho v_z)}{\partial t} + \frac{\partial}{\partial z}(\rho v_z v_z) = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{rz}}{\partial r}$$

Integrating the conservation of momentum over the staggered momentum control volume (shaded control volume in Figure 12) gives:

$$[(\rho v_z)_P - (\rho v_z)_P^o] \frac{\Delta V}{\Delta t} + [\rho v_z A]_e (v_z)_e - [\rho v_z A]_w (v_z)_w$$

$$= -(P_e - P_w) A_P - \bar{\tau}_{rz} \delta \Delta z$$
(4.40)

Define convection values as:

$$F_{w} = [\rho v_{z} A]_{w} \text{ and } F_{e} = [\rho v_{z} A]_{e}$$
 (4.41)

Substitute and formulate this expression into a form to solve the velocities:

$$\left[\rho_{P} \frac{\Delta V}{\Delta t}\right] (v_{z})_{P} + F_{e}(v_{z})_{e} - F_{w}(v_{z})_{w} 
= \left[\rho_{P}^{o} \frac{\Delta V}{\Delta t}\right] (v_{z})_{P}^{o} + (P_{w} - P_{e})A_{P} - \bar{\tau}_{rz} \omega \Delta z$$
(4.42)

Using upwind differencing as the discretisation scheme for the face velocities gives:

$$a_P(v_z)_P = a_W(v_z)_W + a_E(v_z)_E + a_P^{\ o}(v_z)_P^{\ o} + S_C \tag{4.43}$$

where:

$$a_{P} = a_{W} + a_{E} + (F_{e} - F_{w}) + a_{P}^{o} \frac{\rho_{P}}{\rho_{P}^{o}} - S_{P}$$

$$a_{W} = \max(F_{w}, 0) \qquad a_{E} = \max(0, -F_{e})$$

$$a_{P}^{o} = \rho_{P}^{o} \frac{\Delta V}{\Delta t}$$

$$S_{C} = (P_{w} - P_{e})A_{P} - \bar{\tau}_{rz} \wp \Delta z$$

$$S_{P} = 0$$

## 4.8. Algorithm for Simulating a Refrigeration Cycle

The flow is compressible, therefore the usual pressure based algorithms such as SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) are not well suited to solving the flow equations. There is a strong link between density and pressure in compressible flows. Figure 13 shows the density-based algorithm to solve the conservation equations for each time-step. The simulation starts with the initial conditions as described in section 4.2. The boundary conditions as set out in section 4.3 are calculated at the start of each iteration (step 1). Each time-step is solved in a similar fashion as with steady-state problems. To start the simulation of the current time-step a velocity field for the scalar control volume

faces is guessed or taken as zero for the first time-step. With the guessed velocity field the conservation of mass equation is discretised to form an equation to solve for the new density field (step 2). The velocities with the newly obtained densities are then used in the discretisation of the energy equation to form an equation to solve for the new specific internal energy field (step 3).

The newly obtained density and specific internal energy are now used in the equation of state to determine the new pressures and all other properties (step 4). The new pressures, densities and other variables are then used in the discretisation of the momentum equation to form an equation to solve for the new velocity field (step 5). Finally the residuals of each conservation equation are compared to a certain convergence level. If convergence is reached then the iteration stops and the solution is advanced to a new time-step, or else it will reiterate with the new velocity. A relaxation factor,  $\alpha_v$ , is applied to the velocity field in order to facilitate convergence where the new guess for velocity  $v^*$  is defined as:

$$v^* = (1 - \alpha_v)v^* + \alpha_v v \tag{4.44}$$

where  $v^*$  on the right hand side is the previously guessed/used velocity and v is the newly calculated velocity. A relaxation factor of  $\alpha_v=0.050$  proved to produce stable results from initial start-up till steady-state. The script file ltterate\_UD\_density\_based.m, in Appendix C4, performs the function of Figure 13.

The convergence indicator, of how well the current variable satisfies the new coefficients, is determined by the use of a normalised global residual (as given by Versteeg & Malalasekera (2007: 288)) which is defined as:

$$norm\_Global\_residual = \frac{sum(abs(residual))}{sum(abs(norm\_factor))}$$
(4.45)

where the *residual* is defined as the difference between left and right hand sides of the discretised equation for a node:

$$residual = a_P \phi_P - (a_W \phi_W + a_E \phi_E + a_P^o \phi_P^o + S_C)$$

$$(4.46)$$

and the normalisation factor,  $norm\_factor$ , is the left hand side of the discretised equation,  $a_P\phi_P$ . Convergence is reached when the normalised global residuals reach a level of  $10^{-8}$ .

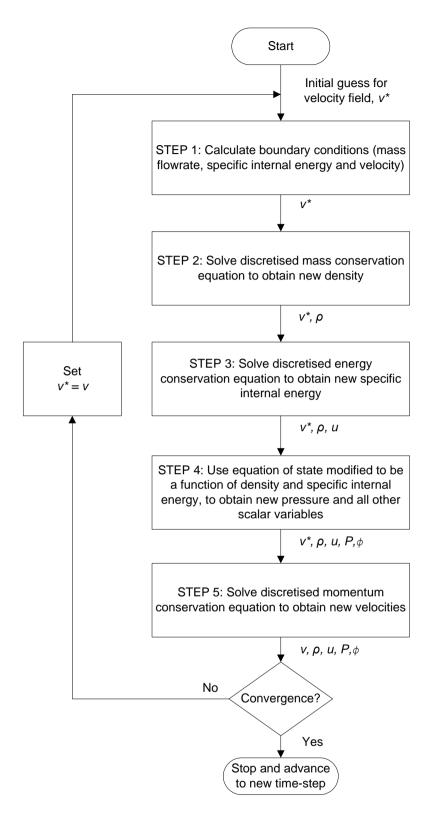


Figure 13: Density-based algorithm for solving compressible flow

#### 5. REFRIGERATOR DESIGN

The system being designed is based on a small household refrigerator. The system serves as a test unit to evaluate refrigeration performance at different operating conditions, and to experimentally validate the simulation program written in this thesis. There are many different routes to designing a refrigerator. The design method explained here serves as an introductory method only.

### 5.1. Compressor Selection

To design a refrigerator an evaporator temperature is selected, an approximate cooling load range is calculated or assumed, and the environment temperature must be known. It was decided to build the system to be capable of reaching an evaporator temperature of -10 °C. The compressor must be capable of producing an outlet pressure that is equal or higher than the saturation pressure of the refrigerant corresponding to the environmental temperature, in order to achieve adequate heat rejection to the environment. Normal household refrigerators have a rated cooling load of about 1 kW. The small EK6210CD CO<sub>2</sub> refrigerant compressor from Embraco (product data attached in Appendix D) is selected since it is capable of working at these conditions with a rated cooling load of 700 W at the selected evaporation temperature of -10 °C. This rated cooling load is deemed adequate for the test unit developed for this project.

## 5.2. Internal Volume of High Pressure Side

The volume of the high pressure (HP) side must be as low as possible in order to ensure a high enough pressure and thus temperature for heat rejection. A density limit for the HP side is placed by the compressor manufacturer (for compressor safety), in the event of expansion device blockage (all refrigerant is in the HP side only). The EK6210CD Embraco compressor specifies a system with a maximum CO<sub>2</sub> refrigerant charge of 500 g and a maximum HP side density of 0.65 g/cm<sup>3</sup> (Embraco, [S.a.]). It was selected to use 435 g of CO<sub>2</sub>, which is well below the 500 g maximum specified.

Based on the mass of refrigerant used, the high side volume must be larger than:

$$V_{\text{HP\_Lower\_limit}} = \frac{\text{Mass used}}{\text{Density limit}} = \frac{435 \text{ g}}{0.65 \frac{\text{g}}{\text{cm}^3}} = 669.231 \text{ cm}^3$$
 (5.1)

The tubes used for the refrigerator are made of copper; most of them are thick-walled in order to handle the high pressure requirements of the CO<sub>2</sub> refrigerant during operation. Table 4 shows the high pressure side tube details used to manufacture the refrigerator.

To connect the different tubes to each other one can either solder them together (a process called swaging of the tubes) or one can use Swagelok tube fittings. Swagelok tube fittings offer easy assembly, disassembly and re-assembly of the tubes therefore providing flexibility in changing the design if needed.

Table 4: Tube details of the high pressure side

Tubes used for the high pressure side	Length, outer diameter, thickness, pressure rating	Inner volume (cm³)
Connecting tube between compressor and gas cooler $(L_{comp\_gc})$	2.15 m, 6.35 mm (1/4"), 0.91 mm, 119.9 bar	34.652
Gas cooler tube $(L_{gc})$	19.7 m, 8 mm, 0.9 mm, 93.9 bar	594.757
Connecting tube between gas cooler and internal heat exchanger $(L_{gc\_IHX})$	1 m, 6.35 mm, 0.91 mm, 119.9 bar	16.117
Internal heat exchanger inner tube $(L_{IHX})$	2.5 m, 4.76 mm (3/16"),0.61 mm, 105.9 bar	24.606
Connecting tube between inner tube of IHX and capillary tube $(L_{IHX\_ct})$	0.45 m, 4.76 mm (3/16"), 0.61 mm, 105.9 bar	4.429
	Total internal volume	674.558

In the simulation program the connection fittings are approximated by adding cone shaped control volumes to account for momentum change at the changing tube diameters and the extra volume added by the connection fittings. Therefore, the high pressure side volume is marginally increased to a value of (as can be seen in the simulation program initialise script in Appendix C2):

$$V_{\rm HP} = 675.75 \, \text{cm}^3 \tag{5.2}$$

This value is larger than the lower limit set in equation (5.1), but not excessively larger; thus it is an acceptable design.

## 5.3. Capillary Tube Design using a Steady-State Capillary Tube Simulation Model

The low pressure (LP) side can now be considered in the design of a capillary tube for the system. The capillary tube operates between inlet conditions at the HP side and evaporator temperature needed at its outlet. It was selected to have an evaporator saturation temperature of -10  $^{\circ}$ C.

The EK6210CD Embraco compressor has a rated cooling capacity of 700 W at an evaporation temperature of -10 °C as shown in the product data attached in Appendix D. The saturation pressure of CO<sub>2</sub> at -10 °C is 26.487 bar. The enthalpy entering the evaporator is equal to the enthalpy entering the capillary tube since the adiabatic throttling process is isenthalpic. The enthalpy entering the capillary tube is determined from the rated compressor discharge pressure of 85 bar and gas cooler return gas temperature of 32 °C. The enthalpy calculated at this pressure and temperature is -217.84 kJ/kg. The compressor inlet temperature from the test conditions is 32 °C. The enthalpy calculated at 32 °C and 26.487 bar is -20.24 kJ/kg. The mass flow rate corresponding to the rated cooling capacity is therefore:

$$\dot{m} = \frac{\text{Cooling load}}{\left(h_{out_{ev}} - h_{in_{ev}}\right)} = \frac{0.7 \text{ kW}}{-20.24 \frac{\text{kJ}}{\text{kg}} - \left(-217.84 \frac{\text{kJ}}{\text{kg}}\right)} = 3.54 \text{ g/s}$$
 (5.3)

A capillary tube now needs to be designed which can provide this mass flow rate at the same operating conditions as shown in the product data from Embraco. Figure 14 shows the steady-state capillary tube model which calculates the mass flow rate based on a capillary tube length and inside diameter.

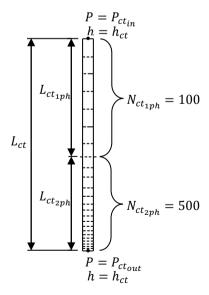


Figure 14: Steady-state capillary tube model

The inlet and outlet pressures and enthalpy of the capillary tube are as mentioned above. Homogenous flow is assumed for the two-phase flow in the simulation model. The steady-state simulation model is written to distinguish between three different operating scenarios:

- 1) Single phase only (if  $P_{ct_{in}}$  and  $P_{ct_{out}}$  are both above the saturation pressure at  $h_{ct}$ ).
- 2) Two-phase only (if  $P_{ct_{in}}$  and  $P_{ct_{out}}$  are both below the saturation pressure at  $h_{ct}$ ).
- 3) Single phase for the first part and then two-phase for the rest of the length of the capillary tube (if  $P_{ct_{in}}$  is above and  $P_{ct_{out}}$  is below the saturation pressure at  $h_{ct}$ ).

The simulation model first determines the saturation pressure at  $h_{ct_{in}}$  and then decides which scenario to follow. Depending on which scenario is encountered the simulation domain is divided into a set number of control volumes of equal pressure drop (and therefore variable length) for the corresponding phase. Scenario three is encountered in the above test conditions; therefore the simulation domain (capillary tube as shown in Figure 14) is divided into 100 control volumes in the single phase region with a pressure drop of:

$$\Delta P_{1ph} = \frac{P_{ct_{in}} - P_{sat@h_{ct}}}{N_{ct_{1ph}}} \tag{5.4}$$

and 500 control volumes in the two-phase region with a pressure drop of:

$$\Delta P_{2ph} = \frac{P_{sat@h_{ct}} - P_{ct_{out}}}{N_{ct_{2ph}}} \tag{5.5}$$

Each control volume is now assigned a pressure based on the constant pressure drop per control volume along the capillary tube and the constant enthalpy as given; thus properties for each control volume can now be calculated. To start the simulation a capillary tube length and inner diameter is specified and a mass flow rate is guessed. Based on the mass flow rate, inner diameter and the pressure drop per control volume a corresponding length for each control volume is calculated. The control volume lengths are then added together to calculate the total length of the capillary tube. If the added length of the capillary tube is more than the specified length, then the mass flow rate guessed is too small and needs to be increased, otherwise it needs to be decreased.

The bisection method (Chapra, 2008: 122) is used to iteratively converge on the correct mass flow rate. The steady-state capillary tube simulation model can be seen in Appendix E. There are a few different capillary tube diameter options available. From trial and error using the simulation program it was decided to

use the TC31 capillary tube with inner diameter of 0.031" (0.79 mm) and length of 3.5 m. It gives a mass flow rate of:

$$\dot{m} = 3.51 \text{ g/s}$$
 (5.6)

which is deemed close enough to the mass flow rate in equation (5.3).

#### 5.4. Internal Volume of Low Pressure Side

Now that the volume of the high pressure side is known, the volume of the low pressure (LP) side may be determined. The volume of the LP side depends on the following two conditions: the evaporator temperature and the rated cooling load of the compressor. The transient simulation program, as discussed in section 4, is used to determine the low pressure side volume by successively trying different volumes (tube lengths) until the one selected suits the conditions mentioned above.

Table 5: Tube details of the low pressure side

Tubes used for the low pressure side	Length, outer diameter, thickness, pressure rating	Inner volume (cm³)
Evaporator tube $(L_{ev})$	12.9 m, 8 mm, 0.9 mm, 93.9 bar	389.460
Connecting tube between evaporator and internal heat exchanger $(L_{ev\_IHX})$	0.93 m, 6.35 mm (1/4"), 0.91 mm, 119.9 bar	14.989
Internal heat exchanger outer tube $(L_{IHX})$	2.5 m, 9.53 mm (3/8"), 0.91 mm, 79.6 bar	72.230
Connecting tube between internal heat exchanger outer tube and compressor ( $L_{IHX\_comp}$ )	0.35 m, 6.35 mm (1/4"), 0.91 mm, 119.9 bar	5.641
	Total internal volume	482.320

Table 5 shows the low pressure side tube details obtained from the simulation and used to manufacture the refrigerator. Again the simulation takes also into account the added volume of the connection fittings between the tubes, therefore the volume increases marginally to a value of (as can be seen in the simulation program initialise script):

$$V_{\rm LP} = 485.15 \,\rm cm^3 \tag{5.7}$$

# 5.5. Heat Exchanger Designs

The design of a heat exchanger depends on the heat transfer rate needed and the convection coefficients of the fluids exchanging the heat. For this project tube-in-tube heat exchangers, with water in the outer tubes, are used for the gas cooler and the evaporator. Water has a high convection heat transfer coefficient and a high specific heat relative to air; therefore, it can absorb/reject more heat per mass and at a faster rate than air. Also it is easy to control and measure its temperature and mass flow rate; therefore it provides for a reliable method for validation of heat transferred during experimentation.

Both evaporator and gas cooler are over designed to handle higher heat transfer rates if needed; thus providing variable operating conditions for the refrigeration system. The water inlet temperature and mass flow rate to the heat exchangers can be varied; also sections of the heat exchangers can be included or excluded in order to accomplish different cooling/heating loads. The refrigerator built thus serves as a good experimental unit, capable of being tested thoroughly at different operating conditions. Table 6 shows the details of the gas cooler - and evaporator outer tubes.

Table 6: Details of the outer tubes of the heat exchangers

Tube lengths for the heat exchanger outer tubes	Length, outer diameter of inner tube, outer diameter of outer tube, thickness of outer tube, pressure rating of outer tube	Inner volume (cm³)
Gas cooler heat exchanger outer tube	14 m, 8 mm, 15.88 mm (5/8"), 0.71 mm, 34.40 bar	1595.365
Evaporator heat exchanger outer tube	12 m, 8 mm, 15.88 mm (5/8"), 0.71 mm, 34.40 bar	1367.456

#### 6. EXPERIMENTAL SETUP

The refrigerator system shown in Figure 15 is now set up with experimental equipment necessary to measure its performance. First the calibration method for the thermocouples used is explained, then the total experimental setup is shown, and finally the experimental test procedure is discussed.

## 6.1. Thermocouple Calibration

The 20 T-type thermocouples used for the experiment were calibrated using a platinum resistance thermometer and a Fluke field metrology well system (manufacturer: model nr: 9142, serial nr: B29291) The Fluke system generates the desired calibration temperature, by heating or cooling the metal bar insert it uses, and measures the resistance of the thermometer. The platinum resistance thermometer details are:

Manufacturer: ISOTECH Model number: 935-14-72 Serial number: 191069

The thermometer was calibrated at Rapid Instrumentation CC (a member of the South African National Accreditation System (SANAS) with Accredited Laboratory Number 366). The calibration certificate number is: RAP15738.

The procedure for calibration is as follows: a number of thermocouples are inserted into a metal bar and then the bar is inserted in the Fluke system. A temperature set point is set for the Fluke system and then allowed sufficient time to reach steady-state. Once the Fluke system reaches steady-state (the Ohm reading of the thermometer remains constant), the Agilent Data Logger scan is started and it is first confirmed that the corresponding thermocouples have indeed reached state-state; only then is the scan restarted to store the steadymeasured temperatures of the corresponding thermocouples. Temperatures are recorded every 5 s for a period of about 4 minutes. At the same time the Ohm reading for the platinum resistance thermometer is recorded manually into a spread sheet from which the corresponding true temperature is calculated. It was deemed sufficient for the refrigerator experiment to have calibration points from -10 °C to 100 °C at 10 °C intervals. Average values for each temperature point are then calculated for each thermocouple. The average measured values are then plotted versus the true values, as shown in Figure 16 for thermocouple 1. The remaining thermocouples all have a good correlation coefficient to their straight trend lines; therefore, it was decided for brevity not to show all the thermocouple calibration plots here (Appendix F provides a table of all the calibration equations and their correlation coefficients).

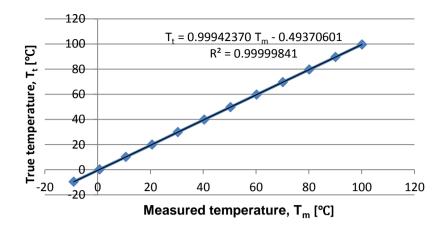


Figure 16: Thermocouple 1 - calibration curve

# 6.2. Experimental System Layout

The experimental setup, shown in Figure 17, consists of the refrigeration system, as shown in Figure 15, with 20 T-type thermocouples, 2 pressure gauges, a control unit for the compressor, a water container, a water pump, a water chiller, a laptop, a data logger and a video camera (CAT B-15 smartphone).



Figure 17: Experimental system

The experimental recording part may now commence as follows:

- First record a set of data to keep as reference of the initial conditions for the experiment. Usually around 3 to 5 minutes of data.
- Place the video camera (CAT B-15 smartphone) at the desired location and start to record the pressure gauges.
- Start recording data on the laptop and then switch on the refrigerator.
- Observe the recording time when the compressor turns on. Usually around 52 seconds after switching the switch on.
- Record data until all temperatures have reached a sufficiently stable value.
- Switch off the data logger and the compressor. Test is complete.

## 7.2. Boundary Conditions and External Heat Exchangers

The boundary conditions, enforced by the compressor, for the simulation domain are as discussed in section 4.3; with a step-input compressor speed at t = 0 s of N = 2400 rpm, a constant compressor volumetric efficiency of 0.954 and a constant isentropic efficiency of 0.716.

The external heat exchangers (gas cooler and evaporator) contain water flowing in the outer tubes at a mass flow rate of 0.050 kg/s, in a counter flow direction in relation to the CO<sub>2</sub> refrigerant flow, and at an inlet temperature of 25 °C.

## 7.3. Grid Independence

A grid independence study is done, as shown here in Figure 20, for the pressure distribution at 150 ms simulation time. It was decided to use the pressure distribution as an indication of grid independence, since all fluid properties are dependent mainly on the operating pressure in the system. The pressure distribution for the different grid sizes show that further grid refinement produces no remarkable difference; thus grid independence has been achieved. Based on this study and in the interest of producing results that are reasonably accurate, in the least amount of time, it was elected to use a grid size of  $N_{tot} = 1390$  i.e. use 1390 control volumes.

