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Master of Research, School of Computing Science and Digital Media

SIMULATION AND OPTIMISATION OF THE SEPARATION PROCESS IN OFFSHORE OIL AND GAS PLATFORMS

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Simulation and Optimisation of the Separation Process in Offshore Oil and Gas Platforms

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Abstract

Hydrocarbon separation in offshore oil and gas platforms is the process that transforms extracted crude oil into transportable oil and gas. Temperatures and pressures of the separation system can be adjusted to modify the separation of the hydrocarbons. Discovery of the optimal settings of the separation system requires the use of simulation and optimisation techniques which are able to identify high quality solutions from a large and complex decision space. The main focus of this research is to find such approach for simulation and optimisation in offshore oil platforms and suggest directions for future research.

In the first part of this thesis, we provide a novel approach for simulation of separation systems based on the flash algorithm. The flash algorithm is an integral part of many reservoir and chemical simulations. The development of a simple, accurate and efficient such algorithm is highly desirable in the oil and gas industry. However, solution of such calculation using the Peng-Robinson equation of state is a complex problem due to the iterative nature of the algorithm and various uncertainties. Our analysis shows that the sources of these uncertainties are poor estimation of initial K-factors, incorrect and/or slow solution of the cubic equation of state and the use of invalid compressibility factors in the approach to the solution. This work presents an improved flash algorithm for real multicomponent hydrocarbon mixtures that can include pure and pseudo components. All computational steps required in order to avoid the various uncertainties are described. Algorithm accuracy was tested and validated by comparing the vapour-feed ratios of different real world hydrocarbon mixtures calculated using both the proposed algorithm and the AspenTech HYSYS tool.

In the second part of the thesis, we formulate an optimisation problem which aims at maximising the profitability of the system by tuning temperatures and pressures in the separation system. The profit is affected by the quality of the separation (market value of hydrocarbons recovered in oil and gas) and the operating costs of the separation process. Our formulation takes into account all the physical constraints of such a system in order to make it as realistic as possible. Finally, we apply differential evolution to three real-world problem instances. We see that optimising the settings of the separation process in an offshore oil and gas platform can save between 10,000 and 100,000 USD per day for the operators.

Keywords: Offshore Oil Platform, Peng-Robinson Equation of State, Flash Calculation, Separation System, Simulation, Optimisation, Differential Evolution

Acknowledgements

I would like to express my sincere gratitude to my supervisors Professor John McCall and Dr. Benjamin Lacroix for the support, patience and guidance during to my Master of Research study and our Knowledge Transfer Partnership (KTP) project with Accord-ESL. Their motivation, immense knowledge, and feedbacks helped me to solve the complex problems which I have met during the research. They helped and supported me in all the time of my research and even during to writing of this thesis while I was far away from Aberdeen. Without their assistance and dedicated support I would not be able to achieve what I have achieved.

My sincere thanks also goes to Phil Stockton, James Arthur, Amy Ross, Clive Ashworth and all other people from Accord Energy Solutions Limited, who provided me an opportunity to join their team as a KTP associate, and who supported me during the KTP project and my research. I thank them for assistance with all my questions about the oil and gas industry. Without they precious support and motivation it would not be possible to conduct the KTP project and this research.

Last but not the least, I would like to thank my mother and father for supporting me spiritually throughout writing this thesis.

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Glossary

Acentric Factor is a measure of the non-sphericity (centricity) of molecules.

K-Factor of a given component is the ratio of the mole fraction of the component in the vapour phase to the mole fraction in the liquid phase.

Bubble point is the pressure and temperature conditions at which the first bubble of gas comes out of solution in oil.

Cloned Component is an allocation method that offers a mechanism to allocate at a component level directly in a simulation.

Crude Oil is a naturally occurring, unrefined petroleum product composed of hydrocarbon components and other organic materials.

Compressor is an equipment used on a offshore oil platform for raising of stream's pressure.

Cooler is an equipment used on a offshore oil platform for dropping of stream's temperature.

Dew point is the temperature and pressure conditions at which the hydrocarbon components of a mixture, such as natural gas, will start to condense out of the gaseous phase.

Flash Algorithm is an algorithm which allows to determine the amounts (in moles or mass) of liquid and vapour hydrocarbons within a reservoir or separator/scrubber at a given pressure and temperature.

Gas export pressure is the pressure of the last scrubber which is required to be achieved in order to meet the gas export conditions.

Hydrocarbon Allocation is the process which determines the quantity of oil and gas products belonging to each operator/company when inputs from different wells are processed together in a commingled system (for example on an offshore oil platform or transportation system).

Hydrocarbon component is an organic compound (such as methane, ethane) made of two elements carbon and hydrogen. Hydrocarbon component can be found in crude oil.

Heater is an equipment used on a offshore oil platform for raising of stream's temperature.

Heavy Hydrocarbon Components are components with significant amount of carbons (more than 6 carbons).

Intermediate Hydrocarbon Components are components such as propane, butane, pentane, hexane with carbons between 2 and 6 but with high amount of hydrogen.

Light Hydrocarbon Components are components such as methane (C1), ethane (C2), propane (C3) and the butanes (C4) which has low amounts of carbon.

Mixture is an equipment used to combine a set of inlet streams into one outlet stream.

Tee is an equipment used to split inlet stream into a few outlet streams.

Oil Well is a boring in the Earth that is drilled to bring hydrocarbons to the surface.

Pseudo-components is a group of various components which are aggregated in one hydrocarbon component. Created pseudo-component has calculated by chemical engineers properties which represent all components include inside.

Critical Pressure of Hydrocarbon Component is the pressure required to liquefy a gas at its critical temperature.

Scrubber is a two-phase separator that is designed to recover liquids from the vapour streams of separators. Liquid quantity in a scrubber is much lower than that in a separator.

Separator is a vessel where under given temperature and pressure a input well stream is separate into gaseous and liquid components.

Critical Temperature of Hydrocarbon Component is the temperature at and above which vapor of the substance cannot be liquefied, no matter how much pressure is applied.

True vapor pressure is a common measure of the volatility of petroleum distillate fuels. It is defined as the equilibrium partial pressure exerted by a volatile organic liquid as a function of temperature as determined by the test method ASTM D 2879.

Valve is an equipment used on a offshore oil platform for dropping of stream's pressure.

Chapter 1

Introduction

1.1 Research Motivation

Over the last two decades, the oil and gas industry has made large financial investments in the offshore oil sector. As a consequence of this, offshore oil and gas production has increased greatly. According to the U.S. Energy Information Administration (EIA) global offshore oil production in 2015 accounted for nearly 30% of total global oil production. Compared with traditional onshore projects, offshore oil projects are more complex and require use of advanced technologies, equipment and materials. As a result of use of advance technologies and engineering, along with the increasing complexity of production operations in offshore oil and gas systems there is a growing incidence of highly complex decision problems. These include: resource-intensive operations management; planning, scheduling and monitoring of complex chemical and industrial processes [1].

An offshore oil platform plays one of the most important roles in the oil industry. The offshore platform is a large structure with facilities to drill new wells into underground reservoirs, to extract and produce transportable oil and gas production and optionally to store extracted production. There are many different classifications and types of offshore oil platforms but all platforms use a separation system where separation of hydrocarbons occurs. Many factors have influence upon the separation process such as changing of oil and gas flow rates from wells or surging and slugging tendencies of wells. Therefore, the separation system needs to be optimised periodically with the aim to improve separation process and optimise production goals. Furthermore, the optimisation of separation systems is a complex decision problem with a large search space where it is important to capture the relationships among the many variables and constraints.

Streams of crude oil are complex mixtures of different compounds of hydrogen and carbon, all with different physical properties. The main purpose of the separation system is to separate crude oil from well streams into two phases (liquid and gas), and process these phases into storable and transportable marketable products. The physical separation of these phases is one of the basic operations and it is based on series of devices called separators. The separator is a vessel where under given temperature and pressure a input stream is separated into gaseous and liquid phase. Therefore, optimisation of the separation system can be done by decision-makers changing the temperatures and pressures of separators. Moreover, tuning temperatures and pressures of separators will change the quantity and quality of extracted oil and gas.

The main focus of this research is to find approaches which will help to decision-makers to explore key scenarios and their consequences for the optimisation of offshore oil separator systems. Nowadays, two major approaches are now increasing in use: simulation and optimisation. Simulation allows decision-makers to explore potential consequences of different scenarios for a range of decisions [2]. Computational optimisation is used to automate the effort of identifying high quality solutions from a large and complex decision space [3]. Together, simulation and optimisation are often combined to present key scenarios and their consequences. In this way, more time is spent on considering high level aims and objectives than on computation and constraint checking, leading to higher quality decision-making.

Approaches to simulation vary according to the system to be modelled but include Discrete Event Simulation, Dynamic Simulation, Monte-Carlo Simulation and a variety of specialised mathematical or logical models embedded in software [4]. Typically a simulation allows the input of instance variables and decision variables. The instance variables define a particular decision scenario to be explored and the decision variables represent the decision to be simulated. Outputs from the simulation are such that they can be formulated into expressions representing key decision objectives, cost efficiency etc. Decision variables may be explored manually by a decision-maker but more frequently computational optimisation techniques are used to automatically explore the decision space to arrive at sets of decision parameters that optimise the objective values output by the simulation. For complex scenarios with heavy constraints and large search spaces, heuristic and metaheuristic techniques are often employed. Examples include genetic and memetic algorithms, particle swarm optimisation, evolution strategies, differential evolution and model-based search [5].

The selection of suitable simulation and optimisation techniques is itself a complex problem. The suitability of those techniques may be affected by the different requirements imposed by the problem such as time and computational limitations or simply their ability to reach satisfactory solutions. It thus requires a clear understanding of the problem and its environment, along with an advanced expertise in the available techniques. The selection of suitable simulation and optimisation techniques for offshore oil platforms is typically complicated. Many factors affect suitability including simulation speed vs available computational power, the effectiveness and efficiency of the optimisation technique vs any existing decision-making approach, the compatibility of the search with decision-support needs and finally confidence of the decision-makers in the validity of each approach (most frequently, the move to simulation and optimisation for decision support requires a considerable change in management processes and culture which can be challenging to achieve successfully).

The main motivation of this research is to find stable and efficient approach for simulation and optimisation of the separation process on offshore oil platforms without additional costs for replacement, adding or removing of any type of equipment. Furthermore, having integration between simulation and optimisation techniques, they can be used by offshore operators as a decision support tool. Furthermore, such a decision support tool will help not only to optimize offshore separation process by increasing the profits but also will help to meet production goals. Likewise, as part of the motivation, the development of a software tool for simulation of separation systems and hydrocarbon allocation was supported by Accord-ESL and Innovate UK under Grant KTP 509146.

1.2 Aims and Objectives

This research has three main aims. The first aim of the project is to develop an novel approach and simulation tool for separation processes of any configuration with the aim to explore range of solutions generated by applied metaheuristics. The secondary aim of the thesis is to analyze the application of state-of-the-art metaheuristics with the aim to identify high quality solutions from a complex decision space which solutions optimise separation processes. The third, and final, aim of the thesis is to test the proposed simulation and optimisation for real world offshore platforms. The aims will be achieved by focusing on the following objectives:

- Investigate a flash algorithm for modelling of separators/scrubbers.
- Develop a novel approach for simulation of separation systems based on flash algorithm.
- Through a literature survey find those decision variables that have the most influence on the optimisation of separation processes.
- Use knowledge gained from the literature survey for mathematical formulation of the optimisation problem and identification of decision variables constraints.
- Apply metaheuristics for optimisation of separation processes.

1.3 Main Contributions of the Thesis

The following contributions have been made and described in this thesis:

- The first contribution of this thesis is the proposed novel approach for simulation of separation processes based on a flash algorithm. The main advantages of the proposed approach are possibility to simulate any configuration of separators/scrubbers and stable and fast chemical calculations which are easy for programming and integration. Moreover, the flash algorithm, which is the key of success simulation and used for modelling of the separator/scrubber, is analysed and found instabilities are resolved during to the research. In addition, the proposed flash algorithm has been released as commercial software, CHARM [1], by Accord-ESL.
- The second contribution of this thesis is the mathematical formulation of the optimisation of offshore oil platforms where the fitness function indicates the quality of provided solution in USD. Here, the fitness function includes two objectives, profit maximisation and utility cost minimisation, which are formulated as a single objective optimisation problem. As a novel contribution of this research, the most valuable decision variables and their limitation are found and described. In addition, formulas for calculations of utility cost in USD for each type of the equipment (cooler, heater and compressor) on the offshore platform are formulated and provided.
- The third main contribution of this thesis are obtained results of applied differential evaluation (DE) and adaptive evaluation algorithms (JADE) which show that integration of the proposed simulation approach with optimisation algorithms allows to increase the profit of offshore oil platform. Furthermore, our results show that depending on the production, the optimised settings increases the profits from 10,000USD to 100,000USD per day.

1.4 Thesis Overview

Chapter 2 provides background information about the offshore oil and gas platforms in specific relation to this research. Also, this chapter briefly describes a traditional approach for simulation of separation systems. Chapter 3 presents novel approach for the simulation of oil and gas separation processes based on a flash algorithm. The flash algorithm is detailed and its validation is provided. The first part of Chapter 4 provides a literature review of

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[1] Compact Hydrocarbon Allocation Reference Model (CHARM), web-site: https://charm.accord-esl.com/

the optimisation of separation system and population-based algorithms which are used for search of optimial separation values. The second part of Chapter 4 gives a formulation of the optimisation problem and experimental evaluation of the proposed optimisation ideas. Finally, the conclusions in Chapter 5 summarize the contributions of the research and suggest possible extensions and directions of future research.

1.5 Thesis Outcomes

The following participations and events are a result of the research conducted in this thesis:

- Stoyan Veleshki, Simulation Software for Hydrocarbon Allocation, KTP Associates Conference 2015, Glasgow, May 2015.
- Stoyan Veleshki, Dr. Benjamin Lacroix, Prof. John McCall and Phil Stockton, Multi-Objectivization for Hydrocarbon Allocation, Design & Technology Symposium 2015, RGU, Aberdeen, May 2015.
- Stoyan Veleshki, Optimisation of separator systems, Seminar at Smart Data Technologies Centre, RGU, Aberdeen, April, 2016
- Stoyan Veleshki, CHARM Simulation Software for Hydrocarbon Allocation, KTP Associate Seminar, Aberdeen, 23 May 2016
- The release event of the CHARM product[2] on 21 June 2016, RGU. During the event was presented the idea of simulation of separation systems based on the flash algorithm and optimisation of offshore oil platform by differential evaluation algorithms. Many engineers from oil companies including BP, Shell attended and the product was well received with follow up enquiries.

The following journal papers are in preparation and planning to be submitted:

- Stoyan Veleshki, Benjamin Lacroix, John McCall, Phil Stockton and Clive Ashworth. "**A robust and efficient flash algorithm for real multicomponent mixtures**". It is planned to be submitted to journal the Computers and Chemical Engineering.

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[2] Compact Hydrocarbon Allocation Reference Model (CHARM) is a simulation software package which models how hydrocarbons behave specifically for hydrocarbon allocation purposes. The development of this tools supported by Accord ESL and Innovate UK under Grant KTP 509146 , web-site: https://charm.accord-esl.com/

- Benjamin Lacroix, Stoyan Veleshki, John McCall, Phil Stockton. "**Optimisation of Separation Process in Offshore Oil and Gas Platforms Using Differential Evolution**".

Chapter 2

Background of Offshore Oil and Gas Platforms

This chapter introduces the background details about the offshore oil and gas platforms related to this research. The definitions of an offshore separation system, used equipment for oil separation and hydrocarbon allocation are given. A brief review of pros and cons of traditional software tools, such as Aspen HYSYS, used for modelling of separation system is provided.

2.1 Definition of Oil Offshore Separation System

Crude oil and gas may be found in hot, high-pressure offshore reservoirs. Based on hydrocarbon compositions, reservoir pressure and temperature, and other physical characteristics some processing is required to be done to extract and enable their safe transfer to onshore, pipeline systems or storage areas. This process is carried out by the offshore oil and gas platform which has a separation system. Example of offshore separation system is presented on Fig. 2.1. This separation system has different type of equipment such as separators, scrubbers, compressors, heaters, coolers, valves and pumps. The main purpose of separation systems is to separate the well stream of crude oil into three components, typically called "phases" (oil, gas, and water), and process these phases into some marketable products(s) or dispose of them in an environmentally acceptable manner [6]. According to Abdel-Aal and Aggour [7], the main target of separation systems is to achieve the following objectives:

- Separate the Ethane (C1) and Methane (C2) from oil. Heavier hydrocarbons tend to condense, forming two-phase flow.
- Maximize the recovery of heavy components of the intermediate hydrocarbons.

- Save the heavy group components in liquid product.

The physical separation of the crude oil is one of the basic and most important operations in the production, processing, and treatment of oil and gas production. Quantities of export oil and gas productions and meeting of environment regulations depend on the equipment used and its settings (temperatures and pressures). After the construction of the offshore oil platform any physical change into the separation system can be very expensive or even impossible due to the offshore platform construction limitation. However, there is a possibility of adjusting the separation system based on changes of temperatures and/or pressures which have influence over the physical separation.