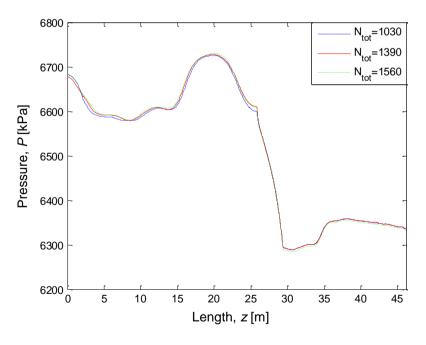


Figure 20: Pressure distribution at 150 ms for grid independence study

## 7.4. Simulation Domain Geometry Properties

From the grid independence study it was chosen to use a total number of 1390 control volumes for the simulation domain. The excerpt below, from the initialise scrip file in Appendix C2, shows the number of control volumes used for the different sections of the simulation domain.

```
%Form the control volumes of the whole solution domain.
N comp gc = 52; %Number of cv's for the connecting tube
                 %between outlet of compressor and inlet of
                 %gas cooler.
N tr1 = 1;
                %Number of cv's for transition between
                %comp gc tube and gas cooler tube.
N gc = 400;
                %Number of cv's for the gas cooler.
N tr2 = 1;
                %Number of cv's for transition between gas
                %cooler tube and gc IHX tube
N gc IHX = 66; %Number of cv's between outlet of gas cooler
                %and IHX.
N tr3 = 1;
                %Number of cv's for transition between
                %qc IHX tube and IHX tube
N IHX = 120; %Number of cv's for the Internal Heat
                 %Exchanger (IHX) inner tube.
N tr4 = 1;
                %Number of cv's for transition between IHX
                %tube and IHX ct tube
N IHX ct = 24; %Number of cv's for the connecting tube
                %between IHX and Capillary tube.
N tr5 = 2;
                %Transition between IHX ct tube and
                %capillary tube
N_ct = 230;
N_tr6 = 2;
                %Number of cv's for the Capillary Tube.
                %Transition between capillary tube and
                %evaporator tube
N_{ev} = 300; %Number of cv's for the Evaporator.

N_{tr7} = 1; %Transition between evaporator tube
                %Transition between evaporator tube and
                %ev IHX tube
N_ev_IHX = 40; %Number of cv's for the connecting tube
                %between outlet of Evaporator and IHX.
N tr8 = 3;
                %Transition between ev_IHX tube and IHX tube
\sqrt[8]{N} IHX = 120;
                %Number of cv's used for outer tube of IHX
N tr9 = 3;
                %Transition between IHX tube and IHX comp
                 %tube
N IHX comp = 23; %Number of cv's for the connecting tube
                %between the IHX outlet and compressor
                 %inlet.
```

Figure 21 shows the control volume lengths for the different sections. A stretch ratio is applied to the different tube sections i.e. variable control volume lengths are used. The minimum control volume length is decided as 15 mm, which is due to transition pieces used between tube sections. The stretch ratio is kept close to a value of one in order to have a good aspect ratio from one control

The slight undershoots and overshoots seen at the transition of tubes (deemed acceptable as is) can be further reduced by refining the mesh locally or by implementing a second-order upwind differencing scheme instead of the first-order upwind differencing scheme currently used.

# 9. EXPERIMENTAL VERSUS SIMULATION RESULTS

In this section the experimental results are compared to the simulation results. The experimental results used are from one of three experiments done at the same conditions to confirm repeatability. The experimental temperatures were measured by tightly tying the thermocouples to the outside of the copper tubes. The simulation temperatures refer to the temperature of the  ${\rm CO_2}$  flowing inside the tubes.

The simulation results shown in section 8, and this section, are for the case where the initial conditions are  $25\,^{\circ}\text{C}$ , water inlet temperature to the heat exchangers are also  $25\,^{\circ}\text{C}$ , the water mass flow rate is  $0.050\,\text{kg/s}$ , and the cooling section of the gas cooler is 14 m long and starts at a distance  $z=2.17\,\text{m}$  from the simulation domain inlet. The experimental refrigerator was however built with the gas cooler cooling section starting at  $z=7.73\,\text{m}$ . It is expected that this discrepancy would not cause much of a difference to the actual operation of the refrigerator. Furthermore, it was not possible to obtain the wanted  $0.050\,\text{kg/s}$  water mass flow rate for the experiment; consequently, the average mass flow rate measured for the evaporator and gas cooler outer tubes was  $0.045548\,\text{kg/s}$ .

Figure 30 shows a comparison of the pressure development predicted by the simulation and what was recorded in the experiment. The initial pressures of the experiment and simulation are 5900 kPa and 6434 kPa, respectively. saturation temperature for CO<sub>2</sub> at 5900 kPa is 21.25 °C. This confirms the initial suspicion that the CO<sub>2</sub> (low conductivity) has not yet reached the new experimental ambient temperature from the previous night's colder temperature. Furthermore, from the figure it is seen that the simulation develops relatively faster than the experiment does, but reaches a steady-state that is relatively close to the experiment. The quick response of pressure is due to the use of a constant isentropic efficiency from start-up and the assumption that the compressor is at full speed from t = 0 s. The water being as close as possible to the compressor outlet dampens the pressure by absorbing heat, thus ensuring that the pressure doesn't reach hazardously high levels. The compressor is a hermetically sealed unit that is intentionally cooled during operation; thus, cooling the gas while it is being compressed. The efficiency would thus be a changing function that is dependent on the transient operating conditions and cooling. It is thus recommended to rather use an isothermal (non-adiabatic) efficiency model

temperature distribution trend agrees well with the experiment, confirming that most of the cooling occurs in the first 7 m of the cooling section. The gas cooler heat rejection rate development through time is shown in Figure 33-(b). The simulation predicts a higher heat transfer rate at the start, but does follow the trend recorded in the experiment. The steady-state temperature increase of the water measured in the experiment is 4.65 °C and the corresponding heat loss rate is 885 W. The simulation predicted steady-state values for water temperature increase and heat loss rate of 5.04 °C and 1050 W, respectively. The higher heat loss predicted by the simulation is due to the use of an isentropic efficiency model for the compressor, which gives a higher compressor outlet temperature. Thus, more heat will now be extracted by the 25 °C incoming water.

Table 7: Comparison of experimental and simulation results

	Experiment	Simulation	
Inlet water temperature to external heat exchangers (°C)	25 ± 0.2	25	
Temperature decrease of water (°C),	4.36	3.70	
water mass flow rate (g/s) and	45.548	50	
corresponding heat transferred to the evaporator (W)	830	772	
Temperature increase of water (°C),	4.65	5.04	
water mass flow rate (g/s) and heat	45.548	50	
transferred from the gas cooler (W)	885	1050	
Measured compressor power input (W)	426	-	
Evaporator temperature (°C)	-9.75	-10.05	
Pressure of HP side (kPa)	7100	7238	
Pressure of LP side (kPa)	2600	2638	

Table 7 shows a summary of the experimental versus simulation results. The experiment shows that the compressor power input is 426 W, but the difference between the gas cooler and evaporator heat transfer rate is only 55 W (885W-830W). This shows that there is a substantial heat loss mostly by the compressor and also along the hot HP side tubes. The simulation on the other hand predicts a compressor energy input to the gas of 278 W. This higher energy input is, as mentioned earlier, due to the incorrect compressor model used. The higher energy input is however absorbed by the gas cooler water

which is 165 W more than in the experiment. This counters the effects of the isentropic compressor model used and explains why the simulation predicted pressures that are relatively close to the experimental pressures. It was however found that if the gas cooler cooling section was moved further away from the compressor outlet, then the pressures reached by the simulation are higher than the experiment. The water cooling section being further away from the compressor amplifies the effects of the incorrect compressor model used. Also the simulation model does not account for axial heat conduction in the copper connecting tubes.

From these results it is evident that a non-adiabatic transient compressor model should be adopted instead of an isentropic compressor model. Due to the inaccurate compressor model used it was decided not to include simulation results for other operating cases, since they would have no further meaning. The results shown by the simulation in this report are nonetheless a confirmation that the simulation model predicts operation within the refrigerator fairly well; and would be more so, if the boundary conditions (compressor model) employed were better. Developing a non-adiabatic transient compressor model is outside the scope of this project.

#### 10. OTHER EXPERIMENTAL RESULTS

Table 8 shows the experimental results for four different operating conditions. Note that the ambient temperature is also maintained at the same temperature as the inlet water to the external heat exchangers. The results show an increase of evaporator temperature with increasing evaporator external water inlet temperature used. From the results it is evident that the refrigerator built was successful in reaching an evaporator temperature close to -10 °C.

The system's measured COP is between 1.86 and 2.12. Additionally, the results show that only 11 to 14 % of the compressor input power is transferred to the gas (determined by the difference between gas cooler and evaporator heat transfer rates measured), while the rest is lost to the environment. The compressor shell temperature was also recorded during experiments. It showed an increase from start-up to steady-state, meaning that the compressor body also absorbs heat from the gas during transient conditions. This confirms the need for using a non-adiabatic transient compressor model for the simulation.

Table 8: Steady-state experimental results for different water inlet temperatures

Inlet water temperature to external heat exchangers (°C)	20	22.5	25	27.5
Temperature decrease of water (°C), water mass flow rate (g/s) and corresponding heat transferred to the evaporator (W)	4.55	4.55	4.36	4.35
	44.675	44.869	45.548	45.554
	851	844	830	828
Temperature increase of water (°C), water mass flow rate (g/s) and heat transferred from the gas cooler (W)	4.8	4.72	4.65	4.65
	44.777	45.161	45.548	45.752
	898	891	885	889
Measured compressor power input (W)	401	416	426	444
Evaporator temperature (°C)	-11.90	-10.70	-9.75	-8.01
Pressure of HP side (kPa)	6800	6950	7100	7800
Pressure of LP side (kPa)	2480	2550	2600	2750
Coefficient of performance	2.12	2.03	1.95	1.86

#### 11. DISCUSSION OF RESULTS

The results obtained by the simulation model are dependent on the compressor model used, since this provides the boundary conditions to the simulation model. The simulation predicts a compressor outlet temperature which is higher than in the experiment, as shown in Figure 31. Also, the experimental results in section 10 show a remarkable heat loss by the compressor, and it was mentioned that the compressor body absorbed heat during the transient process. From the above it is confirmed that the use of a constant isentropic efficiency compressor model (determined from one steady-state point) for the transient simulation model is not appropriate. Therefore, the results shown for the simulation are slightly in error; nonetheless, they still prove that the simulation behaves as expected and confirm that this simulation model can be used for refrigerator designs. The development of a non-adiabatic transient compressor model is outside the scope of this project.

The transient simulation results in section 8 shows how the refrigeration system develops through time. They provide a reasonably accurate description of what occurs within the refrigeration system as the system transitions from standstill through to steady-state conditions. The simulation gives results that correlate well with actual experimental results and expected behaviour.

The pressure wave travels through the domain at the speed of sound, for that corresponding pressure, as shown in Figure 22. The operation of the capillary tube is confirmed in these same graphs by the pressure difference it causes between the low and high pressure side. The constant temperature sections, at about 30 m, shown in the bottom two graphs in Figure 23 confirm that the simulation predicts real life constant temperature (and constant pressure) phase change processes, as encountered in an evaporator. Note there is a small temperature drop with frictional pressure drop here, but it is so small that it's virtually "constant". Heat addition causes phase change from two-phase to saturated gas at a constant temperature, and subsequent heat addition causes a temperature rise.

The velocity graphs in Figure 24 show the high velocity encountered in the capillary tube as expected. Also, it shows how the velocity increases towards its outlet; this is due to a decrease in density along the capillary tube. The mass flow rate graphs in Figure 25 show how the system reaches a steady-state mass flow rate. At the start the compressor has a high mass flow rate due to the high density of the saturated vapour at inlet. The mass flow rate decreases now with decreasing density of the super-heated vapour (at lower pressure) at the inlet; up until the refrigeration system reaches steady-state where the inlet (or inlet density) and outlet conditions of the compressor remain constant. Steady-state

is achieved since the compressor performance is now in equilibrium with the refrigeration system.

The steady-state pressure drop through the sections of the refrigerator shown in Figure 29 confirms the "text-book" assumptions that the LP and HP side could be approximated by constant pressure processes. The capillary tube pressure drop has a slight curve indicating an increase in pressure drop towards the end of the capillary tube; this is due to the increasing friction brought by the higher velocities encountered towards the end of the capillary tube.

The results shown in section 9 confirm that the simulation model correlated well with the experimental system; thus the simulation model is successful. The evaporator temperature, LP and HP pressure achieved by the simulation agrees well with the experiment. The heat transfer rates of the evaporator and gas cooler show trends similar to the experiment and reach steady-state values that are close to the experiment.

# 12. CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

Refrigeration has become a highly essential part of modern day living. Recent abandonment of synthetic refrigerants, due to their damaging effects on the environment, has renewed interest in using  $CO_2$  as refrigerant.  $CO_2$  is a natural gas with no ozone depletion potential and a low global warming potential. The need to obtain a better understanding of  $CO_2$  refrigeration cycles and to design  $CO_2$  refrigerators with a higher COP has led to the development of a transient simulation model for  $CO_2$  refrigerators.

For the development of the transient simulation model a literature study was done covering aspects such as the theoretical vapour-compression refrigeration cycle, the CO<sub>2</sub> transcritical refrigeration cycle, properties of an ideal refrigerant, properties of CO<sub>2</sub> as refrigerant, and finally the use of the control volume method. Furthermore, methods for determining the state of CO<sub>2</sub> in a control volume were developed, which are based on the use of the real gas equation of state for CO<sub>2</sub> from Span and Wagner (1996). These methods cover saturated, single phase and two-phase property determination at a given density and specific internal energy. Finally, assumptions, geometry, boundary conditions and conservation equations (employing the 1D-CFD approach) were defined for the transient simulation model. Lastly, a density-based algorithm to solve the compressible flow equations for the simulation model was developed. The transient simulation model was now complete.

To validate the transient simulation model, a  $CO_2$  refrigerator had to be built. For this reason a  $CO_2$  refrigerator design procedure was developed and used to obtain the design of the experimental refrigerator. The design procedure involved the use of a steady-state capillary tube simulation model to obtain the design of the capillary tube, and used the transient simulation model to validate the design of the entire system.

The refrigerator built was successful in reaching the evaporator design temperature of -10 °C for a cooling load close to the rated cooling load. This proves that the simulation model may be used to design CO<sub>2</sub> refrigerators. Experimentation was conducted successfully for different water inlet temperatures to the external heat exchangers (gas cooler and evaporator). The experimentation focussed on capturing the transient behaviour of the system from start-up till steady-state conditions.

The simulation results all showed a good correlation to the experimental results and provided valuable insight into the processes occurring within the refrigerator. It was found that the constant isentropic efficiency compressor model used for the simulation over predicted energy input to the gas; thus, leading to higher

compressor outlet temperatures than the experiment and subsequently also a higher heat removal rate in the gas cooler. The experimental results show that there is a substantial heat loss by the compressor; therefore, confirming the need for using a non-adiabatic transient compressor model in the simulation. This was however outside the scope of this project.

In conclusion, the transient simulation model of the  $CO_2$  refrigerator runs stably on its own and predicts real life operation fairly accurately; thus, it shows promise in being a valuable tool for designing  $CO_2$  refrigerators if a non-adiabatic transient compressor model is developed. It is recommended for future work to use the experimental refrigerator built to test the system at different operating conditions (different ambient temperatures and different heating or cooling water temperatures to the heat exchangers) and thus ultimately developing a non-adiabatic transient compressor model.

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## APPENDIX A: SAMPLE CALCULATIONS

Sample calculations for values stated in the report.

# A1: Sample Calculations for an Ideal CO<sub>2</sub> Refrigeration Cycle with an Ideal Work Recovering Expansion Device

The sample calculations shown here are for section 2.4.3. The calculations show how the coefficient of performance improves due to the addition of an ideal work recovering expansion device. The operating conditions for the cycle are as mentioned in ASHRAE-Fundamentals (2001: 19.8). The conditions are 258 K evaporation temperature and 303 K condensing temperature. The inlet of the expansion device is at saturated liquid and the inlet of the compressor is at saturated vapour. There is no pressure drop through the tubes.

The cycle performance is evaluated for a cooling load of 1 kW. Calculations for the values stated in table 2 are shown below.

Evaporator pressure is:

$$P_{evaporator} = P_{sat @ T=258 K} = 2.281 \text{ MPa}$$

Condenser pressure:

$$P_{condenser} = P_{sat @ T=303 K} = 7.189 \text{ MPa}$$

Compression ratio:

$$Compression_{ratio} = \frac{P_{condenser}}{P_{evaporator}} = \frac{7.189 \text{ MPa}}{2.281 \text{ MPa}} = 3.15$$

Net refrigerating effect:

$$s \circledast \begin{cases} T = 303K \\ rho = rho_{sat\_liquid} = 599.86 \ kg/m^3 = -1.40 \ kJ/kg \end{cases}$$

$$h_{isentropic} = h \circledast \begin{cases} P = P_{evaporator} = 2.281 \ MPa \\ s = -1.40 \ kJ/kg \end{cases} = -221.62 \ kJ/kg$$

$$Net_{refrigerating_{effect}} = h_{g \circledast T_{evaporator}} - h_{isentropic} = -70.48 - (-221.62)$$

$$= 151.14 \ kJ/kg$$

Refrigerant circulated:

$$Refrigerant_{circulated} = \frac{Cooling\; load}{Net_{refrigerating_{effect}}} = \frac{1\; kW}{151.14\; kJ/kg} = 6.62\; g/s$$

Specific volume of suction gas:

$$\rho_{suction} = \rho_{sat\,vapor} \, @T_{evaporator} = 60.4377 \, \, \text{kg/m}^3$$

$$v_{suction} = \frac{1}{\rho_{suction}} = \frac{1}{60.4377 \frac{\text{kg}}{\text{m}^3}} = 0.0165 \text{ m}^3/\text{kg}$$

Compressor displacement rate:

$$\begin{split} Compressor_{displacement} &= Refrigerant_{circulated} \cdot v_{suction} \\ &= 0.00662 \frac{\text{kg}}{\text{s}} \cdot 0.0165 \frac{\text{m}^3}{\text{kg}} = 0.000109 \frac{\text{m}^3}{\text{s}} = 0.109 \text{ l/s} \end{split}$$

Compressor power needed to compress the vapour:

s @ 
$$\begin{cases} T = 258 \, K \\ rho = rho_{sat\_vapor} = 60.438 \, kg/m^3 \end{cases} = -0.8145 \, kJ/kg$$

$$h_{inlet} = h @ \begin{cases} T = 258 \ K \\ rho = rho_{sat\_vapor} = 60.438 \ kg/m^3 \end{cases} = -70.48 \ kJ/kg$$

$$h_{isentropic\_comp} = h @ \begin{cases} P = P_{condenser} = 7.189 \ MPa \\ s = -0.8145 \ kJ/kg \end{cases} = -21.40 \ kJ/kg$$

$$\dot{W}_{needed} = Refrigerant_{circulated} \cdot (h_{isentropic_{comp}} - h_{inlet})$$
  
= 0.00662(-21.40 - (-70.48)) = 0.3249 kW

Power recovered from isentropic expansion and used to aid the compression process:

s @ 
$$\begin{cases} T = 303 \ K \\ rho = rho_{sat\_liquid} = 599.86 \ kg/m^3 = -1.40 \ kJ/kg \end{cases}$$

$$h_{inlet} = h @ \begin{cases} T = 303 \ K \\ rho = rho_{sat\_liquid} = 599.86 \ kg/m^3 = -203.73 \ kJ/ \ kg \end{cases}$$

$$h_{isentropic\_exp} = h @ \begin{cases} P = P_{evaporator} = 2.281 \text{ MPa} \\ s = -1.40 \text{ kJ/kg} \end{cases} = -221.62 \text{ kJ/kg}$$

$$\dot{W}_{recovered} = Refrigerant_{circulated} \cdot (h_{inlet} - h_{isentropic\_exp})$$
  
= 0.00662(-203.73 - (-221.62)) = 0.1184 kW

Compressor power consumption with the work recovery:

$$\dot{W}_{comp} = \dot{W}_{needed} - \dot{W}_{recovered} = 0.3249 - 0.1184 = 0.2065 = 0.207 \text{ kW}$$

Coefficient of performance:

$$COP = \frac{Cooling\ load}{\dot{W}_{comp}} = \frac{1\ kW}{0.2065\ kW} = 4.84$$

Compressor discharge temperature:

$$T_{comp\_discharge} = T @ \begin{cases} P = P_{condenser} = 7.189 \, MPa \\ h = h_{isentropic\_comp} = -21.40 \, kJ/kg \\ = 343.43 \, K = 343 \, K \end{cases}$$

# **APPENDIX B: Property Function Codes for CO<sub>2</sub>**

The following MATLAB program codes are specifically written to calculate the properties of  $CO_2$  for the control volume method implemented in the refrigeration simulation model, as discussed in section 3. It is based on the use of the real gas equation of Span and Wagner (1996) to calculate the properties of  $CO_2$ .

# **B1:** Function to Calculate the Single Phase Properties at a Given Density and Temperature

```
%CO2 Property.m is a script file written to calculate all derivatives and values
%needed in the equation of Span and Wagner (1996) to calculate the thermodynamic
%properties of CO2 i.e. it is a direct implementation of Span and Wagner's
%equation of %state. The .mat file containing all variables,
%CO2_Property_Workspace.mat, is called %before-hand to import all variables needed
%in the Span and Wagner equation.
%Apply special treatment to avoid using rho=rho_c, for which the equations would
%give meaningless results i.e. properties at the critical density are taken in the
%limit close enough to the actual critical density.
if abs(rho-rho c)<1e-13 %i.e. avoid critical density
   rho=rho_c+1e-13;
end
delta = rho/rho c; %Reduced density
tau = T c/T;
                %Inverse of reduced temperature
%Following Table 28 in Span and Wagner to calculate the ideal-gas part of the
%Helmholtz energy Phi o
%Initialize variables
%Ideal-gas part of the dimensionless Helmholtz function Phi o
Phi o = log(delta) + a o(1) + a o(2) *tau+a o(3) *log(tau);
%1st and 2nd derivative of the dimensionless Helmholtz function Phi o w.r.t. tau
Phi o tau1 = a o(2)+a o(3)/tau; Phi o tau2 = -a o(3)/tau^2;
%Calculate and update variables
    Phi o = Phi o + a_o(p) *log(1-exp(-tau*theta_o(p)));
    \label{eq:phi_o_tau1} Phi_o_tau1 = Phi_o_tau1 + a_o(p) * theta_o(p) * ((1-exp(-tau*theta_o(p))) ^ (-1) - 1);
    Phi_o_tau2 = Phi_o_tau2 - a_o(p) * (theta_o(p)^2) *exp(-tau*theta_o(p)) * ... ((1-exp(-tau*theta_o(p)))^(-2));
%1st and 2nd derivative of the dimensionless Helmholtz function Phi o w.r.t. delta
Phi_o_delta1 = 1/delta;
Phi o delta2 = -1/delta^2;
%Derivative of the dimensionless Helmholtz function Phi o w.r.t. delta and tau
Phi o delta tau = 0;
%Following Table 32 in Span and Wagner to calculate the residual part of
%the Helmholtz energy Phi r
for p = 1:3
PSI(p,1) = exp(-C S4(p)*(delta-1)^2-D S4(p)*(tau-1)^2);
%Derivatives of the exponential function
%1st and 2nd derivative w.r.t. delta

PSI_delta1(p,1) = -2*C_S4(p)*(delta-1)*PSI(p);

PSI_delta2(p,1) = (2*C_S4(p)*(delta-1)^2-1)*2*C_S4(p)*PSI(p);
\$1st and 2nd derivative w.r.t. tau
PSI_taul(p,1) = -2*D_S4(p)*(tau-1)*PSI(p);
PSI_tau2(p,1) = (2*D_S4(p)*(tau-1)^2-1)*2*D_S4(p)*PSI(p);
%Derivative w.r.t. delta and tau
PSI delta tau(p,1) = 4*C S4(p)*D S4(p)*(delta-1)*(tau-1)*PSI(p);
```

```
DELTA_delta1(p,1) = (delta-1)*(A__S4(p)*THETA(p)*(2/beta_S4(p))*((delta-1)^2)^...
(1/(2*beta_S4(p))-1)+2*B__S4(p)*a_S4(p)*((delta-1)^2)^(a_S4(p)-
1));
part1 = 4*B S4(p)*aS4(p)*(aS4(p)-1)*((delta-1)^2)^(aS4(p)-2)+...
                  2*A S4(p)^2*(1/beta S4(p))^2*(((delta-1)^2)^(1/(2*beta S4(p))-1))^2+...
                  A \overline{S4} (p) *THETA(p) * (4/beta S4(p)) * (1/(2*beta S4(p))-1) *...
                                ((delta-1)^2)^(1/(2*beta S4(p))-2);
DELTA delta2(p,1) = 1/(delta-1)*DELTA delta1(p)+(delta-1)^2*part1;
%Derivatives of the distance function DELTA^bi
%1st and 2nd derivative w.r.t. delta
\label{eq:deltal} $$ $ DELTAbi_deltal(p,1) = b_S4(p)*DELTA(p)^(b_S4(p)-1)*DELTA_deltal(p); $$ $
DELTAbi_delta2(p,1) = b_S4(p)*(DELTA(p)^(b_S4(p)-1)*DELTA_delta2(p)+...

(b_S4(p)-1)*DELTA(p)^(b_S4(p)-2)*DELTA_delta1(p)^2);
%1st and 2nd derivative w.r.t. tau
DELTAbi tau1(p,1) = -2*THETA(p)*b S4(p)*DELTA(p)^(b S4(p)-1);
DELTAbi tau2 (p,1) = 2*b S4(p)*DELTA(p)^(b S4(p)-1)+4*THETA(p)^2*b S4(p)*...
                               (b_S4(p)-1)*DELTA(p)^(b_S4(p)-2);
%Derivative w.r.t. delta and tau
DELTAbi_delta_tau(p,1) = -A _ S4(p) *b_S4(p) * (2/beta_S4(p)) *DELTA(p) ^ (b_S4(p)-1) *... (delta-1) * ((delta-1)^2) ^ (1/(2*beta_S4(p))-1) -...
                                          2*THETA(p)*b S4(p)*(b S4(p)-1)*DELTA(p)^(b S4(p)-
2) *DELTA delta1(p);
%Residual part of the dimensionless Helmholtz function Phi r
Phi r = 0;
 %1st and 2nd derivative of the dimensionless Helmholtz function Phi r w.r.t. delta
Phi_r_delta1 = 0;
Phi_r_delta2 = 0;
%1st and 2nd derivative of the dimensionless Helmholtz function Phi r w.r.t. tau
Phi_r_tau1 = 0;
Phi r tau2 = 0;
*Derivative of the dimensionless Helmholtz function Phi_r w.r.t. tau and delta
Phi r delta tau = 0;
        Phi r = Phi r + n S1(p)*delta^d S1(p)*tau^t S1(p);
        Phi_r_delta1 = Phi_r_delta1 + n_S1(p)*d_S1(p)*delta^(d_S1(p)-1)*tau^t_S1(p);
        Phi r delta2 = Phi r delta2 + n S1(p)*d S1(p)*(d S1(p)-1)*delta^(d S1(p)-
2) *tau^t S1(p);
        Phi_r_tau2 = Phi_r_tau2 + n_S1(p)*t_S1(p)*(t_S1(p)-
1) *delta^d S1(p) *tau^(t S1(p)-2);
       Phi r delta tau = Phi r delta tau + n S1(p)*d S1(p)*t S1(p)*delta^(d S1(p)-
1) *tau^(t S1(p)-1);
end
for p=1:27
        Phi_r = Phi_r + n_S2(p)*delta^d_S2(p)*tau^t_S2(p)*exp(-delta^c_S2(p));
        Phi r delta1 = Phi r delta1 + n_S2(p) * exp(-delta^c_S2(p)) * (delta^(d_S2(p) - delta)) * (delta) * (delta
1) *tau^t S2(p) *..
                                 (d S2(p)-c S2(p)*delta^c_S2(p)));
        Phi r delta2 = \overline{Phi} r de\overline{Ita2} + n S2(p)\overline{texp} (-delta^c S2(p))*(delta^(d S2(p)-
2) *tau^{\overline{t}} \overline{S}2(p) *..
                                ((d S2(p)-c S2(p)*delta^c S2(p))*(d S2(p)-1-
c_S2(p)*delta^c_S2(p))-...
c_S2(p)^2*delta^c_S2(p)));
        Phi r tau1 = \overline{Phi} r tau1 + n S\overline{2} (p)*t S2(p)*delta^d S2(p)*tau^(t S2(p)-1)*exp(-
delta^c S2(p));
 \begin{array}{l} \text{Phi} = r \; \text{tau2} \; = \; \text{Phi} = r \; \text{tau2} \; + \; n \; \text{S2} \; (p) \; *t \; \text{S2} \; (p) \; * \; (t \; \text{S2} \; (p) \; -1) \; * \text{delta} \; ^d = S2 \; (p) \; *t \; \text{tau} \; (t \; \text{S2} \; (p) \; -2) \; * \ldots \\ \end{array} 
                                       exp(-delta^c S2(p));
        Phi r delta tau = Phi r delta tau + n S2(p) * exp(-
delta^c_S\overline{2}(p))*\overline{delta}(d_S\overline{2}(p)-1)*\overline{t}S2(p)*...
                                   tau^(t_S2(p)-1)*(d_S2(p)-c_S2(p)*delta^c_S2(p));
end
for p=1:5
```

```
Phi r = Phi r + n S3(p)*delta^d S3(p)*tau^t S3(p)*exp(-alpha S3(p)*...
                     (delta-eps S3(p))^2-beta S3(p)*(tau-gamma S3(p))^2);
    Phi r delta1 = Phi r delta1 + n S3(p)*delta^d S3(p)*tau^t S3(p)*exp(-
alpha S3(p)*...
                  (delta-eps_S3(p))^2-beta_S3(p)*(tau-gamma_S3(p))^2)*...
    (d_S3(p)/delta-2*alpha_S3(p)*(delta-eps_S3(p)));
Phi_r_delta2 = Phi_r_delta2 + n_S3(p)*tau^t_S3(p)*exp(-alpha_S3(p)*(delta-
eps S3(p)^{-}^2-.
                 beta_S3(p)*(tau-gamma_S3(p))^2)*(-2*alpha S3(p)*delta^d S3(p)+...
                 4*alpha S3(p)^2*delta^d S3(p)*(delta-eps S3(p))^2-..
                 4*d S3(p)*alpha S3(p)*delta^(d S3(p)-1)*(delta-eps S3(p))+...
                 d S3(p)*(d S3(p)-1)*delta*(d S3(p)-2));
    Phi r tau1 = Phi r tau1 + n S3(p)*delta^d S3(p)*tau^t S3(p)*exp(-
alpha S3(p)*..
              (delta-eps S3(p))^2-beta S3(p)*(tau-qamma S3(p))^2)*(t S3(p)/tau-...
              2*beta S3(p)*(tau-gamma S3(p)));
    Phi_r_tau2 = Phi_r_tau2 + n_S3(p)*delta^d S3(p)*tau^t S3(p)*exp(-
alpha S3(p)*..
              (delta-eps S3(p))^2-beta S3(p)*(tau-gamma S3(p))^2)*...
              ((t S3(p)/tau-2*beta S3(p)*(tau-gamma S3(p)))^2-...
              t S3(p)/(tau^2)-2*beta S3(p));
    Phi r delta tau = Phi r delta tau + n S3(p)*delta^d S3(p)*tau^t S3(p)*exp(-
alpha S\overline{3}(\overline{p})*...
                   (delta-eps S3(p))^2-beta S3(p)*(tau-gamma S3(p))^2)*...
                   (d S3(p)/delta-2*alpha S3(p)*(delta-eps S3(p)))*...
                   (t S3(p)/tau-2*beta S3(p)*(tau-gamma S3(p)));
end
for p=1:3
    Phi_r = Phi_r + n_S4(p)*DELTA(p)^b S4(p)*delta*PSI(p);
    Phi_r_delta1 = Phi_r_delta1 +
n S4(p)*(DELTA(p)^b S4(p)*(PSI(p)+delta*PSI delta1(p))+...
                 DELTAbi_delta1(p) *delta*PSI(p));
    Phi r delta2 = Phi r delta2 +
n S4(p)^+(DELTA(p)^+b S4(p)^+(2*PSI delta1(p)+delta*PSI delta2(p))+...
                 2*DELTAbi delta1(p)*(PSI(p)+delta*PSI delta1(p))+...
                 DELTAbi delta2(p)*delta*PSI(p));
Phi_r_tau1 = Phi_r_tau1 +
n_S4(p)*delta*(DELTAbi_tau1(p)*PSI(p)+DELTA(p)^b_S4(p)*PSI_tau1(p));
Phi_r_tau2 = Phi_r_tau2 +
n_S4(p)*delta*(DELTAbi_tau2(p)*PSI(p)+2*DELTAbi_tau1(p)*PSI_tau1(p)+...
                     \overline{DELTA}(p)^b S4(p)^*PSI tau2(p));
    part1 = DELTA(p)^b S4(p)*(PSI tau1(p)+delta*PSI delta tau(p));
    part2 =
delta*DELTAbi delta1(p)*PSI tau1(p)+DELTAbi tau1(p)*(PSI(p)+delta*PSI delta1(p));
    part3 = DELTAbi delta tau(p)*delta*PSI(p);
    Phi_r_delta_tau = Phi_r_delta_tau + n_S4(p)*(part1+part2+part3);
end
%The equation of state for carbon dioxide is expressed in the form of the
%dimensionless Helmholtz energy:
Phi = Phi o + Phi r;
%Use the relations to the dimensionless Helmholtz function Phi in Table 3 of Span
%and Wagner to calculate the thermodynamic properties
%Pressure [kPa]
P = (1+delta*Phi_r_delta1)*rho*R*T;
%Specific internal energy [kJ/kg]
u = (tau*(Phi_o_tau1+Phi_r_tau1))*R*T;
%Specific enthalpy [kJ/kg]
h = (1+tau*(Phi o tau1+Phi r tau1)+delta*Phi r delta1)*R*T;
%Specific entropy [kJ/(kg K)]
s = (tau*(Phi_o_tau1+Phi_r_tau1)-Phi)*R;
Specific isochoric heat capacity [kJ/(kg K)]
cv = (-tau^2*(Phi o tau^2+Phi r tau^2))*R;
%Specific isobaric heat capacity [kJ/(kg K)]
cp = (-tau^2*(Phi_o_tau2+Phi_r_tau2)+(1+delta*Phi_r_delta1-...
       delta*tau*Phi_r_delta_tau)^2/(1+2*delta*Phi_r_delta1+...
       delta^2*Phi_r_delta2))*R;
```

## **B2:** Function to Calculate the Saturated Properties at a Given Temperature

```
%CO2 Sat Prop at T.m is a script file written to determine saturated properties
%simultaneously solving equations (2.2a-c) of Span and Wagner (1996:1516) using
%the %Newton-Raphson method
%T = 290; %Given temperature at which to determine saturated properties [K]
%Define initial guesses
%Equation 3.13 in Span and Wagner (1996:1524) to get guess for saturation pressure
Ps = P_c*exp(T_c/T*sum(a_VP.*(1-T/T_c).^t_VP));
%Saturated liquid density guess given by eq 3.14
 rho_f = rho_c * exp(sum(a_rho_sl.*(1-T/T c).^t rho sl)); 
%Saturated vapour density guess given by eq 3.15
\label{eq:rho_g} \mbosebox{$=$ rho_c*exp(sum(a_rho_sv.*(1-T/T_c).^t_rho_sv));}
x = [Ps; rho_f; rho_g]; %Vector of variables to solve
error = 1:
while error>10^-10 %Itterate till convergence
%Determine properties of the saturated liquid
rho = x(2); CO2 Property; %Determine properties at rho and T.
delta f = delta; Phi r delta1 f = Phi r delta1; Phi r delta2 f = Phi r delta2;
Phi rf = Phi r;
%Determine properties of the saturated gas
rho = x(3); CO2 Property; %Determine properties at rho and T.
delta g = delta; Phi r delta1 g = Phi r delta1; Phi r delta2 g = Phi r delta2;
Phi_r_g = Phi_r;
%Define derivatives
f1 Ps = 1/(R*T*x(2)); f1 rho g = 0;
f1 rho f = -x(1)/(R*T*(x(2))^2)-1/rho c*Phi r delta1 f-...
              1/rho c*delta f*Phi r delta2 f;
f2 Ps = 1/(R*T*x(3)); f2 rho f = 0;
f2 rho g = -x(1)/(R*T*(x(3))^2)-1/rho c*Phi r delta1 g-...
              1/rho c*delta g*Phi r delta2 g;
f3 Ps = 1/(R*T)*(1/x(3)-1/x(2));
f3 rho f = x(1)/(R*T*(x(2))^2)-1/x(2)-1/rho c*Phi r delta1 f;
f3 rho g = -x(1)/(R*T*(x(3))^2)+1/x(3)+1/rho c*Phi r delta1 g;
%Matrix of derivatives
J = [f1_Ps f1_rho_f f1_rho_g;...]
     f2_Ps f2_rho_f f2_rho_g;...
f3_Ps f3_rho_f f3_rho_g];
%Calculate function values.
f1 = x(1)/(R*T*x(2))-1-delta f*Phi r delta1 f;
%Define vector of function values
f = [f1; f2; f3];
%Determine updated variables using Newton-Raphson formula applied to a matrix of
error=max(abs(f)); %Define error as the maximum absolute value of any of the
                    %function %values in f.
%Write vector values to Ps, rho f and rho g
Ps = x(1); rho f = x(2); rho g = x(3);
```

## B3: Function to Calculate the Single Phase Properties at a Given Density and Specific Internal Energy

```
%CO2_1Ph_Prop_at_rho_and_u.m is a script file written to calculate single phase %properties from a given density and specific internal energy using the Newton-
%Raphson %method.
Two ph = 0; %Flow is not two phase, i.e. flow is single phase
rho x = rho; %Given density
u x = u; %Given specific internal energy
%T = 300; %Initial guess for temperature [K] error = 1; i = 0;
while error>10^-8
u and cv script; %Call u and cv script.m to calculate %specific internal energy,
                   u=f(rho,T), and isochoric heat capacity, v=f(rho,T).
f1 = -u x+u;
error=abs(f1);
%Update the temperature only if the error is larger than criteria, to iterate
%again.
if error>10^-8
    f1 T = cv;
    T = T-f1/f1 T; %Update the temperature
CO2 Property %Update all properties
%Set rho and u to values as entered to avoid round off errors
rho = rho x; u = u x;
```

## **B4:** Derivatives Used in the Formulation of the Two-Phase Function

This section shows the derivatives used in the development of the two-phase function as explained in section 3.3.2. The relations of the thermodynamic properties to the dimensionless Helmholtz function  $\phi$ , as shown in Table 3, was used to determine the derivatives. Recall from section 3.1 that  $\tau = T_c/T$  is the inverse reduced temperature and  $\delta = \rho/\rho_c$  is the reduced density. Furthermore, from section 3.3.2, the specific Helmholtz energy is  $\phi(\delta,\tau)$  and the specific Gibbs energy is g = h - Ts.

First the derivatives of the inverse reduced temperature and reduced density w.r.t. T and  $\rho$  are stated; as these form the basis of application of the chain rule for derivatives.

$$\frac{\partial \tau}{\partial T} = \frac{\partial}{\partial T} \left( \frac{T_c}{T} \right) = -\frac{T_c}{T^2} = -\frac{\tau}{T} , \quad \frac{\partial \tau}{\partial \rho} = 0$$
 (B1)

$$\frac{\partial \delta}{\partial \rho} = \frac{\partial}{\partial \rho} \left( \frac{\rho}{\rho_C} \right) = \frac{1}{\rho_C} , \quad \frac{\partial \delta}{\partial T} = 0$$
 (B2)

Also the derivatives of the specific Helmholtz energy w.r.t. T and  $\rho$  are given here since these derivatives repeat frequently in derivatives of the thermodynamic properties:

$$\frac{\partial \phi}{\partial T} = \frac{\partial \phi}{\partial \tau} \frac{\partial \tau}{\partial T} = \phi_{\tau} \left( -\frac{\tau}{T} \right) = -\frac{\tau}{T} \phi_{\tau} \tag{B3}$$

$$\frac{\partial \phi}{\partial \rho} = \frac{\partial \phi}{\partial \delta} \frac{\partial \delta}{\partial \rho} = \phi_{\delta} \left( \frac{1}{\rho_{c}} \right) = \frac{1}{\rho_{c}} \phi_{\delta} \tag{B4}$$