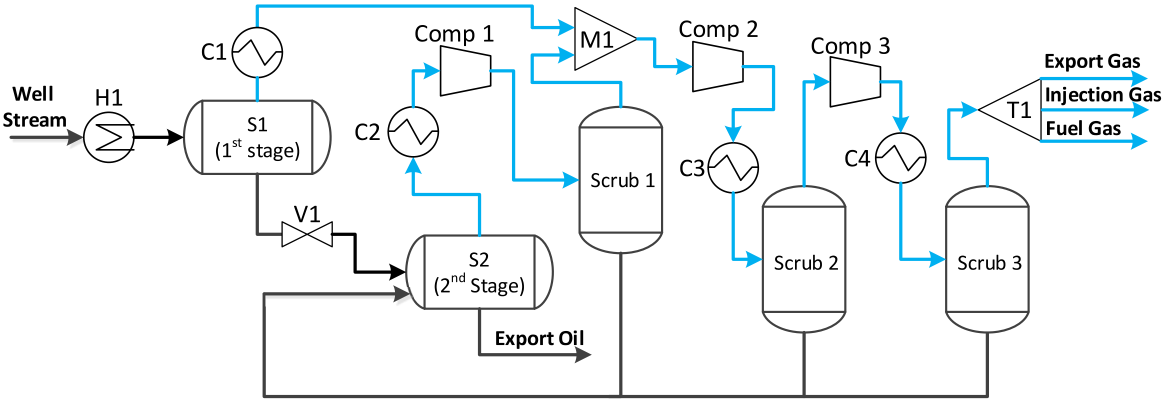


Fig. 2.1 Diagram of offshore oil separation system

The main devices which are used through the whole separation process are the following (see Fig. 2.1):

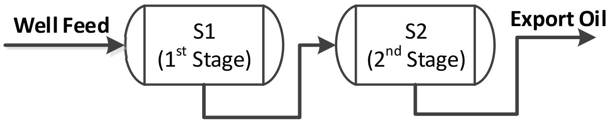
- Separator/Scrubber – a vessel used for separating a well stream into gaseous and liquid components. The separation process is carried out due to the pressure and temperature of the vessel (S1, S2, Scrub 1, Scrub 2, Scrub 3).
- Cooler – drops the temperature of the stream (C1, C2, C3, C4).
- Heater – increase the temperature of the stream (H1).
- Valve – drop the pressure of the stream (V1).
- Compressor – increase the pressure of the stream (Comp 1, Comp 2, Comp 3).
- Mixture – combine a set of inlet streams into one outlet stream (M1).
- Tee – split a inlet stream into a few outlet streams (T1).

The separator is a vessel used to separate liquid (heavy) and gas (light) components from a crude oil. Separators are classified as “two-phase” if they separate gas from the total liquid stream and “three-phase” if they also separate the liquid stream into its crude oil and water components. Typically, a chain of connected separators is used for removal of light components (Ethane, Methane, Propane) and saving of heavy components (i-Butane, n-Butane, and other C7+) into the export oil. This separator chain allows the production of stable export oil meeting sales criteria [8]. Scrubbers are two-phase separators which are especially designed to be used when the ratio of gas rate to liquid rate is very high. They recover liquids carried over from the gas outlets of separators or to catch liquids condensed due to cooling or pressure drops. Liquid loading in a scrubber is much lower than that in a separator [8]. Typically, the vapour stream from the separator is connected to the scrubber via compressor or cooler. Other devices such as cooler, heater, valve, compressor, etc. have simple functions such as to increase or drop the temperature/pressure. Moreover, these devices do not perform separation. The separation process is possible only inside separators or scrubbers. Therefore, those simpler devices can be ignored when modelling the separator system. At the same time, modelling of the separation process into the separator/scrubber is very complex due to the nature of this process. There are many factors which affect the separation such as physical properties of hydrocarbon components, crude flow rate, presence of impurities, and foaming tendencies of the oil.

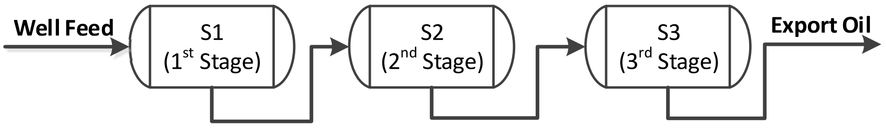
2.2 Stage of separation

The objectives of the separation process are achieved by a chain of separators and chain of scrubbers. The stage of separation is based on a number of separators arranged in series. The well stream of crude oil is passed through these separators in order to achieve export and environment requirements. The first separator is called first-stage separator, the second separator is called second-stage separator and additional separators are named according to their position in the series. The pressures of separators decrease from the first to the final separator. The highest pressure is found at the first separator and the lowest pressure at the final separator. The objective of stage separation is to maximize the hydrocarbon liquid recovery and to provide maximum stabilization to the resultant phases (liquid and gas) leaving the final separator. Stabilization means that considerable amounts of gas or liquid will not evolve from the final liquid and gas phases, respectively, in downstream locations such as stock tanks or gas pipelines. Additionally, staged separation reduces the horsepower required by a compressor, since the gas is fed at higher pressures [8]. Determination of the optimal number of stages is very difficult because the composition of crude oil from well to well can be different and over the time pressure of wells change. Also, more stages (separators) do not guarantee more export oil and hence more profit. This is because after each stage liquid recovery drops, so as a result of it the cost of additional separators (stages) is not justified. Installation of more separators is related with more space, piping, compressors and complexity. Therefore, there are three general separation systems which are more often installed on the offshore oil platforms:

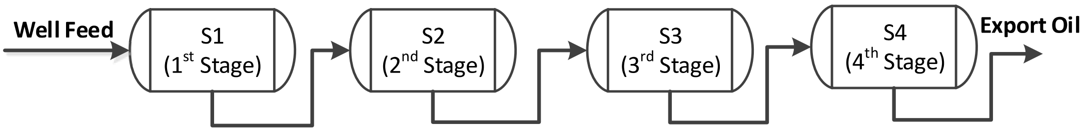
- two-stage separation system (Fig. 2.2a)
- three-stage separation system (Fig. 2.2b)
- four-stage separation system (Fig. 2.2c)



(a) Two-stage separation system



(b) Three-stage separation system



(c) Four-stage separation system

Fig. 2.2 Types of stage of separation

2.3 Hydrocarbon Allocation

Today many oil and gas companies are collaborating in order to reduce their financial cost and risks related with extraction, transportation and storage of oil and gas products. Moreover, according to Oil and Gas UK [9], large oil and gas reserves remain offshore where collaboration is very important for the industry's future. There are a few reasons for that. First, using facilities and construction in offshore location for extraction and transportation of gas and crude oil are more complex and costly than onshore facilities. Secondly, there are risks of accidents, spills and fires which can be catastrophically for marine life and coastal economies [10].

Nowadays, as a result of used shared facilities, there is a need of some process to split export oil and gas production between companies, suppliers or operators which used those facilities. Hydrocarbon allocation (HA) (Fig. 2.3) is the process which determines the quantity of oil and gas products belonging to each operator (which comprises one or more oil and gas companies) when inputs from different wells are processed together in a commingled system (for example on an offshore oil platform). HA is one of the most important processes for oil and gas companies. There are a few reasons for that. First, accurate allocation reduces the exposure of companies to financial loss through allocation error. Secondly, HA can be used not only for multiple operators but also for multiple wells and a single operator when allocation of export oil and gas production between wells is required. Moreover, the results from allocation between wells are input to reservoir models, allowing engineers to optimise production and make decisions on drilling new wells. Thirdly, allocation is used to prepare different types of production reports to governments and partners.

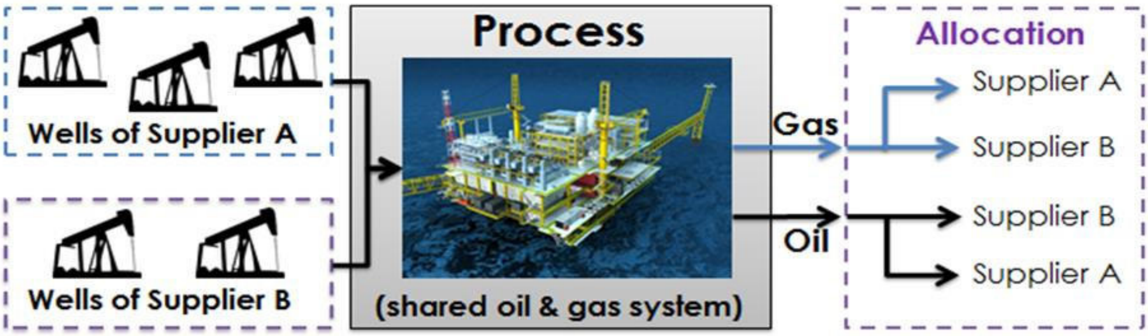


Fig. 2.3 Hydrocarbon Allocation - Suppliers A and B wish to know what fraction of the Export Gas and Oil produced is theirs

A key feature of many hydrocarbon allocation processes is a Flash Calculation (FC). The flash allows for given feed stream (from well or separator) to determine the quantity of each hydrocarbon composition (Methane, Ethane, Propane, etc.) of the resulting vapour and liquid streams which would be achieved under equilibrium at specific temperature and pressure conditions (see Chapter 3.1). Cloned components allocation offers a mechanism to allocate at a component level directly in a simulation. Here, the simulation means a sequence of flash calculations which represents the shared oil and gas system. In case of this allocation all components from different wells are copied with identical properties but tagged as belonging to a well. After that, those tagged streams are used as input information for FC. On Figure 2.4

is shown how cloned components allocation will look like if stream from wells A and B are tagged in “orange” and “purple” colors. After the tagging, components are used as input for simulation which represents complex chemical processes of shared oil and gas system. As can be seen on the Figure 2.4, at the end of the simulation we will have export oil and gas streams which consist of “orange” and “purple” components. So, the quantity of “orange” components shows how much of exported oil and gas production belong to well A while “purple” components shows the production of well B.

Cloned components allocation is not possible for real world but possible in simulation. The main advantage of this allocation is the ability to handle each hydrocarbon component through the chemical processes. As a results of this feature, this allocation is very precise and accurate. Moreover, commercial packages such as Aspentech’s HYSYS use this type of allocation. However, the accuracy of the allocation is directly related with the accuracy of the used FC. Therefore, for the needs of cloned components allocation is required robust, efficient and precise FC.