The derivatives of the thermodynamic properties as well as the specific Gibbs energy can now be developed:

$$\frac{\partial u}{\partial T} = \frac{\partial}{\partial T} \left( \tau \left( \phi^o_{\tau} + \phi^r_{\tau} \right) RT \right) = \frac{\partial}{\partial T} \left( RT_c \left( \phi^o_{\tau} + \phi^r_{\tau} \right) \right) \\
= RT_c \left( \phi^o_{\tau\tau} + \phi^r_{\tau\tau} \right) \left( -\frac{\tau}{\tau} \right) = R \left[ -\tau^2 \left( \phi^o_{\tau\tau} + \phi^r_{\tau\tau} \right) \right] = R \left[ \frac{c_v}{\rho} \right] = c_v$$
(B5)

$$\frac{\partial u}{\partial \rho} = \frac{\partial}{\partial \rho} \left( \tau \left( \phi^o_{\tau} + \phi^r_{\tau} \right) RT \right) = \frac{T_c R}{\rho_c} \left( \phi^o_{\delta \tau} + \phi^r_{\delta \tau} \right) \tag{B6}$$

$$\frac{\partial P}{\partial T} = \frac{\partial}{\partial T} \left( \rho R T \left( 1 + \delta \phi^r_{\delta} \right) \right) = \frac{P}{T} + \rho R T \frac{\partial}{\partial T} \left( 1 + \delta \phi^r_{\delta} \right) \\
= \frac{P}{T} + \rho R T \delta \frac{\partial}{\partial T} \left( \phi^r_{\delta} \right) = \frac{P}{T} + \rho R T \delta \left( -\frac{\tau}{T} \phi^r_{\delta \tau} \right) = \frac{P}{T} - \rho R \delta \tau \phi^r_{\delta \tau}$$
(B7)

$$\frac{\partial P}{\partial \rho} = \frac{\partial}{\partial \rho} \left( \rho RT \left( 1 + \delta \phi^r_{\delta} \right) \right) = \frac{P}{\rho} + \rho RT \frac{\partial}{\partial \rho} \left( 1 + \delta \phi^r_{\delta} \right) \\
= \frac{P}{\rho} + \rho RT \left( \frac{1}{\rho_c} \phi^r_{\delta} + \frac{\delta}{\rho_c} \phi^r_{\delta\delta} \right) = \frac{P}{\rho} + \delta RT \left( \phi^r_{\delta} + \delta \phi^r_{\delta\delta} \right)$$
(B8)

$$\frac{\partial h}{\partial T} = \frac{\partial}{\partial T} \left( u + \frac{P}{\rho} \right) = \frac{\partial u}{\partial T} + \frac{1}{\rho} \frac{\partial P}{\partial T} = c_v + \frac{1}{\rho} \left( \frac{P}{T} - \rho R \delta \tau \phi^r_{\delta \tau} \right) 
= c_v + \frac{P}{\rho T} - R \delta \tau \phi^r_{\delta \tau} = c_v + \left( R \left( 1 + \delta \phi^r_{\delta} \right) \right) - R \delta \tau \phi^r_{\delta \tau} 
= c_v + R \left( 1 + \delta \phi^r_{\delta} - \delta \tau \phi^r_{\delta \tau} \right)$$
(B9)

$$\begin{split} &\frac{\partial h}{\partial \rho} = \frac{\partial}{\partial \rho} \left( u + \frac{P}{\rho} \right) = \frac{\partial u}{\partial \rho} + \frac{\partial}{\partial \rho} \left( \frac{P}{\rho} \right) = \left[ \frac{T_{cR}}{\rho_{c}} \left( \phi^{o}_{\delta \tau} + \phi^{r}_{\delta \tau} \right) \right] + \left( \frac{-1}{\rho^{2}} \right) P + \frac{1}{\rho} \frac{\partial P}{\partial \rho} \\ &= \left[ \frac{T_{cR}}{\rho_{c}} \left( \phi^{o}_{\delta \tau} + \phi^{r}_{\delta \tau} \right) \right] + \left( \frac{-1}{\rho^{2}} \right) P + \frac{1}{\rho} \left[ \frac{P}{\rho} + \delta R T \left( \phi^{r}_{\delta} + \delta \phi^{r}_{\delta \delta} \right) \right] \\ &= \left[ \frac{T_{cR}}{\rho_{c}} \left( \phi^{o}_{\delta \tau} + \phi^{r}_{\delta \tau} \right) \right] + \frac{RT}{\rho_{c}} \left( \phi^{r}_{\delta} + \delta \phi^{r}_{\delta \delta} \right) \\ &= \frac{RT}{\rho_{c}} \left[ \tau \left( \phi^{o}_{\delta \tau} + \phi^{r}_{\delta \tau} \right) + \left( \phi^{r}_{\delta} + \delta \phi^{r}_{\delta \delta} \right) \right] \end{split}$$
 (B10)

$$\frac{\partial s}{\partial T} = \frac{\partial}{\partial T} \left[ R \left( \tau \left( \phi^{o}_{\tau} + \phi^{r}_{\tau} \right) - \phi^{o} - \phi^{r} \right) \right] 
= R \frac{\partial}{\partial T} \left[ \left( \tau \left( \phi^{o}_{\tau} + \phi^{r}_{\tau} \right) - \phi^{o} - \phi^{r} \right) \right] 
= R \left[ \frac{\partial}{\partial T} \left( \tau \left( \phi^{o}_{\tau} + \phi^{r}_{\tau} \right) \right) - \frac{\partial}{\partial T} \left( \phi^{o} + \phi^{r} \right) \right]$$
(B11)

$$= R \left[ \left[ -\frac{\tau}{T} (\phi^o_{\ \tau} + \phi^r_{\ \tau}) - \frac{\tau^2}{T} (\phi^o_{\ \tau\tau} + \phi^r_{\ \tau\tau}) \right] - \left( -\frac{\tau}{T} \right) (\phi^o_{\ \tau} + \phi^r_{\ \tau}) \right]$$

$$= \frac{R}{T} \left( -\tau^2 (\phi^o_{\ \tau\tau} + \phi^r_{\ \tau\tau}) \right) = \frac{R}{T} \left( \frac{c_v}{R} \right) = \frac{c_v}{T}$$

$$\frac{\partial s}{\partial \rho} = \frac{\partial}{\partial \rho} \left[ R \left( \tau (\phi^o_{\ \tau} + \phi^r_{\ \tau}) - \phi^o - \phi^r \right) \right]$$

$$= R \frac{\partial}{\partial \rho} \left[ \tau (\phi^o_{\ \tau} + \phi^r_{\ \tau}) - (\phi^o + \phi^r) \right]$$

$$= R \left[ \frac{\tau}{\rho_c} (\phi^o_{\ \delta\tau} + \phi^r_{\ \delta\tau}) - \frac{1}{\rho_c} (\phi^o_{\ \delta} + \phi^r_{\ \delta}) \right]$$

$$= \frac{R}{\rho} \left[ \tau (\phi^o_{\ \delta\tau} + \phi^r_{\ \delta\tau}) - (\phi^o_{\ \delta} + \phi^r_{\ \delta}) \right]$$

$$\frac{\partial g}{\partial T} = \frac{\partial}{\partial T} (h - Ts) = \frac{\partial h}{\partial T} - \frac{\partial}{\partial T} (Ts) = \frac{\partial h}{\partial T} - s - T \frac{\partial s}{\partial T} 
= \left( c_v + R \left( 1 + \delta \phi^r_{\ \delta} - \delta \tau \phi^r_{\ \delta \tau} \right) \right) - s - T \left( \frac{c_v}{T} \right) 
= R \left( 1 + \delta \phi^r_{\ \delta} - \delta \tau \phi^r_{\ \delta \tau} \right) - s$$
(B13)

$$\frac{\partial g}{\partial \rho} = \frac{\partial}{\partial \rho} (h - Ts) = \frac{\partial h}{\partial \rho} - \frac{\partial}{\partial \rho} (Ts) = \frac{\partial h}{\partial \rho} - T \frac{\partial s}{\partial \rho} 
= \frac{RT}{\rho_c} \left[ \tau (\phi^o_{\delta \tau} + \phi^r_{\delta \tau}) + (\phi^r_{\delta} + \delta \phi^r_{\delta \delta}) \right] 
- \frac{RT}{\rho_c} \left[ \tau (\phi^o_{\delta \tau} + \phi^r_{\delta \tau}) - (\phi^o_{\delta} + \phi^r_{\delta}) \right] 
= \frac{RT}{\rho_c} \left[ 2\phi^r_{\delta} + \phi^o_{\delta} + \delta \phi^r_{\delta \delta} \right)$$
(B14)

# B5: Function to Calculate the Two-Phase Properties at a Given Density and Specific Internal Energy

```
%CO2_2Ph_Prop_at_rho_and_u.m is a script file written to calculate two-phase
%properties from a given homogeneous density and specific internal energy using
%the Newton-Raphson method.
Two ph = 1; %Flow is two-phase
rho x = rho; %Given density
u x = u; %Given internal energy
%T = 260; %Initial guess for temperature or use previous value
%If guess is above critical point temperature then change the guess to an
%appropriate %value.
if T>=T_c
    T=T_c-1e-3;
%If the flow has just changed from single phase to two-phase use these guesses
if (alpha vol==0) | | (alpha vol==1)
%Use saturated liquid density given by eq 3.14 S&W(1996) as %initial guess rho_f = rho_c*exp(sum(a_rho_sl.*(1-T/T_c).^t_rho_sl));
%Use saturated vapour density given by eq \overline{3}.15~\mathrm{S\&W}(1\overline{9}96) as %initial guess
    \label{eq:rho_g} \mbosebox{$=$ rho_c*exp(sum(a_rho_sv.*(1-T/T_c).^t_rho_sv));}
end %else use previous iteration's value
%alpha vol = 0.9; %Initial guess for volume fraction or use previous value
x = [T; rho g; rho f; alpha vol];
error = 1; %Set error level to start while loop
i = 0; %Counter to count nr of iterations within while loop
while error>10^-8
i = i+1;
T = x(1);
```

```
%Calculate saturated vapour properties
rho = x(2); CO2 Property;
cv_g = cv; cp_g = cp; u_g = u; P_g = P; h_g = h; sg = s; deltag = delta;
Phi r g = Phi r; Phi o delta tau g = Phi o delta tau; Phi o delta1 g =
Phi_o delta1;
Phi_r_delta_tau_g = Phi_r_delta_tau; Phi_r_deltal_g = Phi_r_deltal; Phi_r_delta2_g = Phi_r_delta2; Phi_r_taul_g = Phi_r_taul;
%Calculate saturated liquid properties
rho = x(3); CO2 Property;
cv_f = cv; cp_f = cp; u_f = u; P_f = P; h_f = h; s_f = s; delta_f = delta;
Phi_r_f = Phi_r; Phi_o_delta_tau_f = Phi_o_delta_tau; Phi_o_delta_f =
Phi_o_delta1;
Phi r delta tau f = Phi r delta tau; Phi r delta1 f = Phi r delta1;
Phi r delta2 f = Phi r delta2; Phi r tau1 f = Phi r tau1;
f1 = -rho_x*u_x+x(4)*x(2)*u_g+(1-x(4))*x(3)*u_f; f2 = -rho_x+x(4)*x(2)+(1-x(4))*x(3)*u_f; f2 = -rho_x+x(4)*x(4)*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*x(4)+(1-x(4))*
x(4))*x(3);
f3 = P g-P f; f4 = (h g-T*s g)-(h f-T*s f);
f = [f1; f2; f3; f4];
error=max(abs(f)); %Error is defined as the maximum absolute value of f
%Update the values only if the error is larger than criteria, to iterate again.
if error>10^-8
f1 T = x(4)*x(2)*cv g+(1-x(4))*x(3)*cv f;
f1_{rho_g} = x(4) *u g+x(4) *x(2) *T c*R/rho c*...
                          (Phi o delta tau g+Phi r delta tau g);
f1 rho f = (1-x(4))*u f+(1-x(4))*x(3)*T c*R/rho c*...
                          (Phi_o_delta_tau_f+Phi_r_delta_tau_f);
f1 alpha vol = x(2)*u g-x(3)*u f;
f2 T = 0; f2 rho q = x(4); f2 rho f = 1-x(4); f2 alpha vol = x(2)-x(3);
f3 T = P g/T-x(2)*R*tau*delta g*Phi r delta tau g - ...
                    (P f/T-x(3)*R*tau*delta f*Phi r delta tau f);
 \begin{array}{lll} & \text{f3\_rho\_g} &=& \text{P\_g/x}(2) + \text{delta\_g*R*T*} (\text{Phi\_r\_delta1\_g+delta\_g*Phi\_r\_delta2\_g}); \\ & \text{f3\_rho\_f} &=& -\text{P\_f/x}(3) - \text{delta\_f*R*T*} (\text{Phi\_r\_delta1\_f+delta\_f*Phi\_r\_delta2\_f}); \\ \end{array} 
f3 alpha vol = 0;
f4_T = R*(1+delta_g*Phi_r_delta1_g-delta_g*tau*Phi_r_delta_tau_g)-s_g-...
R*(1+delta_f*Phi_r_delta1_f-delta_f*tau*Phi_r_delta_tau_f)+s_f;
f4_rho_g = R*T/rho_c*(2*Phi_r_delta1_g+Phi_o_delta1_g+delta_g*Phi_r_delta2_g);
f4_rho_f = -R*T/rho_c*(2*Phi_r_delta1_f+Phi_o_delta1_f+delta_f*Phi_r_delta2_f);
f4 alpha vol = 0;
J = [f1 T, f1 rho g, f1 rho f, f1 alpha vol; f2 T, f2 rho g, f2 rho f,
f2_alpha vol;
          f3 \overline{T}, f3 rho g, f3 rho f, f3 alpha vol; f4 \overline{T}, f4 rho g, f4 rho f,
f4 alpha vol];
x = x-J \setminus \overline{f};
else
        break; %Leave while loop
end
T = x(1); rho g = x(2); rho f = x(3); alpha vol = x(4); rho = rho x; u = u x;
Determine vapour fraction
xi = (u x-u f)/(u g-u f);
\mbox{\ensuremath{\$Determine}} properties
P=(P_g+P_f)/2; h = xi*h_g+(1-xi)*h_f; s = xi*s g+(1-xi)*s f;
cp = xi*cp g+(1-xi)*cp f; cv = xi*cv g+(1-xi)*cv f;
```

#### **B6:** Function to Calculate the Thermal Conductivity

```
%CO2 Conductivity.m is a script file written to calculate the thermal conductivity
% of carbon dioxide using the equation of Scalabrin G., Marchi P., Finezzo F., and
%Span R. (2006)
%cond [W/m.K]
%The equation to calculate conductivity is a function of density and temperature.
%rho = 12.388; %Density [kg/m^3]
%T = 750; %Temperature [K]
rho_r = rho/rho_c; %Reduced density
                  --
%Reduced temperature
T r = T/T c;
\bar{n} i = [7.\bar{6}9857587;0.159885811;1.56918621;-6.73400790;16.3890156;...
         3.69415242;22.320551400000;66.1420950;-0.171779133;0.00433043347];
g i = [0;0;1.5;0;1;1.5;1.5;1.5;3.5;5.5];
h = [1;5;1;1;2;0;5;9;0;0];
\bar{n} c = 0.775547504;
%Parameters for the critical term
a = [3;6.70697;0.94604;0.3;0.3;0.39751;0.33791;0.77963;0.79857;0.9;0.02;0.2];
%Thermal conductivity enhancement in the near-critical region is given by equation
%5 in R.Span
alpha T r = 1-a(10)*acosh(1+a(11)*((1-T r)^2)^a(12));
cond r ce = rho r*exp(-(rho r^a(1))/a(1)-(a(2)*(T r-1))^2-...
                   (a(3)*(rho r-1))^2)/((((1-1/T r)+a(4)*...

((rho r-1)^2)^(1/(2*a(5))))^2)^a(6)+...
                   ((a(7)*(rho_r-alpha_T_r))^2)^a(8))^a(9));
cond r = sum(n i(1:3).*(T r.^g i(1:\overline{3})).*(rho r.^h i(1:3)))+...
         \exp(-5*\text{rho}_r^2)*\sup(n_i(4:10).*(T_r.^g_i(4:10)).*...
         (rho_r.^h_i(4:10)))+n_c*cond_r_ce;
%Calculate critical conductivity parameter
R_M = 8.314472; %[J/(mol.K)]

N A = 6.0221353*10^23; %[1/mol]
M CO2 = 0.044098; %Molar mass of CO2 [kg/mol]
 \texttt{cond\_c} \ = \ (\texttt{R\_M}^{\wedge}(5/6) * (\texttt{P\_c}*1000)^{\wedge}(2/3)) \, / \ (\texttt{T\_c}^{\wedge}(1/6) *\texttt{M\_CO2}^{\wedge}(1/2) *\texttt{N} \ \texttt{A}^{\wedge}(1/3)); 
%cond_c = 0.00481384; %[W/(m.K)]
cond = cond_r*cond_c; %[W/m.K]
```

### **B7:** Function to Calculate the Dynamic Viscosity

```
%Viscosity.m is a script file written to calculate the dynamic viscosity of carbon
%dioxide using the equation of Fenghour A., Wakeham W.A., and Vesovic V. (1998)
%visc [Pa.s]
%The viscosity equation is a function of T and rho.
%T = 260; %Temperature [K]
rac{1}{6} % The = 64.4166; % Density [kg/m^2]
ao = [0.235156;-0.491266;0.05211155;0.05347906;-0.01537102]; %Coefficients
i v = [0;1;2;3;4];
eps k = 251.196; %Energy scaling parameter used in equations
Tr = T/eps_k; %Reduced temperature
red eff cs = exp(sum(ao.*(log(Tr)).^i v));
visc o = 1.00697*T^0.5/red eff cs;
d11 = 0.4071119*10^{-2}; d21 = 0.7198037*10^{-4}; d64 = 0.2411697*10^{-16};
d81 = 0.2971072*10^{-22}; d82 = -0.1627888*10^{-22};
visc_e = d11*rho+d21*rho^2+d64*rho^6/(Tr^3)+d81*rho^8+d82*rho^8/Tr;
visc = visc o + visc e;
visc = visc \times 10^{-6}; \sqrt[8]{Pa.s}
```

## B8: Function to Calculate the Properties at a Given Density and Specific Internal Energy

```
%CO2 Prop at rho and u.m is a script file written to calculate all properties of
%CO2 based on rho and u.
%Determine if the flow is single phase (1ph) or two phase (2ph) for a given
%density (rho) and internal energy (u), and then call the appropriate functions to %calculate the thermodynamic properties as well as the thermal conductivity and
%dynamic viscosity
%rho = ; %Given density
%u = ; %Given specific internal energy
%rho_fi_2,rho_gi_2 and u_fi_2,u_gi_2 are vectors of saturated density and
%saturated %specific energy. These vectors are used to decide if the flow is two-
%phase or single %phase.
if (rho>=rho_fi_2(1))||(rho<=rho_gi_2(1))</pre>
    CO2_1Ph_Prop_at_rho_and_u;
    CO2 Conductivity; %Calculate conductivity given rho and T
    Viscosity CO2; %Calculate dynamic viscosity given rho and T
else
    if rho>=rho c
        if rho<600
             u f at rho = interp1(rho fi,u fi,rho); %finer vector
        else
             u f at rho = interp1(rho fi 2, u fi 2, rho); %coarser vector (for speed)
        end
        if abs(u-u f at rho)<1 %Only recalculate if it is really close to the
                                    %saturation line
             CO2_Sat_Prop_at_rho_f
u_f_at_rho = u_f;
         if u<(u f at rho-le-8) %Calculate two-phase properties
             CO2_2Ph_Prop_at_rho_and_u;
             rho = rho g; Viscosity CO2; visc g = visc;
             CO2 Conductivity; cond g = cond;
             rho = rho_f; Viscosity_CO2; visc_f = visc;
             CO2 Conductivity; cond f = cond;
             rho = rho x; %Set density to its two-phase value
             visc = 1/(xi/visc_g+(1-xi)/visc_f);
cond = 1/(xi/cond_g+(1-xi)/cond_f);
         elseif abs(u-u f at rho) <=1e-8
             %Assign saturation properties
             T=x(1); Two_ph = 0;
             CO2_Property
CO2 Conductivity
             Viscosity CO2
        else %Calculate single phase properties
             CO2_1Ph_Prop_at_rho_and_u;
             CO2 Conductivity;
             Viscosity CO2;
        end
    elseif rho<rho_c</pre>
        if rho>330
             u_g_at_rho = interp1(rho_gi,u gi,rho);
             u_g_at_rho = interp1(rho_gi_2,u_gi_2,rho);
        end
         if abs(u-u_g_at_rho)<1 %Only recalculate if it is really close to the
                                    %saturation line
             CO2_Sat_Prop_at_rho_g
             u_g_at_rho = u_g;
        end
         if u<(u g at rho-le-8) %Calculate two-phase properties
             CO2_2Ph_Prop_at_rho_and_u;
```

```
rho = rho g; Viscosity_CO2; visc_g = visc;
          CO2 Conductivity; cond_g = cond;
           rho = rho_f; Viscosity_CO2; visc_f = visc;
          CO2 Conductivity; cond f = cond;
          cond = 1/(xi/cond_g+(1-xi)/cond_f);
       elseif abs(u-u g at rho) <=1e-8
          %Assign saturation properties
          T=x(1); Two_ph = 0;
          CO2 Property
          CO2 Conductivity
          Viscosity_CO2
       else %Calculate single phase properties
          CO2_1Ph_Prop_at_rho_and_u;
          CO2 Conductivity;
          Viscosity CO2;
       end
   end
end
```

#### APPENDIX C: TRANSIENT SIMULATION PROGRAM

This section shows the program code for the transient simulation model of the CO<sub>2</sub> refrigeration cycle with capillary tube expansion device, as discussed in section 4.