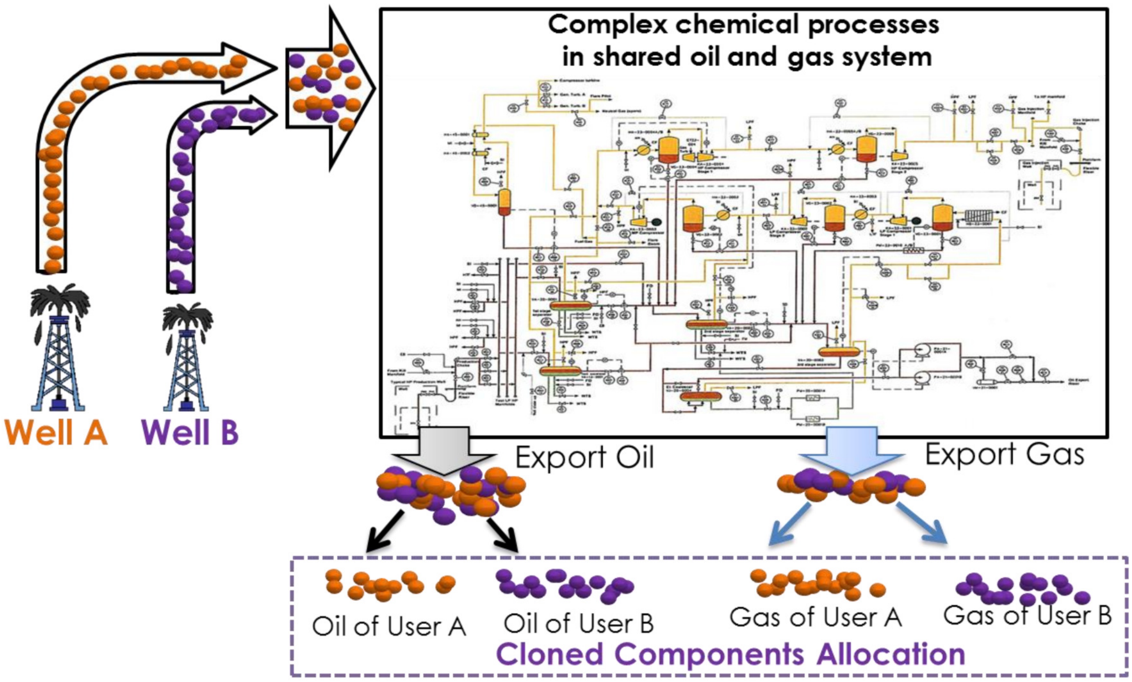


Fig. 2.4 Cloned Component Allocation – example with two wells

2.4 Traditional Approach for the Simulation of Separation Systems

Nowadays, simulations of separation system are routinely used in the oil and gas industry for many purposes. For instance, simulations are widely used during the design of offshore oil separation systems and hydrocarbon allocation. Calculated results have to be accurate and precise because any error in simulation can lead to a poor design or/and financial losses worth thousands or millions dollars.

In oil industry, the simulation of separation systems is normally associated with commercial packages such as Aspentech's HYSYS, Honeywell's UniSim, Simsci-Esscor's PRO/II. Currently, these software packages are a "gold" standard in oil and gas industry and there are many reasons for it. First of all, these packages are developed in order to cover the needs of chemical engineers in oil and gas industry. Therefore, they support wide range of features and chemical calculations, such as process simulations, refinery operations and modeling the gas plant. Secondly, these packages are robust, accurate and have state-of-the-are user interface. However, there are some major disadvantages related with these software tools.

Firstly, due to the wide range of implemented features and the specific of oil industry, it is required training in order to start to use them even in cases where only some small part of features is used. As an example can be provided hydrocarbon allocation where is used only small piece of what these commercial packages can do. Secondly, during the use of some calculations, such as separation system simulation, there can occur a situation where the simulation stops and this requires a chemical engineer to be directly involved in order to solve the problem. For instance, this situation can happen when a convergence in some calculations is not achievable. So, a chemical engineer has to investigate it and change a simulation in a way where simulation will continue and the convergence will be achieved. Thirdly, these software tools are user interface oriented and establishment of connection with other software is very complex and raises many issues. Moreover, interfaces of these packages can change from one version to an other. At the same time, the integration with other tools is highly important in cases where external software use these commercial packages as a tool for simulation and calculations. As a example of the external software can be provided a hydrocarbon accounting system which use commercial packages for daily hydrocarbon allocation. Another example of external software may be some optimization framework launched on a cluster computer which tries to find optimal settings of an oil separation system. The last but not least disadvantage, is the license price of these commercial tools which is very expensive.

Due to the reasons provided above traditional commercial packages are not convenient for use in cases where only small part of their features and calculations are used. In our research, use of these packages only for separation simulation and hydrocarbon allocation is not suitable and appropriate. First of all, the integration of provided above packages with novel optimisation frameworks is not adequate and very complex. This is because these commercial packages can be installed only on Windows machines while today in the era of technology for launched of heavy optimisation frameworks are used supercomputers, clusters or cloud computing. Secondly, optimisation frameworks generate thousands solutions and tested the quality of these solutions so it is impossible direct interaction in order to fix the solutions with problems because there can be hundreds of them. Finally, the price of these packages is to higher for university research.

To sum up, traditional commercial packages are not convenient for hydrocarbon allocation due to the reasons provided above. Therefore, for the needs of this research was used software tool "CHARM"[1] which was developed during to my research and KTP project. The key feature of our software tool is a flash algorithm which performs accurate and fast phase equilibrium calculations. Chapter 3 provides detailed information about the flash algorithm and its use for modelling and simulation of separation systems.

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[1] Compact Hydrocarbon Allocation Reference Model (CHARM), web-site: https://charm.accord-esl.com/

Chapter 3

Simulation of Oil and Gas Separation Processes

This chapter describes a novel approach to the simulation of separation systems based on flash algorithm. The flash algorithm takes a key place into the simulation of separation processes because it provides a computational model of physical separator/scrubber. The chapter covers the description and improvements of the flash calculation algorithm. In addition, this chapter provides results of our investigation which show how and when instabilities in the flash calculation can occur. Sources of these instabilities include a poor estimation of K-factors, an incorrect and/or slow solution of the cubic equation of state and the use of invalid compressibility factors. Finally, the validation of the proposed algorithm is given.

3.1 Vapour-Liquid Equilibrium

Vapour-liquid equilibrium (VLE) calculations are an integral part of chemical engineering: simulations of how hydrocarbons behave in a chemical process. The ability to predict thermodynamic properties of multicomponent mixes, such as density and entropy, depends on a good understanding of phase behaviour. Moreover, modelling and design of many types of equipment for separating vapours and liquids - such as separators, distillation columns and even a pipeline - are based on the vapour and liquid phases being present in equilibrium [8]. Therefore, it is very important to recognize and be able to calculate quickly and efficiently when these phases are in equilibrium with each other, and how much of each component is in each phase. This knowledge is especially important for the simulation of a real separation process. For instance, simulations are routinely used in oil and gas allocation systems. Even a small error in the simulation calculations used for the daily or monthly allocation of oil through an offshore platform can result in accumulated worth thousands or millions dollars.

FC can be used as the phase equilibrium calculation for processes in VLE. Moreover, flash calculation is an integral part of oil and gas engineering simulations. Flash is applicable whenever one needs to know the amounts (in moles or mass) of hydrocarbon liquid and vapour coexisting in equilibrium within a reservoir or vessel at a given pressure and temperature. A typical process that requires this calculation is when a feed stream of n-hydrocarbon components, $Z = (z_1, z_2, ..., z_n)$, is separated into a liquid (oil) stream, $X = (x_1, x_2, ..., x_n)$, and a vapour (gas) stream, $Y = (y_1, y_2, ..., y_n)$, at a given temperature (T) and pressure (P). Here, i-element (z_i, x_i, y_i) of vectors Z, X and Y is the amount in moles or mass of the corresponding hydrocarbon component. Also, flash calculation enables the vapour-feed ratios and K-factors of such hydrocarbons to be determined [11].

The main reasons for those instabilities are related with the iterative nature of the flash calculation

Flash calculation and its constituent steps (Figure 3.1) are well known and are described in many papers [11], [12], [13]. Although relatively simple, there can be instabilities in the flash calculation which can result in a poor or even an absolutely wrong solution. The standard approach to speeding up and improving flash is to use a lumping procedure in order to decrease the number of components [14]. Gaganis and Varotsis [15] present a non-iterative approach based on classification and regression models which are generated in an automated offline way for any given feed composition. Belkadi et al. [16] suggest skipping stability analysis in the single phase region and use approximation based on existing tie-line results. A literature survey of flash calculation gives numerous articles which have proposed how to improve the speed and robustness of flash calculation [17], [18], [19]. Furthermore, such literature can be split in two groups. The first group includes improvement (adaptation) of flash calculation under specified conditions. The second group discusses a reduction of computational effort, for instance reduction of the Jacobian or Hessian matrix [20]. Therefore, the oil industry is still looking for improvements of flash computational steps (Figure 3.1) under wide range of conditions. Moreover, these improvements have to be simple to understand and convenient for coding.

3.2 Approach for Simulation of Oil Separation Systems

Simulation of oil separation systems can generally be represented by a series of separators, scrubbers, stream mixers and splitters and is often implemented using simulation software. At the same time, the modelling of separators/scrubbers can be replicated by analogous flash and mass balance calculations. These calculations employ the flash algorithm that is applicable over a wide range of conditions (temperatures and pressures) and hydrocarbon compositions and can be easily coded. We aim to develop a simple, fast, robust and easy to support and maintain simulation software.