### C1: Main Program Code of the Transient Simulation Model

### C2: Program Code to Assign Initial Conditions of the Simulation Model

```
%Initialise Refrigerator System.m is a script file written to define the
%simulation geometry and initial conditions for the refrigeration cycle
%simulation.
load('CO2_Property_Workspace'); %Load variables that are used in the equation of
                                      %state from Span and Wagner (1996)
        ----- Refrigeration system parameters ------
%Geometric properties of the tube-in-tube gas cooler
%Inner tube is CO2 working fluid of the refrigeration cycle
%Outer tube is cold water
L gc = 19.7 %Length of the gas cooler [m] 15.2; 19.7;
di_gc_i = 0.0062; %Inner diameter of the inner tube [m] do_gc_i = 0.008; %Outer diameter of the inner tube [m]
di_gc_o = 0.01446; %Inner diameter of the outer tube [m]
do_gc_o = 0.01588; %Outer diameter of the outer tube [m]
A_gc_i = pi/4*di_gc_i^2; A_gc_o = pi/4*(di_gc_o^2-do_gc_i^2);
V gc i = L gc*A gc i; V gc o = L gc*A gc o;
1 ct = 3.5; %Length of capillary tube [m]
d ct = 0.00079; %Inner diameter of capillary tube [m]
di ct = d ct;
L_{ct} = l_{ct}
A ct = pi/4*d ct<sup>2</sup>;
L ev = 12.9; %Length of the evaporator pipe [m] 10.92;
di_ev_i = 0.0062; %Inner diameter of inner tube [m]
do_ev_i = 0.008; %Outer diameter of the inner tube [m]
di_ev_o = 0.01446; %Inner diameter of the outer tube [m]
do ev_o = 0.01588; %Outer diameter of the outer tube [m]
A_{ev_i} = pi/4*di_{ev_i^2}; A_{ev_0} = pi/4*(di_{ev_0^2-do_{ev_i^2}});
V_ev_i = L_ev*A_ev_i; V_ev_o = L_ev*A_ev_o;
%Geometric properties of the tube-in-tube internal heat exchanger
%Gas cooler CO2 flows in the inner tube and evaporator CO2 flows in the outer
%tube.
L_IHX = 2.5; %Length of the internal heat exchanger [m]
di_i_HX = 0.00354; %Inner diameter of the inner tube [m] do_i_HX = 0.00476; %Outer diameter of the inner tube [m] di_o_IHX = 0.00771; %Inner diameter of the outer tube [m] do_o_IHX = 0.00953; %Outer diameter of the outer tube [m]
A_i = pi/4*di_i_IHX^2; %Area of inner tube [m^2]
A \circ = pi/4*(di \circ IHX^2-do i IHX^2); %Area of outer tube [m^2]
V_{IHX_i} = L_{IHX*A_i}; V_{IHX_0} = L_{IHX*A_0};
%Geometric properties of the connecting tubes in-between the refrigeration
%components
L_{comp\_gc} = 2.15; %Length of tube connecting compressor and gas cooler [m]
\overline{di} comp gc = 0.00453; %Inner diameter [m]
V comp gc = L comp gc*pi/4*di comp gc^2; %Inner volume [m^3]
L\_gc\_IHX = 0.35 + 0.65; %Length of tube connecting gas cooler and IHX [m]
di gc IHX = 0.00453; %Inner diameter [m]
V_gc_IHX = L_gc_IHX*pi/4*di_gc_IHX^2;
                                             %Inner volume [m^3]
L IHX ct = 0.45; %Length of tube connecting IHX and the capillary tube [m]
di IHX ct = 0.00354; %Inner diameter [m]
V IHX ct = L IHX ct*pi/4*di IHX ct^2; %Inner volume [m^3]
L ev IHX = 0.93; %Length of tube connecting Evaporator and the IHX [m]
```

```
di ev IHX = 0.00453; %Inner diameter [m]
V ev IHX = L ev IHX*pi/4*di ev IHX^2; %Inner volume [m^3]
L IHX comp = 0.35; %Length of tube connecting IHX to inlet of compressor [m]
d\bar{i} IHX comp = 0.00453; %Inner diameter [m]
V IHX comp = L IHX comp*pi/4*di IHX comp^2;
                                                   %Inner volume [m^3]
%Lengths [m] of transition pieces between tubes of different diameters
L_tr1 = 0.015; %Between comp_gc and gc
L tr2 = 0.015; %Between gc and gc IHX
L_tr3 = 0.015; %Between gc_IHX and IHX inner tube (contains gas cooler CO2)
L_tr4 = 0.015; %Between IHX inner tube and IHX ct
L_{\rm tr5} = 0.030; %Between IHX_ct and ct L_{\rm tr6} = 0.030; %Between ct and ev
L tr7 = 0.015; %Between ev and ev IHX
L_{tr8} = 0.045; %Between ev_IHX and IHX outer tube (Contains evaporator CO2) L_{tr9} = 0.045; %Between IHX outer tube and IHX_comp
%Form the control volumes of the whole solution domain.
N comp gc = 52; %Number of cv's for the connecting tube between outlet of
                  %compressor and inlet of gas cooler.
N tr1 = 1;
                  %Number of cv's for transition between comp gc tube and gas
                  %cooler tube.
                  %Number of cv's for the gas cooler.
N gc = 400;
N tr2 = 1;
                  %Number of cv's for transition between gas cooler tube and
                  %gc IHX tube
N gc IHX = 66;
                  %Number of cv's between outlet of gas cooler and IHX.
                  %Number of cv's for transition between gc IHX tube and
N tr3 = 1;
                  %IHX tube
N THX = 120:
                  %Number of cv's for the Internal Heat Exchanger (IHX) inner tube.
N = 1;
                  %Number of cv's for transition between IHX tube and
                  %IHX ct tube
N IHX ct = 24; %Number of cv's for the connecting tube between IHX and
                  %Capillary tube.
N \text{ tr5} = 2;
                  %Transition between IHX ct tube and capillary tube
                  %Number of cv's for the Capillary Tube.
N = 230;
N_{tr6} = 2;
                  %Transition between capillary tube and evaporator tube
N = 300;
                  %Number of cv's for the Evaporator.
N = 1;
                  %Transition between evaporator tube and ev IHX tube
N_ev_IHX = 40; %Number of cv's for the connecting tube between outlet of
                  %Evaporator and IHX.
N tr8 = 3;
                  %Transition between ev IHX tube and IHX tube
                  %Number of cv's used for outer tube of IHX
%N IHX = 120;
_{\rm N} tr9 = 3;
                  %Transition between IHX tube and IHX comp tube
N IHX comp = 23; % Number of cv's for the connecting tube between the IHX outlet
                  %and compressor inlet.
N HP = N comp qc+N tr1+N qc+N tr2+N qc IHX+N tr3+N IHX+N tr4+N IHX ct+N tr5;
N LP = N tr6+N ev+N tr7+N ev IHX+N tr8+N IHX+N tr9+N IHX comp;
N_{tot} = N_{HP+N_{ct+N_{LP}}}
%--Build a vector containing cv lengths--%
\mbox{\ensuremath{\mbox{\$}}\xspace{-1.5ex} Initialise control volume lengths}
L z(1:N tot) = 0;
                      %[m]
%Define lengths of control volumes for the different sections.
%comp_gc connecting pipe lengths
 \label{eq:loss_loss}  \texttt{L\_z} \, (1: \texttt{N\_comp\_gc/2}) \, = \, \texttt{Changing\_Size\_Mesh} \, (\texttt{L\_comp\_gc/2,1/0.9322,N\_comp\_gc/2}) \, ; 
Lz(N comp gc/2+1:N comp gc) = Changing Size Mesh(L comp gc/2, <math>\overline{0}.9322, N comp gc/2);
%tr1 cv lengths
\label{eq:loss_loss}  \mbox{L\_z}\left(\mbox{N\_comp\_gc+1:N\_comp\_gc+N\_tr1}\right) \ = \ \mbox{L\_tr1/N\_tr1;}
%Gas cooler cv lengths
L z(N comp gc+N tr1+1:N comp gc+N tr1+N gc/2) =
Changing_Size_Mesh(L_gc/2,1/0.98981,N gc/2);
L_z(N_comp_gc+N_tr1+N_gc/2+1:N_comp_gc+N_tr1+N_gc) =
Changing_Size_Mesh(L_gc/2,0.98981,N_gc/2);
%tr2 cv lengths
L z(N comp gc+N tr1+N gc+1:N comp gc+N tr1+N gc+N tr2) = L tr2/N tr2;
```

```
%gc IHX cv lengths
L z(N comp gc+N tr1+N gc+N tr2+1:N comp gc+N tr1+N gc+N tr2+N gc IHX) =
L_gc_IHX/N_gc_IHX; %tr3 cv lengths
 \texttt{L\_z} \; (\texttt{N\_comp\_gc+N\_tr1+N\_gc+N\_tr2+N\_gc\_IHX+1:N\_comp\_gc+N\_tr1+N\_gc+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr
3) = L tr3/N tr3;
%IHX cv lengths
%Gas cooler side of IHX's cv lengths
L z (N HP-(N IHX+N tr4+N IHX ct+N tr5)+1:N HP-(N IHX/2+N tr4+N IHX ct+N tr5)) =
Changing Size Mesh (L IH\overline{X}/2, \overline{1}/0.9895, N IH\overline{X}/2);
L z (N HP-(N IHX/2+N tr4+N IHX ct+N tr5)+1:N HP-(N tr4+N IHX ct+N tr5)) =
Changing_Size_Mesh(L_IHX/2,0.9895,N_IHX/2);
%tr4 cv lengths
L z(N HP-(N tr4+N IHX ct+N tr5)+1:N HP-(N IHX ct+N tr5)) = L tr4/N tr4;
%IHX ct cv lengths
L z(N HP-(N IHX ct/2+N tr5)+1:N HP-(N tr5)) =
Changing Size Mesh (L IHX ct/2, 0.9619, N IHX ct/2);
%tr5 cv lengths (Transition to capillary tube)
L_z(N_HP-(N_tr5)+1:N_HP) = L_tr5/N_tr5;
%ct (capillary tube) cv lengths
L z(N HP+1:N HP+N ct) = L ct/N ct;
%tr6 cv lengths (Transition from capillary tube to evaporator tube)
L_z(N_HP+N_ct+1:N_HP+N_ct+N_tr6) = L_tr6/N_tr6;
%Evaporator cv lengths
L z(N HP+N ct+N tr6+1:N HP+N ct+N tr6+N ev/2) =
Changing Size Mesh (L ev/2, 1/\overline{0}. 98779, N ev/2);
L z(N HP+N ct+N tr6+N ev/2+1:N HP+N ct+N tr6+N ev) =
Changing_Size_Mesh(L_ev/2,0.98779,N_ev/2);
%tr7 cv lengths
L z(N HP+N ct+N tr6+N ev+1:N HP+N ct+N tr6+N ev+N tr7) = L tr7/N tr7;
 %ev IHX cv lengths
Changing Size Mesh (L ev IHX/2,1/0.958,N ev IHX/2);
L z(N HP+N ct+N tr6+N \overline{\text{ev}}+N tr7+N \overline{\text{ev}} th tr7+N \overline{\text
Changing Size Mesh (L ev IHX/2, 0.958, N ev IHX/2);
%t.r8 cv lengths
L z(N HP+N ct+N tr6+N ev+N tr7+N ev IHX+1:N HP+N ct+N tr6+N ev+N tr7+N ev IHX+N tr
8) = \overline{L}_{tr8/N_tr8}
 %IHX cv lengths
%Evaporator side of IHX's cv lengths
 %k is outer tube
for k=(N \text{ tot-}(N \text{ tr9+N IHX comp})):-1:((N \text{ tot-}(N \text{ IHX+N tr9+N IHX comp})+1))
             %k i is cv number of inner tube cv exchanging heat with the outer k'th cv
            k = ((N \text{ tot-}(N \text{ tr9+N IHX comp}))-k+1)+
 (N comp gc+N tr1+N gc+N tr2+N gc IHX+N tr3);
            L z(k) = L z(k i);
end
%tr9 cv lengths
L_z(N_{tot-(N_tr9+N_IHX_comp)+1:N_tot-(N_IHX_comp))) = L_tr9/N_tr9;
%IHX comp cv lengths
L z (N tot-(N IHX comp)+1:N tot) = L IHX comp/N IHX comp;
%Define area and hydraulic diameter of control volumes
A v(1:N tot+1) = 0; %[m^2]
d\overline{h}(1:N \ \overline{tot}) = 0; \ %[m]
%comp_gc
A v(1) = pi/4*di comp gc^2; %Inlet area of 1st cv
 for k=1:N comp_gc
           end
for k=(N_comp_gc+1):(N_comp_gc+N_tr1)
dh(\overline{k}) = sqrt(((A_v(k)+\overline{A}_v(\overline{k}+1))/2)*4/pi);
```

```
for k=(N comp gc+N tr1+1):(N comp gc+N tr1+N gc)
                   A v(k+1) = pi/4*di gc i^2; dh(k) = di gc i;
end
%tr2
for k=(N comp gc+N tr1+N gc+1):(N comp gc+N tr1+N gc+N tr2)
                  A_v(k+1) = (pi/4*(di_gc_IHX^2-
di_gc_i^2)/L_tr2)*sum(L_z(N_comp_gc+N_tr1+N_gc+1:k))+pi/4*di_gc_i^2;
                   dh(k) = sqrt(((A v(k)+A v(k+1))/2)*4/pi);
 %gc IHX
for k=(N comp gc+N tr1+N gc+N tr2+1):(N comp gc+N tr1+N gc+N tr2+N gc IHX)
                  A v(k+1) = pi/4*di gc IHX^2; dh(k) = di gc IHX;
%tr3
for
k = (N\_comp\_gc+N\_tr1+N\_gc+N\_tr2+N\_gc\_IHX+1): (N\_comp\_gc+N\_tr1+N\_gc+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc\_IHX+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_gc+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N\_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_tr2+N_t
                  A v(k+1) = (pi/4*(di i IHX^2-
di gc IHX^2)/L tr3)*sum (\overline{L} z(N comp gc+N tr1+N gc+N tr2+N gc IHX+1:k))+pi/4*di gc I
HX^{-2};
                  dh(k) = sqrt(((A v(k)+A v(k+1))/2)*4/pi);
end
 %THX
for
k=(N comp gc+N tr1+N gc+N tr2+N gc IHX+N tr3+1):(N comp gc+N tr1+N gc+N tr2+N gc I
HX+N tr3+N IHX)
                  \overline{A} v(k+\overline{1}) = pi/4*di i IHX^2; dh(k) = di i IHX;
end
8+r4
for k = (N_{HP} - (N_{tr4} + N_{IHX_{ct}} + N_{tr5}) + 1) : (N_{HP} - (N_{IHX_{ct}} + N_{tr5}))
  \underline{A} \underline{v} (\overline{k}+1) = (pi/4*(di \underline{IHX} \underline{ct}^2 - \underline{di} \underline{i} \underline{IHX}^2) / \underline{L} \underline{tr4}) * \underline{sum} (\underline{L} \underline{z} (\underline{N} \underline{HP} - \underline{N} \underline{HP} - \underline{N} \underline{HP} - \underline{N} \underline{HP} - \underline{HP} \underline{
                  dh(k) = sqrt(((A_v(k)+A_v(k+1))/2)*4/pi);
end
%IHX ct
for k=(N HP-(N IHX ct+N tr5)+1):(N HP-N tr5)
                  A v(k+1) = pi/4*di IHX ct<sup>2</sup>; dh(k) = di IHX ct;
end
%tr5
for k=(N HP-N tr5+1):(N HP)
                  A_v(k+1) = (pi/4*(di_ct^2-di_IHX_ct^2)/L_tr5)*sum(L_z(N_HP-1)
N_tr5+1:k))+pi/4*di IHX ct^2;
                   dh(k) = sqrt(((\overline{A} v(\overline{k}) + A v(k+1))/2)*4/pi);
 %ct
for k=(N HP+1):(N HP+N ct)
                   A_v(k+1) = pi/4*di_ct^2; dh(k) = di ct;
end
 %tr6
for k=(N HP+N ct+1):(N HP+N ct+N tr6)
                  A_v(k+1) = (pi/4*(di_ev_i^2-
di_ct^2)/L_tr6)*sum(L_z(N_HP+N_ct+1:k))+pi/4*di_ct^2;
                  dh(k) = sqrt(((A_v(k)+A_v(k+1))/2)*4/pi);
end
%evaporator
for k=(N HP+N ct+N tr6+1):(N HP+N ct+N tr6+N ev)
                   A v(k+1) = pi/4*di ev i^2; dh(k) = di ev i;
end
8+r7
for k=(N HP+N ct+N tr6+N ev+1):(N HP+N ct+N tr6+N ev+N tr7)
                  A v(k+1) = (pi/4*(di ev IHX^2-
di ev i^2)/L tr7)*sum(L z(N HP+N ct+N tr6+N ev+1:k))+pi/4*di ev i^2;
                  dh(k) = sqrt(((A_v(k) + A_v(k+1))/2)*4/pi);
end
for k=(N HP+N ct+N tr6+N ev+N tr7+1):(N HP+N ct+N tr6+N ev+N tr7+N ev IHX)
                  A v(\bar{k}+1) = pi/4*di ev IHX^2; dh(k) = di ev IHX;
end
%tr8
```

```
k=(N HP+N ct+N tr6+N ev+N tr7+N ev IHX+1):(N HP+N ct+N tr6+N ev+N tr7+N ev IHX+N t
   A_v(k+1) = (pi/4*((di_o_IHX^2-do i IHX^2)-
di ev IHX^2)/L tr8)*sum(L z(N HP+N ct+N tr6+N ev+N tr7+N ev IHX+1:k))+pi/4*di ev I
HX^2;
   dh(k) = sqrt(((A v(k)+A v(k+1))/2)*4/pi);
end
%THX outer tube
for
k=(N HP+N ct+N tr6+N ev+N tr7+N ev IHX+N tr8+1):(N HP+N ct+N tr6+N ev+N tr7+N ev I
HX+N tr8+N IHX)
   \overline{A} v(k+\overline{1}) = pi/4*(di o IHX^2-do i IHX^2); dh(k) = (di o IHX-do i IHX);
%tr9
for k=(N tot-(N tr9+N IHX comp)+1):(N tot-(N IHX comp))
    (N_tr9+N_IHX_comp)+1:k))+pi/4*(di_o_IHX^2-do_i_IHX^2);
   dh(k) = sqrt(((A v(k)+A v(k+1))/2)*4/pi);
%THX comp
for \overline{k} = (N \text{ tot-N IHX comp+1}): N \text{ tot}
   A v(k+1) = pi/4*di IHX comp<sup>2</sup>; dh(k) = di IHX comp;
%-----%
%Calculate total volume of the refrigerator system
Vol HP = 0; %Calculate the volume of the high pressure side
for k=1:N HP
    Vol HP = Vol_{HP} + (A_v(k) + A_v(k+1))/2*L_z(k);
end
Vol ct = 0; %Calculate the volume of the capillary tube
for k=(N HP+1):(N HP+N ct)
   Vol_ct = Vol_ct + (A_v(k) + A_v(k+1))/2*L z(k);
Vol LP = 0; %Calculate the volume of the low pressure side
for k=(N HP+N ct+1):(N tot)
    Vol_{LP} = Vol_{LP} + (A_v(k) + A_v(k+1))/2*L_z(k);
end
Vol Total = Vol HP+Vol ct+Vol LP;
\label{eq:m_Total_CO2} $$m_Total_CO2 = 0.435; $$\%Total mass of CO2 in system [kg] $$rho_initial = m_Total_CO2/Vol_Total; $$Initial average density in the system $$$
T initial = 25+273.15; %Assume the system is in equilibrium with its environment
%Determine the state of the CO2 working fluid at the start
rho = rho_initial;
T = T initial;
CO2 Prop at rho and T; %Determines all properties of CO2 at the given initial
state
P initial = P; %Pressure at the start (kPa)
%Define and initialise vectors to hold the vapour quality and other values of CO2
alpha_vol_z(1:N_tot)=0.9; %Initialise
xi z(\overline{1}:N tot)=1; %Initialise
%If two phase is present in the initial state
if Two ph==1
    m \overline{f} = (1-xi) * m Total CO2;
    Vol f = m f/rho f;
    if Vol HP<=Vol f
        for k=1:N_tot
    %Assume for the simulation that at all liquid is contained in the first
    %control volumes of the HP side at start-up. (This is a fair assumption
    %since the refrigerator is charged in the HP side and also most CO2 settles
    %in the HP side at the end of operation).
        m_z(k) = rho_f*(A_v(k)+A_v(k+1))/2*L_z(k); rho_z(k) = rho_f;
        u z(k) = u f; z(k) = cp f; cv z(k) = cv f; h z(k) = h f; s z(k) = s f;
```

```
cond z(k) = cond f; mu z(k) = visc f;
                rho_f z(k) = rho_f; rho_g z(k) = rho_g;
                 alpha_vol_z(k) = 0; xi_z(k) = 0;
                 if sum(m z(1:k))>m f
                          %Correct the properties of the current control volume (transition cv)
                         m f k = m f-sum(m z(1:k-1));
                         vol_f = m_f k/rho_f;

vol_g = (A_v(k)+A_v(k+1))/2*L_z(k))-vol_f k;
                         m \ g \ k = vol \ g \ k*rho \ g;
                         xi = m g k/(m g k+m f k); %vapour fraction
                          \label{eq:m_z(k) = m_f_k+m_g_k; rho_z(k) = m_z(k)/((A_v(k)+A_v(k+1))/2*L_z(k)); } \\  \mbox{m_z(k) = m_f_k+m_g_k; rho_z(k) = m_z(k)/((A_v(k)+A_v(k+1))/2*L_z(k)); } 
                         u_z(k) = xi*u_g+(1-xi)*u_f; h_z(k) = xi*h_g+(1-xi)*h_f; s_z(k) = xi*s_g+(1-xi)*s_f; cp_z(k) = xi*cp_g+(1-xi)*cp_f;
                         cv z(k) = xi*cv g+(1-xi)*cv f; cond z(k) = (xi/cond g+(1-xi)/cond f)^-
1:
                         mu_z(k) = (xi/visc_g+(1-xi)/visc_f)^-1; rho_f_z(k) = rho_f;
                         rho g z(k) = rho g; alpha vol z(\overline{k}) = vol g \overline{k}/(\text{vol g k+vol f k});
                         xi z(k) = xi;
                         k trans = k;
                         break %Leave the for loop
                 end
                 %Remainder of refrigeration system will contain saturated gas only
                 for k=(k trans+1):N tot
                         m_z(k) = rho_g*(A_v(k)+A_v(k+1))/2*L_z(k); rho_z(k) = rho_g;
                          u z(k) = u g; cp z(k) = cp g; cv z(k) = cv g; h z(k) = h g;
                         z(k) = s_g; cond_z(k) = cond_g; mu_z(k) = visc_g;

rho f z(k) = rho f;
                         rho_gz(k) = rho_g; alpha_vol_z(k) = 1; xi_z(k) = 1;
                 end
        else
                 for k=N HP:-1:1
                         m \ z(k) = rho_f*(A_v(k)+A_v(k+1))/2*L_z(k); rho_z(k) = rho_f;
                         u z(k) = u f; cp z(k) = cp f; cv z(k) = cv f; h z(k) = h f;
                          s^{-}z(k) = s_{f};
                         cond z(k) = cond f; mu z(k) = visc f; rho f z(k) = rho f;
                         rho_{g}z(k) = rho_{g}; alpha_{vol}z(k) = 0; xi_{z}(k) = 0;
                          if sum(m z(N HP:-1:k))>m f
                                  %Correct the current properties for the transition control volume
                                  m f k = m f-sum(m z(N HP:-1:k+1));
                                  vol_f_k = m_f_k/rho_f;
                                  vol_g_k = ((A_v(k)+A_v(k+1))/2*L_z(k))-vol_f_k;
                                  m g k = vol g k*rho g;
                                  xi = m_g k/(m_g k+m_f k); %vapour fraction
                                  m_z(k) = m_f_k+m_g_k; rho_z(k) =
m_z(k)/((A_v(k)+A_v(k+1))/2*L_z(k));
                                 u_z(k) = xi*u_g + (1-xi)*u_f; h_z(k) = xi*h_g + (1-xi)*h_f;

s_z(k) = xi*s_g + (1-xi)*s_f; cp_z(k) = xi*cp_g + (1-xi)*cp_f;
                              cv z(k) = xi*cv g+(1-xi)*cv f; cond z(k) = (xi/cond g+(1-xi)*cv f)
xi)/cond f)^-1;
                                  mu z(k) = (xi/visc g+(1-xi)/visc f)^-1; rho f z(k) = rho f;
                                  \label{eq:rho_g_z(k) = rho_g; alpha_vol_z(k) = vol_g_k/(vol_g_k+vol_f_k);} \\ \text{rho_g_z(k) = rho_g_k/(vol_g_k+vol_f_k);} \\ \text{
                                  xi_z(k) = xi;
                                  k trans = k;
                                  break %Leave the for loop
                         end
                 end
                 %Remainder of HP side will contain saturated gas only
                 for k=(k trans-1):-1:1
                         m_z(k) = rho_g*(A_v(k)+A_v(k+1))/2*L_z(k); rho_z(k) = rho_g;
                         u_z(k) = u_g;
                         cp_z(k) = cp_g; cv_z(k) = cv_g; h_z(k) = h_g; s_z(k) = s_g;
```

```
cond z(k) = cond g; mu z(k) = visc g; rho f z(k) = rho f;
            rho g z(k) = rho_g; alpha_vol_z(k) = 1; xi_z(k) = 1;
        end
        %Remainder of refrigeration system will contain saturated gas only
        for k=N HP+1:N tot
            m z(k) = rho g*(A v(k)+A v(k+1))/2*L z(k); rho z(k) = rho g;
            u^{z}(k) = u^{z}(k)
            cp_z(k) = cp_g; cv_z(k) = cv_g; h_z(k) = h_g; s_z(k) = s_g; cond_z(k) = cond_g; mu_z(k) = visc_g; rho_f_z(k) = rho_f; rho_g_z(k) = rho_g; alpha_vol_z(k) = 1; xi_z(k) = 1;
    end
end
%If only single phase is present in the initial state
if Two ph==0
    fprintf('Warning check that CO2 is charged to the level required');
        %If flow is only single phase define rho_f and rho_g as values that
        %may be obtained if the flow at that temperature T becomes two-phase
        %abruptly (Their use is to speed up the simulation program in
        %providing a better guess once the flow changes to two-phase.)
        %Use saturated liquid density given by eq 3.14 S&W(1996) as initial guess
        rho f = rho c*exp(sum(a rho sl.*(1-T/T c).^t rho sl));
        %Use saturated vapour density given by eq 3.15 S&W(1996) as initial guess
        rho g = rho c*exp(sum(a rho sv.*(1-T/T c).^t rho sv));
    for k=1:N tot
        cond z(k) = cond; mu z(k) = visc; rho f z(k) = rho f; rho g z(k) = rho g;
        alpha vol z(k) = 1; \overline{x}i z(k) = 1;
    end
end
%Initialise vectors that are used and tracked during the simulation.
P_z(1:N_tot) = P_initial; %Pressure [kPa]
T z(1:N tot) = T initial; %Temperature [K]
T z(1:N tot) = T initial;
u z old = u z;
u_z_latest_upd = u_z;
\frac{1}{2} rho z old = rho z;
rho z latest upd = rho z;
v z(1:N tot+1) = 0; %Initial velocity at each velocity node [m/s]
vz old = vz;
v z older = v z old;
v_z_oldest = v_z_older;
% Gas cooler
% Initial state of the gas cooler outer tube (Water used as cooling medium)
T initial gc o = T initial; %Temperature of fluid in outer tube [K]
%Determine the initial state of the outer tube fluid
rho initial gc o = rho f w func(T initial gc o);
%Properties of each control volume of the outer tube at the start
*Outer tube shares the same control volume lengths as the inner tube.
mz gc o(1:N gc)=(rho initial gc o*A gc o)*L z(N comp gc+N tr1+1:N comp gc+N tr1+N
ac);
rho z gc o(1:N gc) = rho initial gc o;
uz_gc_o(1:N_gc) = u_f_w_func(T_initial_gc_o); %Internal energy of each control
cpz gc o(1:N gc) = cp f w func(T initial gc o); %Specific heat cp of each control
volume
T_{gc_0}(1:N_{gc}) = T_{initial_{gc_0}}
```

```
cond gc o(1:N gc) = cond_f_w_func(T_initial_gc_o);
mu_gc_o(1:N_gc) = mu_f_w_func(T_initial_gc_o);
uz_gc_o_latest_upd = uz_gc_o;
%Fixed operating conditions for the gas cooler outer tube (Cooling water)
mdot gc o = 0.045; %Mass flow rate through outer tube [kg/s]
\ensuremath{^{\circ}} Temperature of entering fluid in outer tube
T_{in}gc_{o} = 25 + 273.15; %Water at 25 deg C enters the outer tube of gas cooler h_{in}gc_{o} = h_{f}w_{f}unc(T_{in}gc_{o}); %Enthalpy of incoming flow for the outer tube
%[kJ/kq]
u in gc o = u f w func(T in gc o); %Internal energy of incoming flow for the
outer %tube [kJ/kg]
               ______
% Evaporator
% Initial state of the evaporator outer tube
T initial ev o = T initial; %Temperature of fluid in outer tube [K]
%Determine the initial state of the outer tube fluid
rho initial ev o = rho f w func(T initial ev o);
%Mass in each control volume of the outer tube at the start
mz ev o(1:N ev)=(rho initial ev o*A ev o)*L z(N HP+N ct+N tr6+1:N HP+N ct+N tr6+N
ev):
rho z ev o(1:N ev) = rho initial ev o;
uz ev o(1:N ev) = u f w func(T initial ev o); %Internal energy of each control
cpz ev o(1:N ev) = cp f w func(T initial ev o); %Specific heat cp of each control
volume
hz ev o(1:N ev) = h f w func(T initial ev o); %Enthalpy of each control volume
hz new ev o(1:N ev) = hz ev o;
\overline{T} ev o(1:\overline{N}) ev) = \overline{T} initial ev o;
cond ev o(1:N ev) = cond f w func(T initial ev o);
mu ev o(1:N ev) = mu f w func(T initial ev o);
uz ev o latest upd = uz ev o;
%Fixed operating conditions for the evaporator outer tube (Heating water)
mdot \ ev \ o = 0.045; %Mass flow rate through outer tube [kg/s]
%Temperature of entering fluid in outer tube
T in ev o = 25 + 273.15; %Water at 25 deg C enters the outer tube of evaporator
h in ev o = h f w func(T in ev o); %Enthalpy of incoming flow for the outer tube
u in ev o = u f w func(T in ev o); %Internal energy of incoming flow for the
outer tube [kJ/kg]
§______
alpha vol = 0.1; %Initial guess to determine two-phase properties
%-----%
dt = 1e-4; %Time step size [s]
t = 0; %Initialise time
rho out comp = rho g/2; %Define an initial guess for the outlet density of the
%compressor
%Define vector to store location of cell centered nodes
L(1:N_tot)=0;
L(1) = L z(1)/2;
for k=2:\overline{N} tot
   L(k) = L(k-1) + L z(k-1)/2 + L z(k)/2;
%Initialise variables used in the discretisation of conservation equations
%Variables for scalar control volumes
F w = 0; F e = 0;
a_{w}(1:N_{tot}) = 0; a_{e}(1:N_{tot}) = 0; a_{p}(1:N_{tot}) = 0; a_{p}old (1:N_{tot}) = 0;
S_u(1:N_{tot}) = 0; S_p = 0; Qdot_ht(1:N_{tot}) = 0;
%Variables for momentum control volumes (on the staggered grid)
```

```
F_w_mom = 0; F_e_mom = 0;
a_w_mom(1:N_tot+1) = 0; a_e_mom(1:N_tot+1) = 0; a_p_mom(1:N_tot+1) = 0;
S_u_mom(1:N_tot+1) = 0; S_p_mom(1:N_tot+1) = 0; a_p_old_mom(1:N_tot+1) = 0;
rho_e(1:N_tot-1) = 0; %Initialise for later use

rho_z_new = rho_z;
u_z_new = u_z;
v_z_new = v_z;
```

### C3: Program Code to Update Variables for the New Time-Step

```
%Time_stepping_UD_density_based.m is a script file written to update the old
values, %hence to advance the simulation to the new time-step.
%Update to new time level
v z oldest old = v z oldest; v z oldest = v z older; v z older = v z old;
v z old = v z;
*Use Taylor series expansion combined with backward-finite difference formulas for
the %derivatives to provide a projection method for determining a good guess for
the new %velocity field.
%Third order projection method gives:
v_z = 8/3*v_z_old-2.5*v_z_older+v_z_oldest-1/6*v_z_oldest_old; %Gives fastest
performance
rho_z_old = rho_z; u_z_old = u_z; T_z_old = T_z;
%Gas cooler water (outer tube)
uz gc o old = uz gc o;
%Evaporator water (outer tube)
uz ev o old = uz ev o;
```

## C4: Program Code to Solve the Three Conservation Equations

```
%Itterate UD density based.m is a script file written to iteratively solve the
%three conservation equations for a time-step using a density based algorithm.
sum u mom residuals=1; norm Global mom Residual=1;
i count = 0;
while (norm Global mom Residual>10^-6)||(norm Global c Residual>10^-6)...
             || (norm Global e Residual>10^-6)
i count = i count+1; % Count number of iterations per time-step
% Calculate boundary conditions
%-----%
%Input variables
rho in comp = rho z(N tot); %Exit of last control volume is entrance to the
compressor
h1 = h_z(N_tot); s1 = s_z(N_tot); rho1 = rho_in_comp;
eff_volumetric = 0.954; eff_isentropic = 0.716;
N = 2400; %Compressor speed [rev/min]
s2 isen = s1;
P2 = P z(1); %Outlet pressure of the compressor [kPa]
s = s2 isen; P = P2;
           %Use old value as initial guess
T = T \overline{z}(1);
```

```
rho = rho out comp; %Use old value as initial quess (Note this is only a quess)
CO2 1Ph Prop at P and s;
h2 \overline{isen} = h;
h_comp_out = h1+(h2_isen-h1)/eff_isentropic;
h = h comp out; P = P2;
T = T_z(1); %Use old value as initial guess
rho = rho out comp; %Use old value as initial guess
CO2 1Ph Prop at P and h;
%Obtained boundary conditions for the inlet of the simulation domain.
rho out comp = rho;
u_out_comp = u;
\ensuremath{\overline{\text{5C}}}\xspace mass flow rate boundary condition for the simulation domain.
mdot comp = rho1*V comp*N/60*eff volumetric;
v_in = mdot_comp/(rho_out_comp*A_v(1));
v_out = mdot_comp/(rho_z(N_tot)*A_v(N_tot+1));
%Incorporate velocity boundary conditions for the simulation domain
v z(1) = v in; %Inlet boundary velocity of first control volume
v z (N tot+1) = v out; %Outlet velocity of last control volume
%--Continuity equation--%
%First control volume
k=1:
L PE = L z(k)/2+L z(k+1)/2; fe = (L z(k+1)/2)/L PE;
F w = 0; F e = v z(k+1)*A v(k+1);
a_{w}(k) = 0; a_{e}(k) = max(0, -F_{e}); a_{p}old(k) = (A_{v}(k) + A_{v}(k+1))/2*L_{z}(k)/dt;
S u(k) = mdot comp+a p old(k)*rho z old(k);
a_p(k) = a_w(k) + a_e(k) + (F_e-F_w) + a_p old(k);
for k=2:N_tot-1 %Interior control volumes
    \label{eq:local_pe}  \mbox{$\mathbb{L}$_PE = $\mathbb{L}$_z(k)/2+$\mathbb{L}$_z(k+1)/2; fe = $(\mathbb{L}$_z(k+1)/2)/$\mathbb{L}$_PE;}
    LWP = Lz(k-1)/2+Lz(k)/2; fw = (Lz(k-1)/2)/LWP;
    \begin{array}{l} F_{-w} = v_{-z}\left(k\right)*A_{-v}\left(k\right); \;\; F_{-e} = v_{-z}\left(k\!+\!1\right)*A_{-v}\left(k\!+\!1\right); \\ a_{-w}\left(k\right) = \max\left(F_{-w},0\right); \;\; a_{-e}\left(k\right) = \max\left(0,-F_{-e}\right); \end{array}
     a p old(k) = (\overline{A} \text{ v}(k) + \overline{A} \text{ v}(k+1))/2*L \text{ z}(k)/dt;
     S_u(k) = a_p_old(k)*rho_z_old(k);
     a p(k) = a w(k) + a e(k) + F e - F w + a p old(k);
%Last control volume
L WP = L z(k-1)/2+L z(k)/2; fw = (L z(k-1)/2)/L WP;
F w = v z(k) *A v(k); F e = 0;
%Check how well the current density satisfies the continuity equation:
%Calculate density(continuity) residuals at each cv
c_{residual(1:N_{tot})} = 0;
%For first control volume
c residual(k) = a p(k)*rho z(k)-(a e(k)*rho z(k+1)+S u(k));
c_norm_factor(k) = a p(k)*rho_z(k);
for k=2:(N_tot-1) %Interior control volumes
    c residual(k) = a p(k)*rho z(k)-(a w(k)*rho z(k-1)+a e(k)*rho z(k+1)+S u(k));
    c_{norm_factor(k)} = a_p(k) * rho_z(k);
end
%For the last control volume
k=N tot;
c residual(k) = a p(k)*rho z(k)-(a w(k)*rho z(k-1)+S u(k));
c_{norm_factor(k)} = a_p(k) * rho_z(k);
%Calculate sum of absolute momentum residuals
sum c residuals = sum(abs(c residual(:)));
```

```
sum c norm factor = sum(abs(c norm factor(:)));
%This gives an indication of how well the continuity equation is satisfied
norm Global_c_Residual = sum_c_residuals/sum_c_norm_factor;
%TDMA solver for continuity equation (calculate new densities)
   %alpha = a_e_c(k); %beta = a_w_c(k); %Dj = a_p_c(k);
%Boundary control volume
k=1:
Aj(k) = a e(k) / (a p(k) - 0);
Cj_aks(k) = (0+S_u(k))/(a_p(k)-0);
for k=2:N tot-1
                 %Interior control volumes
    Aj(k) = a_e(k) / (a_p(k) - a_w(k) * Aj(k-1));
    Cj_aks(k) = (a_w(k) * Cj_aks(k-1) + S_u(k)) / (a_p(k) - a_w(k) * Aj(k-1));
k=N tot; %Last control volume
Aj(\overline{k}) = 0;
Cj_aks(k) = (a_w(k) *Cj_aks(k-1) + S_u(k)) / (a_p(k) - a_w(k) *Aj(k-1));
for k=N tot:-1:1
    if k==N tot, rho z(k) = Cj aks(k);
      else rho z(k) = Aj(k) * rho z(k+1) + Cj aks(k);
    end
end
%Obtain face values for density
for k=1:N tot-1
    %Upwind differencing used for density
    if v z(k+1)>0, rho e(k) = rho z(k);
     else rho e(k) = \overline{rho} z(k+1);
    end
end
%--Energy equation--%
%Calculate heat transfer (Radial heat transfer)
%Innitialise heat transfer and afterwards change the required cv's that do
%have heat transfer.
Qdot ht(1:N tot) = 0;
%--Gas cooler heat transfer rate--%
%Heat transfer rate for control volumes transferring heat between the
%gas cooler outer tube (water) and inner tube (CO2);
%Heat transfer rate defined positive as heat from the outer tube to the
%inner tube i.e. as heat addition to the CO2.
for k=(N_comp_gc+N_tr1+1):(N_comp_gc+N_tr1+N_gc)
    %control volume nr for outer tube
    k_o = k-(N_comp_gc+N_tr1);
    if k>299 \sqrt[8]{\text{Only}} 14 m of water cooling used, the rest has no heat transfer
        Qdot ht(k) = 0;
    else %Heat exhange with water in the outer tube
        Re_flow = rho_z(k)*abs((v_z(k)+v_z(k+1))/2)*di_gc_i/mu_z(k);
        k_Cu = 400; %Thermal conductivity of copper [W/m.K]
        Thermal resistance for conduction through copper inner tube
         \texttt{R\_i\_Cu = log(do\_gc\_i/di\_gc\_i)/(2*pi*k\_Cu*L\_z(k));} \quad \texttt{\%[K/W]} 
        %Calculate inner tube heat transfer coefficient (ht i)
        %mu_z(k); %[Pa.s]
%cp z(k); %[kJ/kg.K]
        %cond_z(k); %[W/m.K]
        Pr = mu z(k)*(cp z(k)*1000)/cond z(k);
        Nu = 0.\overline{0}23*Re flow^0.8*Pr^0.3; \frac{8}{9}0.3 used since cooling of the inner fluid
        %expected
        ht_i = Nu*cond_z(k)/di_gc_i; %[W/m^2.K]
        %Calculate outer tube heat transfer coefficient (ht o)
        %mu_gc_o(k_o); %[Pa.s]
%cpz_gc_o(k_o); %[kJ/kg.K]
%cond_gc_o(k_o); %[W/m.K]
        Pr = mu gc o(k o)*(cpz gc o(k o)*1000)/cond gc o(k o);
```

```
mdotz = mdot gc o;
         Re_Do = mdotz*(di_gc_o-do_gc_i)/(mu_gc_o(k_o)*A_gc_o);
         Nu = 0.023*Re D o^0.8*Pr^0.4; %0.4 used since heating of the outer tube
         %fluid is expected
         ht_o = Nu*cond_gc_o(k_o)/(di_gc_o-do_gc_i); %[W/m^2.K]
         %Calculate thermal resistances [K/W]
         R_i_CO2 = 1/(ht_i*pi*di_gc_i*L_z(k));
R_o_CO2 = 1/(ht_o*pi*do_gc_i*L_z(k));
         R \text{ tot} = R \text{ i } CO2 + R \text{ i } Cu + R \text{ o } CO2;
    %Calculate heat transfer rate as from outer tube (water) to inner tube (CO2).
         Qdot ht(k) = (T gc o(k o) -T z(k))/R tot/1000; %[kW]
    %Outer tube %Flow is in opposite direction (steady flow)
    mdotz_out = mdot_gc_o;
    mdotz in = mdot gc o;
    %Update internal energy of outer tube (Outer tube flow is in opposite
    %direction)
    if k o==N gc
         uz gc o(k o) = uz gc o old(k o)+dt*...
              (mdotz in*h in gc o-mdotz out*hz gc o(k o)-Qdot ht(k))/mz gc o(k o);
         uz_gc_o(k_o) = uz_gc_oold(k_o)+dt*...
              (mdotz in*hz_gc_o(k_o+1)-mdotz_out*hz_gc_o(k_o)-
Qdot_ht(k))/mz_gc_o(k_o);
    end
%--Evaporator heat transfer rate--%
%Heat transfer rate for control volumes transferring heat between the
%evaporator outer tube (water) and inner tube (CO2);
%Heat transfer rate defined positive as heat from the outer tube to the
%inner tube i.e. as heat addition to the CO2.
for k=(N HP+N ct+N tr6+1):(N HP+N ct+N tr6+N ev)
    %control volume nr for outer tube
    k \circ = k-(N HP+N ct+N tr6);
    %12 m of water cooling used, the last part has no heat transfer
    if k>1155
        Qdot ht(k) = 0;
    else %Heat exhange with water in the outer tube
         Re flow = rho z(k)*abs((v z(k)+v z(k+1))/2)*di ev i/mu z(k);
         k \overline{Cu} = 400; %Thermal conductivity of copper [\overline{W/m.K}]
         %Thermal resistance for conduction through copper inner tube
         R_i_Cu = \log(do_ev_i/di_ev_i)/(2*pi*k_Cu*L_z(k)); %[K/W]
         %Calculate inner tube heat transfer coefficient (ht i)
         %mu z(k); %[Pa.s]
         %cp_z(k); %[kJ/kg.K]
         %cond z(k); %[W/m.K]
         Pr = mu z(k)*(cp z(k)*1000)/cond z(k);
          \begin{aligned} Nu &= 0.023 \, ^{*}\text{Re} \, \text{flow} \, ^{*}0.8 \, ^{*}\text{Pr} \, ^{*}0.4; & \text{\%}\text{Heating expected} \\ \text{ht\_i} &= Nu \, ^{*}\text{cond\_z} \, (k) \, / \text{di\_ev\_i}; & \text{\%} \, [\text{W/m} \, ^{2}.\text{K}] \end{aligned} 
         %Calculate outer tube heat transfer coefficient (ht o)
         %mu_ev_o(k_o); %[Pa.s]
         %cpz_ev_o(k_o); %[kJ/kg.K]%cond_ev_o(k_o); %[W/m.K]
         Pr = \overline{\text{mu ev o(k o)}} * (cpz ev o(k o)*1000)/cond ev o(k o);
         mdotz = mdot ev o;
         Re D_o = mdotz*(di_ev_o-do_ev_i)/(mu_ev_o(k_o)*A_ev_o);
         Nu = 0.023*Re_D_o^0.8*Pr^0.3; %Cooling expected
         ht o = Nu*cond ev o(k o)/(di ev o-do ev i);
         %Calculate thermal resistances [K/W]
         R_iCO2 = 1/(ht_i*pi*di_ev_i*L_z(k));
         R_oCO2 = 1/(ht_o*pi*do_ev_i*L_z(k));
         R \text{ tot} = R \text{ i } CO2 + R \text{ i } Cu + R \text{ o } CO2;
```

```
%Calculate heat transfer rate as from outer tube (water) to inner tube (CO2).
         Qdot_ht(k) = (T_ev_o(k_o)-T_z(k))/R_tot/1000;
                                                                %[kW]
    %Outer tube %Flow is in opposite direction (steady flow)
    mdotz out = mdot ev o;
    mdotz in = mdot ev o;
    %Update internal energy of outer tube
    if k o==N ev
         \overline{uz} ev o(k o) = uz ev o old(k o) + dt*...
              (mdotz in*h in ev o-mdotz out*hz ev o(k o)-Qdot ht(k))/mz ev o(k o);
         uz ev o(k o) = uz ev o old(k o)+dt*...
              (mdotz_in*hz_ev_o(k_o+1)-mdotz_out*hz_ev_o(k_o)-
Qdot_ht(k))/mz_ev_o(k_o);
    end
end
%--Internal heat exchanger heat transfer rate--%
for k=(N comp gc+N tr1+N gc+N tr2+N gc IHX+N tr3+1):...
              (N comp gc+N tr1+N gc+N tr2+N gc IHX+N tr3+N IHX)
    dh cv = dh(k);
    Re flow = rho z(k) *abs((v z(k)+v z(k+1))/2)*dh cv/mu z(k);
    k \ Cu = 400; %Thermal conductivity of copper [W/m.K]
    %Thermal resistance for conduction through copper inner tube
    R_i_Cu = \log(do_i_IHX/di_i_IHX)/(2*pi*k_Cu*L_z(k)); \ %[K/W]
    %Calculate inner tube heat transfer coefficient (ht i)
    %mu_z(k); %[Pa.s]
%cp_z(k); %[kJ/kg.K]
    % cond z(k); %[W/m.K]
    Pr = mu z(k) * (cp z(k) * 1000) / cond z(k);
    Nu = 0.023*Re flow^0.8*Pr^0.3; %Cooling expected
    ht_i = Nu*cond_z(k)/dh_cv; %[W/m^2.K]
    %Calculate outer tube heat transfer coefficient (ht_o)
    k \circ = (N \text{ tot-}(N \text{ IHX comp+N tr9})+1)-(k-
(N_comp_gc+N_tr1+N_gc+N_tr2+N_gc_IHX+N tr3));
    %mu_z(k_o); %[Pa.s]
%cp z(k o); %[kJ/kg.K]
    %cond z(k o); %[W/m.K]
    Re_flow = rho_z(k_o)*abs((v_z(k_o)+v_z(k_o+1))/2)*(di_o_IHX-v_a)
do i IHX)/mu z(k o);
     \begin{array}{lll} {\tt Pr} &= & {\tt mu\_z}\,(k\_o)\,*\,({\tt cp\_z}\,(k\_o)\,*1000)\,/{\tt cond\_z}\,(k\_o)\,; \\ {\tt Nu} &= & 0.023\,*{\tt Re\_flow}\,^\circ\!0.8\,{\tt Pr}\,^\circ\!0.4\,; & {\tt Heating}\,\,{\tt expected} \end{array} 
    ht_o = Nu*cond_z(k_o)/(di_o_IHX-do_i_IHX);
    %Calculate thermal resistances [K/W]
    R i_CO2 = 1/(ht_i*pi*di_i_IHX*L_z(k));

R_o_CO2 = 1/(ht_o*pi*do_i_IHX*L_z(k));

R_tot = R_i_CO2 + R_i_Cu + R_o_CO2;
    %Heat transferred to inner tube CO2 (i.e. gas cooler side CO2)
    %(Defined as heat addition to the inner tube.)
    Qdot_ht(k) = (T_z(k_0)-T_z(k))/R_tot/1000; %[kW]
    %Heat transferred to the outer tube CO2 (i.e. evaporator side CO2)
    % (Defined as heat addition to the outer tube.)
    Qdot_ht(k_o) = -Qdot_ht(k);
end
%----- Calculate discretisation values for the energy equation ------%
k=1; %First control volume
L_PE = L_z(k)/2+L_z(k+1)/2;
fe = (L z(k+1)/2)/L PE;
if (abs(P z(k)-P c)<10) | | (abs(P z(k+1)-P c)<10)
```

```
cond e = 0;
else
   cond e = fe*cond z(k)+(1-fe)*cond z(k+1);
end
%Axial heat conduction in the gas
dh cv = dh(k);
Re flow = rho z(k) *abs((v z(k)+v z(k+1))/2)*dh cv/mu z(k);
if Re flow>2300 %flow assumed turbulent
   C\overline{f} = 0.078*Re flow^-0.25;
elseif Re flow <= 1e-200 %if there is no flow then there is no friction
                          %(this prevents numerical errors)
    Cf = 0;
else %flow assumed laminar
   Cf = 16/Re flow;
end
tau x = 0.5 \text{ Cf*rho } z(k) \text{ ((v } z(k) + \text{v } z(k+1))/2)^2;
F_w = 0; F_e = rho_e(k) *v_z(k+1) *A_v(k+1);
a^{-}w(k) = 0; a e(k)^{-} = max(0, -F e);
a_p_old(k) = rho_z_old(k) * (A_v(k) + A_v(k+1)) / 2*L_z(k) / dt;
Su(k) = -Pz(k)*(Av(k+1)*vz(k+1)-Av(k)*vz(k))+...
            tau x/1000*(pi*dh cv*L z(k))*abs(((v z(k)+v z(k+1))/2))+...
            \verb| mdot_comp*u_out_comp+Qdot_ht(k)+a_p_old(k)*u_z_old(k)+Qdot_e; \\
a_p(k) = a_w(k) + a_e(k) + (F_e-F_w) + a_p_old(k) / rho_z_old(k) * rho_z(k);
for k=2:N tot-1 %Interior control volumes
    dh cv = dh(k);
    Re_flow = rho_z(k) * abs((v_z(k) + v_z(k+1))/2) * dh_cv/mu_z(k);
    L PE = L z(k)/2+L z(k+1)/2; fe = (L z(k+1)/2)/L PE;
    LWP = Lz(k-1)/2+Lz(k)/2; fw = (Lz(k-1)/2)/LWP;
    \overline{\text{rho}} w = \overline{\text{rho}} e(k-1);
    if (abs(Pz(k-1)-Pc)<10) \mid (abs(Pz(k)-Pc)<10) % Ignore axial conduction when
close to the critical pressure
       cond w = 0;
    else
        cond w = fw*cond z(k) + (1-fw)*cond z(k-1);
    if (abs(P z(k)-P c)<10) || (abs(P z(k+1)-P c)<10)
       cond e = 0;
        cond e = fe*cond z(k)+(1-fe)*cond z(k+1);
    %Calculate skin friction factor for CO2 in current cv
    if Re flow>2300 %flow assumed turbulent
        C\bar{f} = 0.078*Re_flow^{-0.25};
    elseif Re flow <= 1e-200 %if there is no flow then there is no friction
       Cf = 0;
    else %flow assumed laminar
        Cf = 16/Re flow;
    end
    tau x = 0.5*Cf*rho z(k)*((v z(k)+v z(k+1))/2)^2;