Generally, in an allocation system, the simulation of oil separation system is only used to determine how hydrocarbons entering the process are distributed between the various liquid and gas products exiting the process; stream enthalpies, equipment performances, etc. are not of interest. The only important unit operations in the flow scheme are those where material streams are combined or separated. Therefore, the allocation simulation can be constructed simply as a series of flashes, mixers and splitters, provided that the operating conditions in the flashes are known or specified. The fact that there may be a number of equipment items between the flashes does not affect the vapour-liquid equilibria in the vessels, which are determined by the operating conditions therein. According to the practice at Accord-ESL, which has global expertise in the subject, the results from these simplified schemes are almost identical to those generated by the more complex “full-blown” simulations, with the advantage of improved speed and lightness of solution.

Since the process scheme can be represented as a series of flashes (separators/scrubbers) and mixtures and splitters, the calculations associated with these unit operations can be performed outwith commercial simulation packages, such as Aspen HYSYS. Nevertheless, the main difficulties of implementation of stable and accurate simulation represented by a series of separators, scrubbers, stream mixers and splitters are related with the instabilities of the flash algorithm. Therefore, in this research are provided results of an investigation showing how and when instabilities in flash calculation can occur. Sources of these instabilities include a poor estimation of K-factors, an incorrect and/or slow solution of the cubic equation of state and the use of invalid compressibility factors. The following sections present our development and application of a robust flash calculation algorithm. The result of this investigation into VLE and flash calculation is a more robust and efficient flash calculation algorithm which has been validated on thousands of realistic examples and used for development of oil simulation software.

3.3 Modelling of a Separator with Flash Algorithm

The general flowchart diagram of the flash algorithm for determination of the phase-behaviour calculation is given in Figure 3.1. An explanation of the blocks in Figure 3.1 and our proposed improvement inside each block is given below.

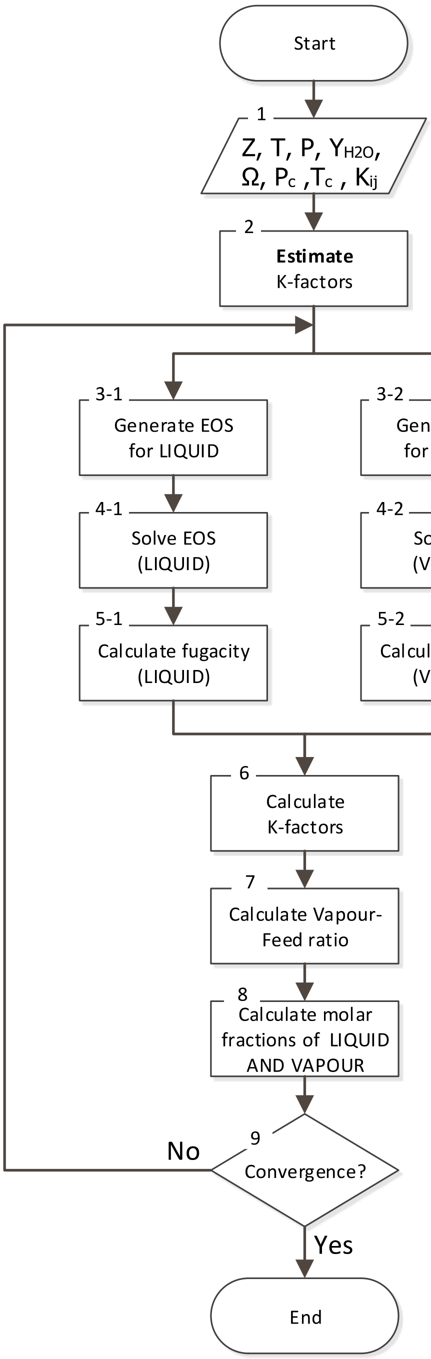


Fig. 3.1 The flowchart diagram of flash calculation

Block 1: Input data

Input data of the flash algorithm are the component fractions ($Z = (z_1, z_2, ..., z_n)$), the vessel's temperature (T) and pressure (P), the water fraction (Y_{H2O}) in the vapour phase, the acentric factors ($\Omega = (\omega_1, \omega_2, ..., \omega_n)$), the critical pressures ($P_c = (p_{c_1}, p_{c_2}, ..., p_{c_n})$), the critical temperatures ($T_c = (t_{c_1}, t_{c_2}, ..., t_{c_n})$) and the binary interaction coefficients (K_{ij} - matrix (n x n)). In all notation, n is number of components.

The following assumes that the water mole fraction in the vapour phase (Y_{H2O}) is provided as an input. If there is no water present, the water mole fraction in the vapour phase (Y_{H2O}) is set to zero. Otherwise, the water saturated vapour can be estimated by a suitable method, e.g. the Antoine Equation [21] as a function of the pressure (P) and temperature (T). The presence of water in the vapour needs to be accounted for as it has an impact on the hydrocarbon component phase split. In the method it is also assumed that liquid water is completely immiscible with the hydrocarbon liquid and forms a second liquid free water phase. Hence the quantity of free water does not need to be determined explicitly if it is assumed that there is sufficient present to saturate the vapour phase.

Block 2: Estimate Initial K-values

The proposed algorithm for the calculation of initial K-factors uses Wilson's formula (equation 3.18). This was found to be the best method for reasons presented in Section 3.4.1.

Block 3-1, 3-2: Generate Peng-Robinson Equation of State

In a flash calculation, an equation of state (EOS) is used to calculate the compressibility factor for the liquid (Z_L) and vapour (Z_V) phases. Generating the Peng-Robinson cubic equation of state (equation 3.27) for the vapour and liquid phases requires the solution of equations 3.25, 3.23, 3.24, 3.21, 3.22, 3.28 and 3.29 (Section 3.4.2).

Block 4-1, 4-2: Solve Peng-Robinson Equation of State

Figure 3.4 summarises the algorithm proposed for the solution of the PR-EOS (Section 3.4.3).

Block 5-1, 5-2: Calculate fugacity coefficients

After calculation of the compressibility factors for the liquid (Z_L) and vapour (Z_V) phases (equation 3.27), fugacity coefficients ($\phi_{i\alpha}$) for components in both phases are calculated using following equation:

$$\phi_{i\alpha} = exp\left(\frac{b_i}{b}(Z_\alpha - 1) - ln(Z_\alpha - B) - \frac{A}{2\sqrt{2}B}\left(\frac{2}{a}\sum_{j=1}^{n} x_j\sqrt{a_i a_j}(1-k_{ij}) - \frac{b_i}{b}\right)\right.$$
$$\left.\ln\left(\frac{Z_\alpha + (1+\sqrt{2})B}{Z_\alpha + (1-\sqrt{2})B}\right)\right) \tag{3.1}$$

where α indicates the phase type L (liquid) or V (vapour).

Block 6: Calculate K-factors

The K-factor, k_i, of a given hydrocarbon component can be expressed as a ratio of the fugacity of the component in the liquid phase, (ϕ_{i_L}), to the fugacity of the component in the vapour phase, (ϕ_{i_V}) (equation 3.2).

$$k_i = \frac{\phi_{i_L}}{\phi_{i_V}} \tag{3.2}$$

Block 7: Calculate Vapour-Feed ratio

The Rachford-Rice equation [22] (equation 3.6) is used to calculate the vapour-feed ratio (V_f). However, before applying the Rachford-Rice equation, it is very important to check that we have a two-phase equilibrium, otherwise the procedure can determine an invalid vapour-feed ratio. In order to avoid this problem, we have to check first of all for a bubble point and after that for a dew point [23]. The bubble point can be checked using equation 3.3 and, if the value of $f_{bubble} >= 0$ then a bubble point exists and $V_f = 0$.

$$f_{bubble} = 1 - Y_{H2O} - \sum_{i=1}^{n} z_i k_i \tag{3.3}$$

If no bubble point exists then the dew point has to be checked using equation 3.4. If $f_{dew} <= 0$ then a dew point exists and $V_f = 1$.

$$f_{dew} = \sum_{i=1}^{n} \frac{z_i(1-k_i)(1-Y_{H2O})}{k_i} - Y_{H2O} \tag{3.4}$$

Finally, if there is multiphase flow (i.e. the mixture lies between the bubble and dew point) the Newton-Raphson method [24] (equation 3.5) can be applied iteratively for an efficient solution of the Rachford-Rice equation.

$$V_{f_{new}} = V_{f_{old}} - \frac{S}{dS} \tag{3.5}$$

where S is given by the Rachford-Rice equation and dS its derivative with respect to vapour feed ratio.

$$S = \sum_{i=1}^{n} \frac{z_i(1-k_i)}{\left(1 - V_{f_{old}}(1 - k_i - Y_{H2O})\right)} - Y_{H2O} \tag{3.6}$$

$$dS = \sum_{i=1}^{n} \frac{z_i(1-k_i)(1-k_i-Y_{H2O})}{\left(1 - V_{f_{old}}(1 - k_i - Y_{H2O})\right)^2} \tag{3.7}$$

Block 8: Calculate molar fraction of hydrocarbons

Calculate the molar fraction of each component in the liquid phase based on the following equation:

$$x_i^L = \frac{z_i}{\left(1 - V_{f_{new}}(1 - k_i - Y_{H2O}\right)} \tag{3.8}$$

Calculate the molar fraction of each component in the vapour phase using:

$$x_i^V = x_i^L k_i \tag{3.9}$$

Block 9: Check Convergence

Two parameters are used when checking for convergence of the proposed algorithm so as to guarantee accurate and correct results. The first parameter is a mass balance combined with changes in vapour-feed ratio (V_f) from one iteration to the next (equation 3.10). The second parameter measures changes in the K-factors over all components between iterations (equation 3.11).

$$dr = \left| \sum_{i=1}^{n} \frac{z_i(1-k_{i_{new}})}{1 - V_{f_{new}}(1 - k_{i_{new}} - Y_{H2O})} - Y_{H2O} \right| + \left| V_{f_{new}} - V_{f_{old}} \right| \tag{3.10}$$

$$k_{err} = \sum_{i=1}^{n} \frac{(k_{i_{new}} - k_{i_{old}})^2}{k_{i_{new}} k_{i_{old}}} \tag{3.11}$$

After calculation of each iteration, the calculations are deemed complete if both $dr \leq \varepsilon_{dr}$ and $k_{err} \leq \varepsilon_k$. Otherwise, the calculation is repeated from blocks 3-1 and 3-2. For this paper, testing of the flash algorithm was performed using $\varepsilon_{dr} = 0.001$ and $\varepsilon_k = 0.001$.