   F_w = rho_w^*v_z(k)^*A_v(k); F_e = rho_e(k)^*v_z(k+1)^*A_v(k+1); a_w(k) = max(F_w,0); a_e(k) = max(0,-F_e);
    a_p_old(k) = rho_z_old(k) * (A_v(k) + A_v(k+1))/2*L z(k)/dt;
    S_u(k) = -P_z(k) * (A_v(k+1) * v_z(k+1) - A_v(k) * v_z(k)) + ...
                tau_x/1000*(pi*dh_cv*L_z(k))*abs(((v_z(k)+v_z(k+1))/2))+...
                \label{eq:condition} {\tt Qdot\_ht\,(k)\,+a\_p\_old\,(k)\,*u\_z\_old\,(k)\,+Qdot\_e+Qdot\_w;}
    a p(k) = a w(k) + a e(k) + F e - F w + a p old(k) / rho z old(k) * rho z(k);
%Last control volume
k=N tot;
L_WP = L_z(k-1)/2+L_z(k)/2;
\overline{fw} = (L \overline{z}(k-1)/2)/L \overline{WP};
```

```
rho w = rho e(k-1);
if (abs(P z(k)-P c)<10) | (abs(P z(k-1)-P c)<10)
    cond w = 0;
    cond w = fw*cond z(k) + (1-fw)*cond z(k-1);
dh cv = dh(k);
Re flow = rho z(k) *abs((v z(k)+v z(k+1))/2)*dh cv/mu z(k); %Use old velocity to
%approximate friction
if Re flow>2300 %flow assumed turbulent
    Cf = 0.078*Re_flow^-0.25;
elseif Re flow <= le-200 %if there is no flow then there is no friction
   Cf = \overline{0};
     %flow assumed laminar
else
    Cf = 16/Re_flow;
end
tau x = 0.5 \text{ Cf*rho } z(k) \text{ ((v } z(k) + \text{v } z(k+1))/2)^2;
F_w = rho_w*v_z(k)*A_v(k);
F = 0;
a^{-}w(k) = max(F w, 0); a e(k) = 0;
a_p_old(k) = rho_z_old(k) * (A_v(k) + A_v(k+1))/2*L z(k)/dt;
Su(k) = -Pz(k)*(Av(k+1)*vz(k+1)-Av(k)*vz(k))...
            +tau x/1000*(pi*dh cv*L z(k))*abs(((v z(k)+v z(k+1))/2))+...
            -mdot\_comp*u\_z\_old(k)+Qdot\_ht(k)+a\_p\_old(k)*u\_z\_old(k)+Qdot\_w;
a_p(k) = a_w(k) + a_e(k) + F_e - F_w + a_p_old(k) / rho_z_old(k) * rho_z(k);
%Check how well the internal energy currently satisfies the energy equation:
%Calculate specific internal energy residuals at each cv node
e residual(1:N tot) = 0;
k=1; %For first control volume
e_r = a_p(k) * u_z(k) - (a_e(k) * u_z(k+1) + S u(k));
e norm_factor(k) = a_p(k)*u_z(k);
for k=2:(N \text{ tot-1}) %Interior control volumes
    e residual(k) = a p(k)*u z(k)-(a w(k)*u z(k-1)+a e(k)*u z(k+1)+S u(k));
    e_{norm_factor(k)} = a p(k) *u z(k);
end
k=N tot; %For the last control volume
e residual(k) = a p(k)*u z(k)-(a w(k)*u z(k-1)+S u(k));
e norm factor(k) = a p(k)*u z(k);
%Calculate sum of absolute specific internal energy residuals
sum e residuals = sum(abs(e residual(:)));
sum e norm factor = sum(abs(e norm factor(:)));
%This gives an indication of how well the energy equation is satisfied
norm_Global_e_Residual = sum_e_residuals/sum_e_norm_factor;
%TDMA solver for energy equation (calculate specific internal energy)
80-----
   %alpha = a_e_c(k); %beta = a_w_c(k); %Dj = a_p_c(k);
%Boundary control volume
k=1:
Aj(k) = a_e(k)/(a_p(k)-0);
Cj_aks(k) = (0+S_u(k))/(a_p(k)-0);
for k=2:N tot-1 %Interior control volumes
    Aj(k) = a e(k) / (a p(k) - a w(k) * Aj(k-1));
    Cj_aks(k) = (a_w(k) * Cj_aks(k-1) + S_u(k)) / (a_p(k) - a_w(k) * Aj(k-1));
end
k=N tot; %Last control volume
Aj(\overline{k}) = 0;
C_{j}^{-} aks(k) = (a w(k)*C<sub>j</sub> aks(k-1)+S u(k))/(a p(k)-a w(k)*A<sub>j</sub>(k-1));
for k=N tot:-1:1
    if \overline{k}==N tot
        u z(k) = Cj aks(k);
```

```
else
               u z(k) = Aj(k)*u z(k+1)+Cj aks(k);
       end
end
%Update refrigerant side i.e. CO2 side
%Update pressure and other variables using equation of state P = f(rho, u)
for k=1:N tot.
        %Recalculate properties only if one of the two variables has changed
        %considerably i.e. changed more than 10^-7
 if ((abs(rho z(k)-rho z latest upd(k))>10^-7)||(abs(u z(k)-rho z latest upd(
u_z_{atest_upd(k))>10^{-7})
                %Find properties at rho and u.
               rho = rho z(k); u = u z(k);
               T = T_z(k); %Use previous iteration's value as initial guess %If the flow is two-phase pre-assign initial guesses based on the
               %previous iteration's values.
                rho f = rho f z(k);
               rho_g = rho_g_z(k);
alpha_vol = alpha_vol_z(k);
%Only use the following code if the program runs into an error with properties too
close to the critical region. It is rarely needed.
                %If T>304.1281, and rho and u are in the two-phase region but very
                %close to the critical point i.e. if they fall within the T=304.1281
               %saturated lines then assign critical point values for other properties.
                if (((rho<468.2)&&(rho>467))&&...
                                ((u)-1.904331870237819e+02) \&\& (u<1.901891527564772e+02)) \&\&
(abs(P z(k)-P c)<10)
                        %Assign critical point properties
                        T = T_c;
rho = rho c;
                        CO2_Property
CO2_Conductivity;
                        Viscosity CO2;
                        Two ph = \overline{0};
                        %Set i=2 so that new properties can be saved
                        i=2
               else
                응 }
                        %Calculate properties
                        if P z(k) > 7390 %i.e. if previous pressure is above this level then
                                                      %expect it to remain single phase.
                                CO2 1Ph Prop at rho and u;
                                CO2 Conductivity;
                                Viscosity_CO2;
                        elseif (k>1) && (k<N_tot) && (xi_z(k-1) == xi_z(k+1))
                                CO2 1Ph Prop at rho and u;
                                CO2 Conductivity;
                                Viscosity CO2;
                        elseif (k>1) \&adeta (k<N_tot) && (xi_z(k-1)>0) && (xi_z(k-1)<1) &&...
                                                                         (xi_z(k+1)>0) && (xi_z(k+1)<1)
                                CO2 2Ph Prop at rho and u
                                rho = rho g; Viscosity CO2; visc g = visc;
                                CO2 Conductivity; cond g = cond;
                                rho = rho f; Viscosity CO2; visc f = visc;
                                CO2_Conductivity; cond_f = cond;
                                rho = rho x; %Set density to its two phase value
                                visc = 1/(xi/visc_g+(1-xi)/visc_f);
                               cond = 1/(xi/cond g+(1-xi)/cond f);
                                CO2_Prop_at_rho_and_u
                        end
               %end
                %Error prevention in case of wrong phase selection previously
                %was incorrectly identified
```

```
%as single phase instead of two-phase
                 T=T z(k);
                 z rho=rho z(k); u=u z(k);
                 CO2 2Ph Prop at rho and u
                 rho = rho g; Viscosity CO2; visc g = visc;
                 CO2 Conductivity; cond q = cond;
                 rho = rho f; Viscosity CO2; visc f = visc;
                 CO2 Conductivity; cond f = cond;
                 rho = rho x; %Set density to its two phase value
                 visc = 1/(xi/visc_g+(1-xi)/visc_f);
cond = 1/(xi/cond_g+(1-xi)/cond_f);
             elseif ((Two ph==1)&&((isreal(cp)==0))||(cp<0))</pre>
                 T=T_z(k);
                 rho=rho_z(k); u=u_z(k);
                 CO2 1Ph Prop at rho and u
                 CO2 Conductivity;
                 Viscosity CO2;
        end
        if i>1 %Only update properties if the first property iteration does not
             %already satisfy the error margin.
             %Store updated density and specific internal energy for use later
             %in deciding if the properties need recalculating or not.
             rho z latest upd(k) = rho z(k);
             u z latest upd(k) = u z(k);
             %Assign new properties
P_z(k) = P; T_z(k) = T; cp_z(k) = cp; cv_z(k) = cv; h_z(k) = h;
             s z(k) = s; cond z(k) = cond; mu z(k) = visc;
             if Two ph==1 %Update two-phase vectors
                 rho f z(k) = rho f;
                 rho_g_z(k) = rho_g;
                 alpha_vol_z(k) = alpha_vol; xi_z(k) = xi;
             else %Two ph==0 thus flow is single phase
                 if rho>rho c
                     alpha vol z(k) = 0; xi z(k) = 0;
                 else
                      alpha_vol_z(k) = 1; xi_z(k) = 1;
                 end
             end
        end
    end
end
%Update gas cooler outer tube side i.e. water side
%Calculate new properties for outer tube
for k=1:N ac
    Recalculate properties only if the specific internal energy has
    %changed considerably i.e. changed more than 10^-7
    if (abs(uz\_gc\_o(k)-uz\_gc\_o\_latest\_upd(k))>10^-7)
        u = uz_gc_o(k);
        T = T gc o(k); %Use old value as initial guess
        %Update to new values
        uz gc o latest upd(k)=uz gc o(k);
        T_gc_o(k) = T_w_at_u_f_func(u,T); %New temperature
hz_gc_o(k) = h_f_w_func(T_gc_o(k)); %New h
cpz_gc_o(k) = cp_f_w_func(T_gc_o(k)); %New cp
cond_gc_o(k) = cond_f_w_func(T_gc_o(k)); %New conductivity
        mu gc o(k) = mu f w func(T gc o(k)); %New viscosity
    end
%Update evaporator outer tube side i.e. water side
%Calculate new properties for outer tube
for k=1:N ev
    \ensuremath{\,^{\circ}} Recalculate properties only if the specific internal energy has
    %changed considerably i.e. changed more than 10^-7
    %Calculate new properties for outer tube
```

```
u = uz ev o(k);
                     T = T \text{ ev } o(k); %Use old value as initial quess
                     uz ev o latest upd(k) = uz ev o(k);
                     T_{ev_o(k)} = T_{w_at_u} f func(u,T); %New temperature
                    hz_ev_o(k) = h_f_w_func(T_ev_o(k)); %New h

cpz_ev_o(k) = cp_f_w_func(T_ev_o(k)); %New cp

cond_ev_o(k) = cond_f_w_func(T_ev_o(k)); %New conductivity
                     mu ev o(k) = mu f w func(T ev o(k)); %New viscosity
end
%--Solve momentum equation to get new velocity field--%
%First momentum control volume
%rho w refers to the scalar control volume k and not the momentum control volume
L_PE = L_z(k)/2+L_z(k+1)/2; fe = (L_z(k+1)/2)/L_PE;
LWP = Lz(k-1)/2+Lz(k)/2; fw = (Lz(k-1)/2)/LWP;
\frac{1}{2} rho w = \frac{1}{2} rho e(k-1);
a_p_old_mom(k) = rho_p_old*A_v(k)*(L_z(k-1)/2+L_z(k)/2)/dt;
a w mom(k) = max(F w mom, 0); a e mom(k) = max(0, -F e mom);
dh cv = sqrt((dh(k-1)^2+dh(k)^2)/2);
Cf = 0.078*Re_flow^-0.25;
elseif Re flow <= le-200 %if there is no flow then there is no friction</pre>
        Cf = \overline{0};
else %flow assumed laminar
          Cf = 16/Re flow;
 \begin{array}{lll} tau_z &=& 0.5 \\ ^*Cf^*rho_p^*abs(v_z(k)) \\ ^*v_z(k); \\ S_u_mom(k) &=& (P_z(k-1) - P_z(k)) \\ ^*1000 \\ ^*A_v(k) - tau_z^*pi^*dh_cv^*(L_z(k-1) - P_z(k)) \\ ^*v_z(k) - tau_z^*pi^*dh_cv^*(k) \\ ^*v_z(k) - tau_z^*pi^*dh_cv^*
\frac{1}{2}+L_z(k)/2)+a_p_old_mom(k)*v_z_old(k);
S_p_mom(k) = 0; -0.5*Cf*rho_P*abs(v_z(k))*pi*(L_z(k-1)/2+L_z(k)/2)*dh_cv;
for k=3:N tot-1 %For interior nodes (momentum control volumes)
          L PE = L z(k)/2+L z(k+1)/2; fe = (L_z(k+1)/2)/L_PE;
          L_WP = L_z(k-1)/2+L_z(k)/2; fw = (L_z(k-1)/2)/L_WP;
          \overline{\text{rho}} w = \overline{\text{rho}}_e(k-1);
          L_WWP = L_z(k-2)/2+L_z(k-1)/2; fww = (L_z(k-2)/2)/L_WP;
          \overline{\text{rho}} ww = \overline{\text{rho}} e(k-2);
          F_w_mom = (rho_ww^*v_z(k-1)^*A_v(k-1) + rho_w^*v_z(k)^*A_v(k))/2;
          F e mom = (\text{rho w*v z}(k) * A v(k) + \text{rho e}(k) * v z(k+1) * A v(k+1)) / 2;
          a_w \mod (k) = \max (F_w \mod , 0); a_e \mod (k) = \max (0, -F_e \mod );
          dh cv = sqrt((dh(k-1)^2+dh(k)^2)/2);
          Re flow = (rho z(k-1)+rho z(k))/2*abs(v z(k))*dh cv/((mu z(k-1)+mu z(k))/2);
          if Re flow>2300 %flow assumed turbulent
                     Cf = 0.078*Re_flow^-0.25;
          elseif Re flow <= 1e-200 %if there is no flow then there is no friction
                   Cf = \overline{0};
          else %flow assumed laminar
                   Cf = 16/Re_flow;
          end
           tau z = 0.5*Cf*rho p*abs(v z(k))*v z(k);
           S = mom(k) = (P z(k-1)-P z(k))*1000*A v(k)-tau z*pi*dh cv*(L z(k
1)/2+L_z(k)/2)+a_p_old_mom(k)*v_z_old(k);
           S p mom(k) = 0; %-0.5 Cf*rho P*abs(v z(k))*pi*(L z(k-1)/2+L z(k)/2)*dh cv;
```

```
a p mom(k) = a w mom(k) + a e mom(k) + (F e mom-F w mom) -
S_p_mom(k)+a_p_old_mom(k)*rho_p/rho_p_old;
%Last momentum control volume
k=N tot;
L WP = L z(k-1)/2+L z(k)/2; fw = (L z(k-1)/2)/L WP;
\overline{\text{rho}} \text{ w} = \overline{\text{rho}}_{\text{e}}(k-1);
L \overline{WWP} = L z(k-2)/2+L z(k-1)/2; fww = (L z(k-2)/2)/L WP;
\overline{\text{rho}} ww = \overline{\text{rho}} e(k-2);
F w mom = (\text{rho ww*v } \overline{z(k-1)*A} \overline{v(k-1)+rho w*v } \overline{z(k)*A} \overline{v(k)})/2;
F e mom = (\text{rho } w*v z(k)*A v(k)+mdot comp)/2;
Re_flow = (rho_z(k-1) + rho_z(k))/2*abs(v_z(k))*dh_cv/((mu_z(k-1) + mu_z(k))/2);
if Re flow>2300 %flow assumed turbulent
          C\overline{f} = 0.078*Re flow^-0.25;
elseif Re flow <= 1e-200 %if there is no flow then there is no friction
         Cf = \overline{0};
else %flow assumed laminar
          Cf = 16/Re flow;
tau z = 0.5*Cf*rho_p*abs(v_z(k))*v_z(k);
S = mom(k) = (P z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k-1) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k) - P z(k))*1000*A v(k) - tau z*pi*dh cv*(L z(k) - P z(k))*1000*A
1)/2+L_z(k)/2)+a_p_old_mom(k)*v_z_old(k);
 S_p mom(k) = 0; \$-0.5*Cf*rho_P*abs(v_z(k))*pi*(L_z(k-1)/2+L_z(k)/2)*dh_cv; a_p_mom(k) = a_w_mom(k)+a_e_mom(k)+(F_e_mom-F_w_mom)- 
S p mom(k)+a p old mom(k)*rho p/rho p old;
%Check that the velocity used currently satisfies the momentum equation:
%Calculate momentum residuals at each velocity node
u mom residual(1:(N tot+1)) = 0;
%For velocity node \overline{1}, i.e. k=1
k=1:
u mom residual(k) = a p mom(k)*v z(k)-(a e mom(k)*v z(k+1)+S u mom(k));
u_norm_factor(k) = a_p_mom(k)*v_z(k);
for k=2:(N \text{ tot}) %For interior control volumes
         u_{mom} residual(k) = a_p_{mom}(k) * v_z(k) - (a_w_{mom}(k) * v_z(k
1) +a e mom(k) *v z(k+1) +S u mom(k));
          \overline{u} norm factor(k) = \overline{a} p mom(k)*v z(k);
%For the last control volume
k=(N tot+1);
u_{mom\_residual(k)} = a_{p\_mom(k)} v_{z(k)} - (a_{w\_mom(k)} v_{z(k-1)} + S_{u\_mom(k)});
u norm factor(k) = a p mom(k)*v z(k);
%Calculate sum of absolute momentum residuals
sum_u_mom_residuals = sum(abs(u_mom_residual(:)));
sum_u_norm_factor = sum(abs(u_norm_factor(:)));
{
m \$This} gives an indication of how well the momentum equation is satisfied
norm_Global_mom_Residual = sum_u_mom_residuals/sum_u_norm_factor
                                 _____
%Store velocity variable for use later in under-relaxation of velocity
          v z interim = v z;
%TDMA solver to calculate new velocities
         alpha = a e(k); beta = a w(k); Dj = a p(k);
%Boundary conditions have velocities
Aj_mom(k) = 0;
Cj_aks_mom(k) = v_in;
for k=2:N tot %Interior control volumes
end
k=N tot+1; %Last control volume
```

#### APPENDIX D: COMPRESSOR PRODUCT DATA

The Embraco EK6210CD compressor is selected for this project. Product data below shows that the rated cooling load at -10 °C is 700 W.



#### Product Data - R-744 (M/HBP)

Compressor	Voltage / Frequency	Displacement		Cooling Capacity
		66	ou in	w
EK6160CD	100V 50•60Hz 1	1.00	0.06	380*
EK6175CD	100V 50•60Hz 1~-	1.30	0.08	500*
EK6210CD	220 <b>⊾</b> 240V 50Hz 1~	1.75	0.11	700
EK6210CD	115V 60Hz 1~	1.75	0.11	805
EK6210CD	220V 60Hz 1~	1.75	0.11	805
EK6214CD	220-240V 50Hz 1~	2.45	0.15	905

<sup>\*</sup> at 50Hz

### **Testing Conditions**

	Evaporating	Discharge	Return Gas	Ambient	Approach
	Temperature	Pressure	Temperature	Temperature	Temperature
	°C (°F)	bar	°C (°F)	°C (°F)	'C ('F)
MBP	-10.0 (14.0)	85.0	32.0 (89.6)	32.0 (89.6)	32.0 (89.6)

Figure D1: EK6210CD product data

# APPENDIX E: STEADY-STATE CAPILLARY TUBE SIMULATION MODEL

```
%Capillary Tube.m is a script file containing a steady-state model for the
%capillary tube. It is used to determine the steady-state mass flow rate for a
%particular capilaary tube design and operating conditions.
%-----% Expansion device modelling (State 3-4) ------%
% Expansion device is a capillary tube
1 ct = 3.5; %Length of capillary tube [m]
d ct = 0.00079; %Diameter of capillary tube [m]
mdot cap = 1*10^-16; %Initialise mass flow rate through capillary tube [kg/s]
*Define lower bound for mass flow rate
xj(1) = mdot cap; %Mass flow rate through capillary tube [kg/s]
Pct in = 8500; %Pressure at inlet of capillary tube [kPa]
Tct in = 32+273.15; %Inlet temperature of capillary tube [K]
Pct out= 2648.677254832481; %Pressure at outlet of capillary tube (Psat ev) [kPa]
P=Pct in; T=Tct in; CO2 1Ph Prop at P and T;
h ct = h; %Assume stays constant for the capillary tube
%Determine pressure at which flow becomes two-phase (i.e. crosses the saturation
line)
hsat = h ct;
if (hsat<h fi(length(h fi))), P sat cross = interp1(h fi,Pi,hsat);</pre>
 elseif (hsat>h_gi_1(length(h_gi_1))), P_sat_cross = interp1(h_gi_1,Pi 1,hsat);
%Can calculate the actual crossing if interpolation is not good enough
%CO2 Sat Prop at hsat
%P sat cross = P;
Ac ct = pi/4*d ct^2; %Area of capillary tube [m]
%--Determine regions of single and two-phase flow in the capillary tube. --%
if (Pct in>=P sat cross) && (Pct out>=P sat cross) % Flow is single phase only
    Scenario = 1;
    N ct 1ph = 200; %Number of control volumes for the single phase flow
                     %in the capillary tube.
    dP ct k 1ph = (Pct in-Pct out) / (N ct 1ph);
elseif (Pct_in>=P_sat_cross) && (Pct_out<P_sat_cross)</pre>
    %Flow is single phase at the start and changes to two phase flow downstream
    Scenario = 2;
    N \text{ ct 1ph} = 200;
                     %Number of control volumes for the single phase flow
                     %in the capillary tube.
    dP_ct_k_lph = (Pct_in-P_sat_cross) / (N_ct_lph);
    N ct 2ph = 500; %Number of control volumes for the two phase flow
                     %in the capillary tube.
   dP_ct_k_2ph = (P_sat_cross-Pct_out) / (N_ct_2ph);
else %Flow is two-phase only
    Scenario = 3;
    N \text{ ct } 2ph = 500;
                    %Number of control volumes for the two phase flow
                     %in the capillary tube.
   dP ct k 2ph = (Pct_in-Pct_out) / (N_ct_2ph);
end %end if
%Calculate properties of the flow
if (Scenario == 1) | | (Scenario == 2)
for k=1:N_ct_1ph
    if k==1
       Pct(k)=Pct in-dP ct k 1ph/2;
    else
       Pct(k) = Pct(k-1) - dP ct k 1ph;
    end
if k==1 %Inlet conditions of 1st control volume
   P = Pct(k)+dP_ct_k_1ph/2; h=h_ct; CO2_1Ph_Prop_at_P_and_h;
   rho_in_1ph(k) = rho;
else %Inlet conditions of k'th control volume
    rho in 1ph(k) = rho out <math>1ph(k-1);
```

```
end
```

```
%Determine rho and viscosity of the k'th control volume
P = Pct(k); h = h ct; CO2 1Ph Prop at P and h;
rho 1ph(k)=rho;
Viscosity CO2 %Determine the viscosity at T and rho
visc 1ph(\bar{k}) = visc;
%Outlet conditions of k'th control volume
rho out 1ph(k) = 2*rho 1ph(k)-rho in 1ph(k); %Approximation to save computation
                                               %time
end %end for loop
end %end if
if (Scenario == 2) | | (Scenario==3)
for k=1:N ct_2ph
    if k==1
        if Scenario==2, Pct(k)=P_sat_cross-dP_ct_k_2ph/2;
         else Pct(k)=Pct in-dP ct k 2ph/2;
        end
    else
        Pct(k) = Pct(k-1) - dP ct k 2ph;
    end
if k==1
        %Inlet conditions of 1st control volume
    P = Pct(k)+dP_ct_k_2ph/2; h = h_ct; CO2_2Ph_Prop_at_P_and_h;
    rho in 2ph(k) = rho;
     %Inlet conditions of k'th control volume
   rho_in_2ph(k) = rho_out_2ph(k-1);
end
%Determine rho and viscosity of the k'th control volume
P = Pct(k); h = h ct; CO2 2Ph Prop at P and h;
rho 2ph(k) = rho; %Homogenous density
rho f 2ph(k) = rho f;
Determine gas viscosity
rho = rho g; Viscosity CO2; visc g = visc;
%Determine fluid viscosity
rho = rho f; Viscosity CO2; visc f = visc;
%Determine the homogenous mixture's viscosity
visc_2ph(k) = 1/(xi/visc_g+(1-xi)/visc_f);
visc_f_2ph(k) = visc_f;
                         %Fluid viscosity
%Outlet conditions of k'th control volume
rho out 2ph(k) = 2*rho 2ph(k)-rho in 2ph(k); %Approximation to save computation
end %end for loop
end %end if
%Initialise length parameter for itteration
Length = 1 ct*2;
%Define upper bound for mass flow rate
mdot cap = 0.2; %Mass flow rate through capillary tube [kg/s]
xj(2) = mdot cap;
while (abs(Length-l ct)>10^-6) && (p<1000)
p=p+1;
for j=1:3
    if j=3, xj(3)=(xj(1)+xj(2))/2; end %Define mid value for mass flow rate
   mdot cap = xj(j);
*Calculate pressure drop length of the single phase flow region
if (Scenario == 1) | (Scenario == 2)
for k=1:N ct 1ph
Re_ct = mdot_cap*d_ct/(visc_1ph(k)*Ac_ct);
    if Re ct>2300
       C\overline{f} = 0.078*Re_ct^-0.25;
        Cf = 16/Re ct;
    end
L_1ph(k) = (dP_ct_k_1ph*1000 - (mdot_cap/Ac_ct)^2*(1/rho out 1ph(k) - ...)
            1/rho_in_1ph(k)) * (0.5*rho_1ph(k)*d_ct/(Cf*(mdot_cap/Ac_ct)^2));
end %end for-loop
```

```
end %end if
%Calculate pressure drop length of the two-phase flow region
if (Scenario == 2) | | (Scenario == 3)
for k=1:N_ct_2ph
%Determine Reynolds number based on liquid only (lo)
Re_ct_lo = mdot_cap*d_ct/(visc_f_2ph(k)*Ac_ct);
    if Re_ct_lo>2300, Cf_lo = 0.078*Re_ct_lo^-0.25;
      else \overline{Cf} lo = 16/Re \overline{Cf} ct lo;
    end
%Determine Reynolds number of homogenous flow
Re_ct_h = mdot_cap*d_ct/(visc_2ph(k)*Ac_ct);
    if Re_ct_h>2300, Cf_h = 0.078*Re_ct_h^-0.25;
      else Cf_h = 16/Re_ct_h;
%Determine two-phase flow friction multiplier
Phi_2ph_fr = (Cf_h/Cf_lo) * (rho_f_2ph(k)/rho_2ph(k));
L 2ph(k)=(dP ct k 2ph*1000-(mdot cap/Ac ct)^2*(1/rho out 2ph(k)-...
             1/rho in 2ph(k)))*(0.5*rho 2ph(k)*d ct/...
              (Cf lo*Phi 2ph fr*(mdot cap/Ac ct)^2));
     %end for-loop
end
end %end if
end %end for j=1:3 for-loop
%Initialise variable
Negative = 0;
%Calculate pressure drop length of the different scenario's
if Scenario==1, Length = sum(L_1ph);
    for k=1:N ct 1ph
        if L \overline{1}ph(k)<0, Negative = 1; end
    end
elseif Scenario==2, Length = sum(L_1ph)+sum(L_2ph);
    for k=1:N ct 1ph
        if L \overline{lph(k)} < 0, Negative = 1; end
    end
    for k=1:N ct 2ph
        if L_{2ph}(k) < 0, Negative = 1; end
    end
elseif Scenario==3, Length = sum(L 2ph);
    for k=1:N ct 2ph
        if L_2ph(k)<0, Negative = 1; end</pre>
    end
end
%Perform interval halving
if Negative==1, xj(2) = xj(3); %Decrease mass flow rate
      if Length<=l ct, xj(2) = xj(3); %Decrease mass flow rate
       else xj(1) = xj(3); %Increase mass flow rate
      end
end
end
mdot cap = (xj(1)+xj(2))/2 %Output mass flow rate [kg/s]
```

### APPENDIX F: THERMOCOUPLE CALIBRATION

The table below shows the calibration equations for the 20 T-type thermocouples used in the experimental setup of the refrigeration system built.  $T_t$  is the true temperature (or adjusted temperature) and  $T_m$  is the measured temperature.

Table F1: Thermocouple calibration equations

Thermocouple	Calibration equation	Correlation
number	T (°C)	coefficient (R <sup>2</sup> )
1	$T_t = 0.99942370T_m - 0.49370601$	0.99999841
2	$T_t = 0.99662053T_m - 0.46347229$	0.9999932
3	$T_t = 0.99612638T_m - 0.39243544$	0.9999925
4	$T_t = 0.99573481T_m - 0.44906098$	0.99999972
5	$T_t = 1.00381498T_m - 0.81235311$	0.99999691
6	$T_t = 1.01093105T_m - 1.23826485$	0.99999027
7	$T_t = 1.01932787T_m - 1.25745816$	0.99999359
8	$T_t = 1.00898747T_m - 0.97542669$	0.99999086
9	$T_t = 1.01625036T_m - 0.91917934$	0.99999372
10	$T_t = 1.00678267T_m - 0.41303334$	0.99999861
11	$T_t = 1.01231436T_m - 0.52143400$	0.99999795
12	$T_t = 1.00453218T_m - 0.40867565$	0.99999929
13	$T_t = 1.00426377T_m - 0.30859600$	0.99999927
14	$T_t = 1.00563168T_m - 0.24162925$	0.9999913
15	$T_t = 1.01621751T_m - 0.69554083$	0.99999573
16	$T_t = 1.01554791T_m - 0.49523630$	0.99999312
17	$T_t = 1.02193689T_m - 0.57046826$	0.99999183
18	$T_t = 1.00888846T_m + 0.25065085$	0.99999110
19	$T_t = 1.01736623T_m + 0.12794252$	0.99999170
20	$T_t = 1.00356127T_m + 0.55267316$	0.99999817

#### APPENDIX G: EXPERIMENTAL APPARATUS

The following section contains details of the experimental apparatus used in this project.

#### G1: Embraco EK6210CD Compressor

The Embraco EK6210CD compressor is a small compressor working with CO<sub>2</sub> as refrigerant. It is ideal for the development of a small household refrigerator.



Figure G1: Embraco EK6210CD Compressor

The compressor specifications as listed in the Embraco EK6210CD compressor application manual (Embraco, [S.a.]) are:

Rated voltage and frequency: 220-240 V/50 Hz

Number of phases: 1 PH

Locked rotor amperage (LRA); 13.4 A Refrigerant: R744 (Carbon dioxide) Displacement volume: 1.75 cm<sup>3</sup>

#### **G2:** Pressure Gauges

The pressure gauges used to measure the low - and high side pressure of the refrigeration system during operation are B model pressure gauges manufactured by Swagelok. B model pressure gauges are general-purpose stainless steel gauges with safety glass lenses.



Figure G2: Swagelok pressure gauges

The pressure gauge specifications as listed in the product data sheet are:

LP pressure gauge model designator: PGI-63B-BG100-LAQX HP pressure gauge model designator: PGI-63B-BG250-LAQX

HP pressure gauge range: 0 to 250 bar LP pressure gauge range: 0 to 100 bar

Type: Positive-pressure gauge

Dial size: 63 mm

Model: B

End Connection: 1/4" Accuracy: ± 1.5 % of span

Weather protection: Weather-tight (NEMA 4X/IP65)
Ambient operating temperature (unfilled): -40 to 60 °C
Media operating temperature (unfilled): 200 °C maximum

Temperature error: ± 0.4 % for every 10 °C temperature change from 20 °C

### G3: B.I.C.I.SA-5500 Water Pump

The B.I.C.I.SA-5500 is a submersible water pump used for aquarium water circulation.



Figure G3: B.I.C.I.SA-5500 water pump

The pump specifications as listed on the pump product data sheet are:

Rated voltage and frequency: 220-240 V/50 Hz

Power: 200 W

Maximum pumping head height: 5.5 m Maximum volume flow rate: 6800 L/h Maximum water temperature: 35 °C

#### G4: Hailea HS-28A Water Chiller

The Hailea HS-28A is a small aquarium water chiller using a standard refrigeration cycle and temperature control unit to cool the water to the required temperature.



Figure G4: Hailea HS-28A water chiller

The water chiller specifications are as listed in the product data sheet:

Model: HS-28A

Rated voltage and frequency: 220-240 V/50 Hz

Working current: 1.1 A

Power: 1/10 HP Refrigerant: R134a

Refrigerant weight: 160-180 g Rate of water flow: 250-1200 L/h

Weight: 13 kg

Size: 400x218x415 mm

### G5: Agilent 34970A Data Acquisition/Data Logger Switch Unit

The Agilent 34970A Data Acquisition/Data Logger Switch Unit is now manufactured by Keysight Technologies. It contains a built-in 6 1/2 digit digital multimeter capable of measuring 250 channels per second. It has a 3-slot mainframe, thus allowing 60 2-wire measurements (20 per slot). On-module screw-terminal connections are used to connect the various measuring probes.



Figure G5: Agilent 34970A Data Acquisition/Switch Unit

The Agilent 34970A Data Acquisition/Data Logger Switch Unit specifications as obtained from Keysight Technologies (2015) are:

3-slot mainframe with built-in GPIB and RS232 interfaces
6 1/2-digit (22-bit) internal DMM, with scanning up to 250 channels per second
8 switch and control plug-in modules to choose from
Built-in signal conditioning measures thermocouples, thermistors and RTDs,
ac/dc volts and current, frequency and period, resistance
50k readings of non-volatile memory holds data when power is removed
Hi/Lo alarm limits on each channel, plus 4 TTL alarm outputs
Free Benchlink data logger software to create tests without programming

A 34901A plug-in module was used with the data logger. This module provides 20 two-wire channels and has a built-in thermocouple reference.

#### **G6:** Efergy Energy Monitoring Socket

The efergy energy monitoring socket measures the energy efficiency of any appliance plugged into it. It is used in this project to measure the compressor power consumption.



Figure G6: Efergy energy monitoring socket

The specifications of the efergy energy monitoring socket as given by the product data sheet are:

Model name: Energy Monitoring Socket

Model number: EMS-RSA Operating voltage: 230 V Operating current: 16A max. Working voltage: 170 V-276 V

Accuracy: ±2%

Measuring Features: Watt(W), Kilowatt Hours (kWh), Voltage (V), Current (A),

Frequency (Hz), Power Factor (%), Max. Watts (W)

Also: Measures time on, and cost if electricity tariff is programmed into it.

Display range: Time (0s-9999 days), Power (0 W-9999 W), Energy (0-

9999 kWh),

Voltage (0-9999 V), Current (0.000-16.00 A), Frequency (0.000-9999 Hz), Price (00.00-99.99 R)