3.4 Proposed Improvements of Flash Algorithm

3.4.1 Estimation of equilibrium ratio

Equilibrium ratios or K-factors play a fundamental role in predicting the phase behaviour of mixtures. They are important for forecasting the compositional changes under varying temperatures and pressures in flash calculations [25]. While laboratory experiments can provide precise and accurate values of K-factors, more often chemical engineers get such values from a chart or from difficult and time-consuming calculations [26].

Accurate estimation of K-factors is one of the challenges in the development of a stable algorithm for flash calculation. According to Almehaided et al. [25] K-values are critical for the effective and successful simulation of compositional reservoirs. Unfortunately, because of the complex nature of hydrocarbon mixtures, accurate estimations of K-values are hard to obtain for the higher pressures where most phase behaviour problems occur. So, poor estimation of K-values can result in significant errors during flash calculation. Conversely, good initial estimates of equilibrium K-values reduces iteration in the flash calculation algorithm and hence improves its speed. Therefore, for the needs of this research a review of exist formulas for estimation of K-values has done by us and provided below.

In a multicomponent system, the equilibrium K-factor of a given component, k_i, is defined as the ratio of the mole fraction of the component in the vapour phase, y_i, to the mole fraction in the liquid phase, x_i (equation 3.12) [11] .

$$k_i = \frac{y_i}{x_i} \tag{3.12}$$

For the real solution, the equilibrium ratios $K = (k_1, k_2, ..., k_n)$ are a function of the pressure (P), temperature (T) and composition $Z = (z_1, z_2, ..., z_n)$ of the hydrocarbon mixture, as per equation 3.13.

$$K = f(T, P, Z) \tag{3.13}$$

As was mentioned above, K-factors can be estimated based on empirical correlations. There are numerous methods which have been proposed for predicting the equilibrium ratios of real hydrocarbon mixtures. These correlations range from a simple mathematical expression to expressions containing several composition-dependent variables. A search of the literature reveals that only a few authors have attempted to obtain a direct general correlation for K-factors from experimental data, especially for high-pressure systems.

In 1953, Hoffman et al. [27] investigated a number of gas-condensate experimental data sets. As a result of this work, the authors suggested that the K-factor of any pure hydrocarbon or non-hydrocarbon component could be uniquely characterized as a function of the critical temperature (T_{ci}), boiling point temperature (T_{bi}) and critical pressure (P_{ci}) (equation 3.14).

$$\begin{aligned} \log(k_i, P) &= b_i\left(\frac{1}{T_{bi}} - \frac{1}{T}\right) \\ b_i &= log\frac{P_{ci}}{14.7}/\left(\frac{1}{T_{bi}} - \frac{1}{T_{ci}}\right) \end{aligned} \tag{3.14}$$

Standing [26] derived a set of equations that fit the equilibrium ratio data of Katz and Hachmuth at pressures less than 1000 psia and temperatures below 200F, which are appropriate for surface-separator conditions. The proposed form of the correlation is based on a modified Hoffmann's equation (equation 3.14) with additional parameters, as per equation 3.15.

$$\log(k_i, P) = a + c\left(b_i\left(\frac{1}{T_{bi}} - \frac{1}{T}\right)\right) \tag{3.15}$$

Solving for the equilibrium ratio, k_i, gives:

$$\begin{aligned} k_i &= \frac{1}{p}10^{a+c\left(b_i\left(\frac{1}{T_{bi}} - \frac{1}{T}\right)\right)} \\ a &= 1.2 + 0.00045p + 15(10^{-8})p^2 \\ c &= 0.89 - 0.00017p - 3.5(10^{8})p^2 \end{aligned} \tag{3.16}$$

Galimberti and Campbell [28] suggested another useful approach for relating K-factors to critical temperatures (T_{ci}) (equation 3.17). The proposed formula can be used for pressures up to $206 * 10^5$Pa and temperatures from 288K to 422K.

$$\log(k_i) = A_0 + A_1 T_{ci}^2 \tag{3.17}$$

The Wilson correlation (equation 3.18) is a simplified thermodynamic expression for estimating K-factors which is a function of more common properties such as the critical pressure (P_{ci}), critical temperature (T_{ci}) and acentric factory (ω_i) [11].

$$k_i = \frac{p_{ci}}{p}\exp\left(5.37(1+\omega_i)\left(1 - \frac{T_{ci}}{T}\right)\right) \tag{3.18}$$

Whitson and Torp [29] reformulated the Wilson equation to yield accurate results at higher pressures by incorporating the convergence pressure, P_k (equation 3.19). The convergence pressure is used to correlate the effect of the composition on equilibrium ratios. Unfortunately, calculation of the convergence pressure requires additional calculations which can be time consuming. Therefore, use of this formula for the estimation of K-factors in the flash algorithm was not adopted.

$$k_i = \left(\frac{p_{ci}}{p_k}\right)^{(A-1)} \left(\frac{p_{ci}}{p}\right) \exp\left(5.37A(1+\omega_i)\left(1-\frac{T_{ci}}{T}\right)\right) \tag{3.19}$$

The right choice of one of the formulae given above (i.e. equations 3.14 to 3.19) for the calculation of K-factors is highly important for both correct results and for the speed of the flash calculation. At the same time selected formulae should not be computationally heavy.

The first proposed formula for estimation of k-factors was proposed in 1953 by Hoffman and since, more accurate formulas have been proposed. The formula suggested by Galimberti and Campbell has two main disadvantages. Firstly, the formula is applicable for temperatures from 288K to 422K and there is also pressure limitation. Secondly, the value of k-factor is estimated only based on the critical temperature of the hydrocarbon component and other parameters, such as critical pressure and acentric factor, are not taken into account during the estimation. So, such estimation can be insufficient for theoretical hydrocarbon components. Due to this reasons, this formula is inappropriate for our flash algorithm. Standing's k-factor formula is also inapplicable due to pressures limitation. According to the authors, the formula applies for pressures which are less than 1000 psia and those pressures are very low for real separation systems. Whitson's formula looks to be a good candidate for initial estimation of k-factors, because there is no temperatures or pressures limitation and a lot of parameters are taken into account during estimation. However, using the Whitson's formula requires heavy calculation of the convergence pressure which is time consuming and not efficient for initial estimation and respectively for the flash calculation algorithm.

Ghafoori et al. [30] provide a wide comparison of various K-formulae, including those provided above. In this paper, authors have compared calculated K-values for different K-formulas with the experimental data. According to results given in this paper, the Wilson's equation has an average relative deviation from empirical values of 38% which is good enough for the initial estimation formula without additional calculation, such as the convergence pressure (P_k) in the Whitson's equation. Moreover, Wilson's equation does not have any temperature or pressure limitations. Neto et al. [31] use the Wilson's correlation in their flash algorithm and recommend to use it because of the reasonably well approximation of the K-values. Also, Ahmed [11] advises use of the Wilson's correlation for good initial values. Therefore, based on reviewed literature and provided results there we have decided to apply the Wilson's formulae for obtaining of the starting K-values in our flash algorithm.

3.4.2 Peng-Robinson Equation of State

VLE calculations use an equation of state (EOS) which provides a mathematical relationship between pressure (P), temperature (T) and volume (V). This PVT relationship is very important for real mixtures in order to determine phase behaviour, describe fluid properties or calculate other properties (for instance, the density) of the hydrocarbon fluid. Likewise, an EOS is used to calculate the equilibrium ratio for each hydrocarbon component. Therefore, this equation and determination of its accurate solution is key to a flash calculation algorithm.

There are many EOS, such as the Redlich-Kwong Equation (RK) [32], the Soave-Redlich-Kwong Equation (SRK) [33] and the Peng-Robinson Equation (PR) [34]. They are mainly developed for pure substances and are applicable under specific conditions, such as certain temperatures and pressures. Application of an EOS requires additional variables and appropriate mixing rules which are different for each EOS. Unfortunately, there is no single equation that accurately predicts the properties of all substances under all conditions. Nowadays, one of the most widely used EOS in the oil and gas industry for the modelling and simulation of chemical processes is the Peng-Robinson cubic equation of state (PR-EOS) – see equation 3.20. The main reasons for this are that it achieves good accuracy near the critical region and better results over a wide range of pressures and temperatures[34]. In addition, the PR-EOS is capable of describing substances in both liquid and vapour phases.

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)} \tag{3.20}$$

Here, P is the system pressure, T is the system temperature, R is the standard gas constant, a is the attraction parameter, b is repulsion parameter and V is the molar volume. The calculation of parameters a and b uses mixing rules which are solved using the following formulas:

$$a = \sum_{i=1}^{n} \sum_{j=1}^{n} z_i z_j \sqrt{a_i a_j}(1-k_{ij}) \tag{3.21}$$

$$b = \sum_{i=1}^{n} z_i b_i \tag{3.22}$$

Where, z_i is the molar fraction of component i, k_{ij} is the binary interaction parameter between components i and j. Parameters a_i and b_i are calculated for each pure component using equations 3.23 and 3.24.

$$a_i = 0.457235\alpha_i \frac{(RT_{ci})^2}{P_{ci}} \tag{3.23}$$

$$b_i = 0.077796\frac{RT_{ci}}{P_{ci}} \tag{3.24}$$

Here, parameters P_{ci} and T_{ci} are the critical pressure and temperature of the pure component i. The correlation parameters $\alpha(T)$ (the temperature-dependent parameters) are calculated for each pure component i by the following relationship:

$$\alpha_i(T) = \left(1+m\left(1-\sqrt{\frac{T}{T_{ci}}}\right)\right)^2 \tag{3.25}$$

$$m = \begin{cases} 0.37464+1.54226\omega_i-0.2699\omega_i^2, & \omega_i<0.49 \\ 0.379642+1.48503\omega_i-0.1644\omega_i^2+0.016667\omega_i^3, & \text{otherwise} \end{cases} \tag{3.26}$$

Where ω_i is the acentric factor of the pure component i.

Equation 3.20 can be rearranged in a cubic form in terms of the volume, V, which after the substitution $V = ZRT/P$ gives:

$$f(Z) = Z^3-(1-B)Z^2+(A-3B^2-2B)Z-(AB-B^2-B^3) = 0 \tag{3.27}$$

$$A = \frac{aP}{R^2T^2} \tag{3.28}$$

$$B = \frac{bP}{RT} \tag{3.29}$$

Now, having determined the compressibility factor (Z) from the cubic PR-EOS (equation 3.27), the fugacity coefficient of component i (ϕ_i) in the mixture can be obtained from

$$\begin{aligned} \ln\phi_i = {} & \frac{b_i}{b}(Z-1)-\ln(Z-B) \\ & -\frac{A}{2\sqrt{2}B}\left(\frac{2}{a}\sum_{j=1}^{n} z_j(1-k_{ij})\sqrt{a_ia_j}-\frac{b_i}{b}\right) \\ & .\ln\left(\frac{Z+(1+\sqrt{(}2))B}{Z-(1-\sqrt{2})B}\right) \end{aligned} \tag{3.30}$$

Solving the cubic PR-EOS (equation 3.27) for both the liquid and vapour phases allows calculation of the fugacity coefficients of component *i* in the liquid phase (ϕ_i^L) and the vapour phase (ϕ_i^V), respectively.

3.4.3 Solution of Peng-Robinson Equation of State

The speed and accuracy of solution of the cubic PR-EOS is related to the mathematical method used. Gundersen [35] suggest to use a second order Newton iterative method [24] or a third order iterative method presented by Asbjornsen [36]. However, we have decided to use an accurate analytical calculation for the PR-EOS, instead of a numerical iterative method in order to increase the speed and precision of the flash algorithm. For solution of the cubic equation we suggest to use the analytical formulae of Vieta (Appendix A). Once the real roots of the cubic PR-EOS are correctly calculated then the compressibility factor can be found.

According to the theory [11], solution of the cubic equation yields one or three real roots. Gundersen [35] explains the existence of three real roots with the situation when the actual composition exists as a liquid and as a vapour, but not necessarily in equilibrium. In the latter case, the smallest positive root corresponds to the compressibility factor of the liquid phase, Z^L, while the largest positive root corresponds to that of the vapour phase, Z^V (see Figure 3.2). In the former case, with one real root, the compressibility factor is given by this single root (see Figures 3.3a and 3.3b).

Unfortunately, Gundersen [35] analysis of the cubic function of the SRK-EOS during iterations of the flash calculation shows that the solution of this equation can be incorrect due to the use of invalid compressibility factors. This situation can happen for the cubic equation that represents either the liquid or vapour phase compressibility (Z_L or Z_V). Our analysis confirmed that this is happening also for the cubic PR-EOS. Gundersen [35] shows that this situation can occur in some of the first iterations of the flash algorithm as a result of poor starting values of the phase compositions. As can be seen in Figures 3.3c and 3.3d it is possible to calculate the real root (Z_1) which does not correspond to the compressibility factor. Mathias and Buston [37] have found that this happens because of the iterative nature of the calculations the liquid or the vapour compressibility factor may not exist at the beginning. Therefore, the authors have used pseudo properties for convergence in their process simulator called ASPEN.

Gundersen [35] provides a deep analysis of the selection of invalid compressibility factors for the cubic SRK equation of state (SRK-EOS). Furthermore, the author suggests an alternative approach for the selection of this value – specifically, how to “slip” from the point Z_1 to Z_0 (see Figures 3.3c and 3.3d). According to the author, selection of Z_0 has

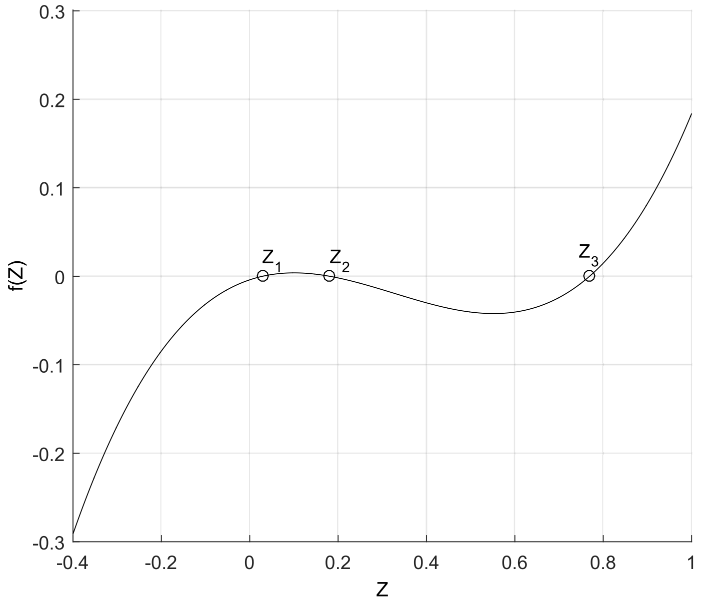


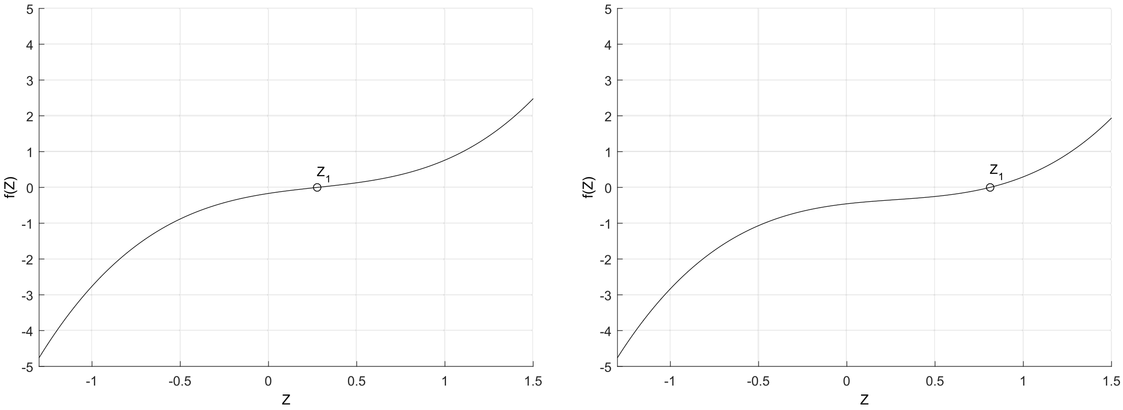
Fig. 3.2 Cubic equation of state with three real root

a positive effect on the iteration procedure and generates accurate results from the flash calculation. Based on this suggested procedure for the SRK-EOS we have developed an analogous procedure for the PR-EOS (Figure 3.4).

The inputs of the proposed procedure for selection of the compressibility factor are the values of A and B (equations 3.28 and 3.29), and also the type of the fluid phase ($IPH = 0$ for liquid and $IPH = 1$ for vapour) which these A and B values represent. The variables A and B do not require tuning and they are set with existing formulas 3.28 and 3.29 based on the composition of the stream. In proposed procedure, the values of A and B are used for calculation of V, Q and R (equations 3.31). The procedure also needs the solutions of the first (equation 3.32) and second derivatives (equation 3.33) of the cubic PR-EOS. Solutions of derivatives indicate the possibility of one or three roots in the range of Z from 0 to 1.

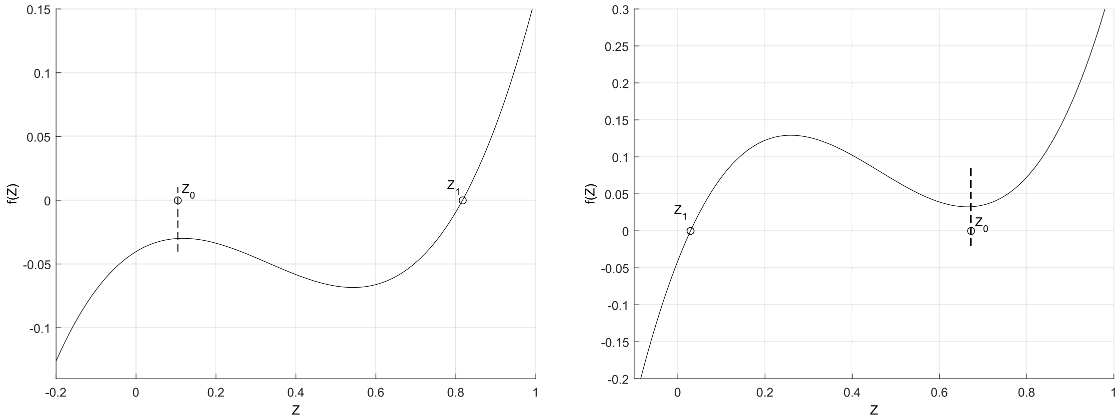
Clarify the fact that variables A and B do not require tuning and can be set with existing formula based on the composition of the stream.

$$\begin{aligned} & F(Z) = Z^3 + VZ^2 + QZ + R = 0 \\ & Where \\ & \quad V = -(1-B) \\ & \quad Q = A - 3B^2 - 2B \\ & \quad R = -(AB - B^2 - B^3) \end{aligned} \tag{3.31}$$



(a) Liquid phase

(b) Vapour phase



(c) Invalid root for liquid phase

(d) Invalid root for vapour phase

Fig. 3.3 Functions of the Peng-Robinson cubic equation of state

The first derivative of the cubic PR-EOS and its solution (Z-values of extreme points, $Z'_{1,2}$) are:

$$\begin{gathered} F'(Z) = 3Z^2 + 2VZ + Q = 0 \\ Where \\ Z'_{1,2} = -\frac{V}{3} \pm \frac{\sqrt{V^2 - 3Q}}{3} \end{gathered} \tag{3.32}$$

The second derivative of the cubic PR-EOS and its solution (the point of inflection, Z'') is:

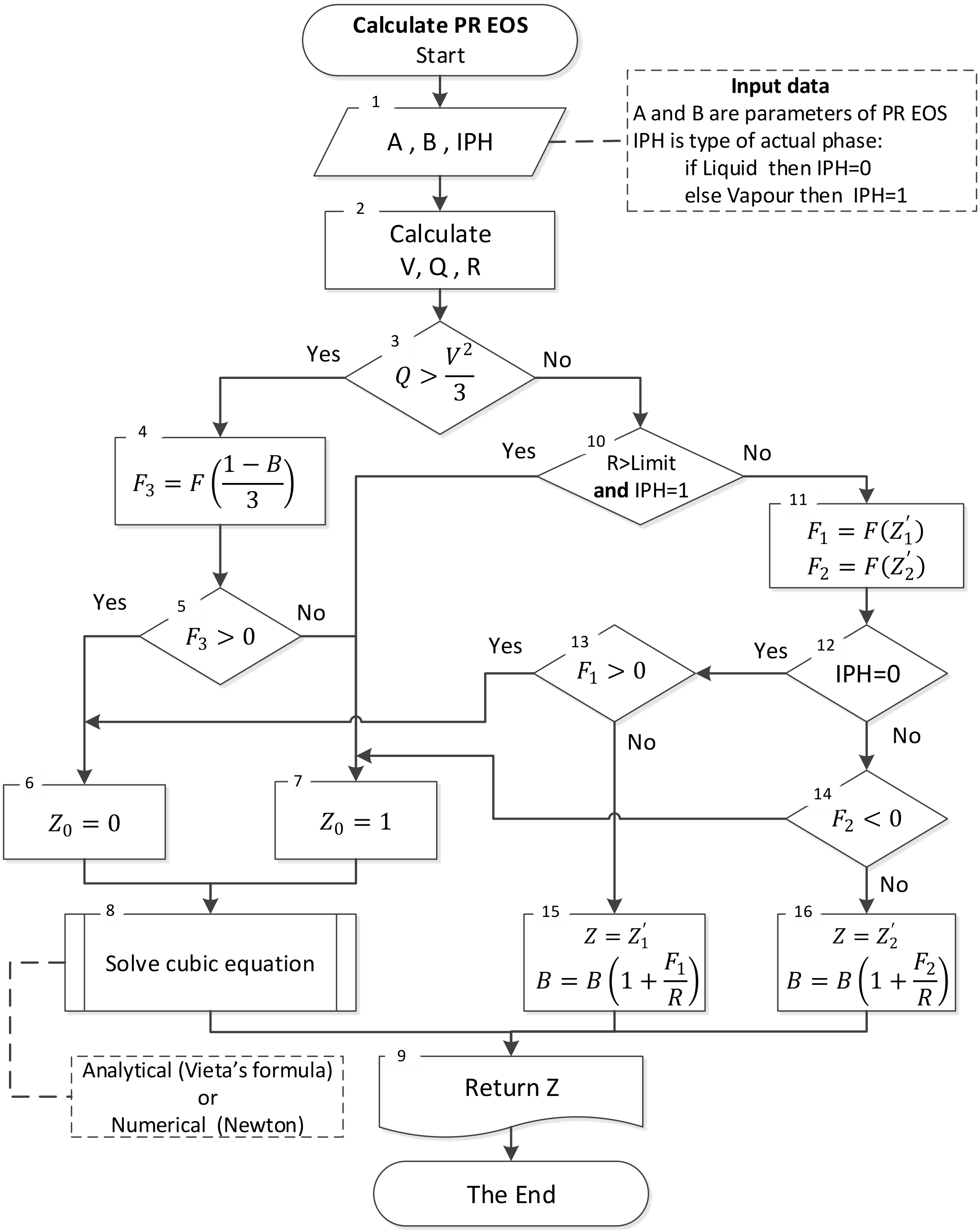


Fig. 3.4 Interpretation and Solution of PR-EOS

$$\begin{aligned} &F''(Z) = 6Z + 2V = 0 \\ &Where \\ &Z'' = -\frac{V}{3} = \frac{1-B}{3} \end{aligned} \tag{3.33}$$

The variables Q and R play an important role in the proposed solution of the PR-EOS. Coward et al. [38] show that, based on the values of these variables, the equation of state can have either one or three real roots. Information provided by Gundersen [35] for the SRK-EOS allows the limit values for Q and R to be determined. These limit values are found by calculating the first and second derivatives. The limit value of $Q = \frac{V^2}{3}$ (Figure 3.4, block 3) is based on the solution of the first derivative. In this case (when $Q = \frac{V^2}{3}$), the solutions of the first and second derivatives match, i.e. the extreme points and the inflection point match ($Z'_{1,2} = z'' = -\frac{V}{3} = \frac{1-B}{3}$). Applying these values (Q and $Z'_{1,2} = Z''$) to equation 3.31 gives the limit value of R (Figure 3.4, block 10), as a following equation:

$$Limit = \left(\frac{1-B}{3}\right)^3 + V\left(\frac{1-B}{3}\right)^2 + \frac{V^2}{3}\left(\frac{1-B}{3}\right) \tag{3.34}$$

3.5 Validation of proposed algorithm

Today, AspenTech HYSYS is the leading simulation software in the energy industry. Its advanced features mean that it is regarded as the gold standard for many chemical calculations, including the flash calculation. Therefore, AspenTech HYSYS was used to validate our proposed algorithm.

In order to validate our proposed flash algorithm, seven hydrocarbon mixtures were used (Table 3.1). Compositions A, B and C consist only of pure hydrocarbon components; the difference between them being the number of components. In practice, hydrocarbon mixtures (especially heavy oils) contain a very large number of components. In such cases, chemical engineers group various components into a smaller number of pseudo-components [39]. So, some compositions with pseudo-components were also used for validation of the proposed flash algorithm. Mixtures D and E are real compositions with different type of pseudo-components. At the same time, G and I are derived artificially from mixture E. Mixture G and I are generated by reducing (removing) the number of pure component in mixture E. Moreover, the main purpose of mixture G and I is to check the behavior of our algorithm with a low number of pure components and a high number of pseudo-components.

To demonstrate the accuracy and performance of our proposed algorithm, 251 cases were generated for each hydrocarbon mixture (A, B, C, D, E, G, I) by a uniform random generator

Table 3.1 Hydrocarbon mixtures used to validate the proposed flash algorithm

Hydrocarbon Compositions						
A	B	C	D	E	G	I
Nitrogen	Nitrogen	Nitrogen	Nitrogen	Nitrogen	Nitrogen	Nitrogen
CO2	CO2	CO2	CO2	CO2	CO2	CO2
Methane	Methane	Methane	Methane	Methane	Methane	Methane
Ethane	Ethane	Ethane	Ethane	Ethane	Ethane	Ethane
Propane	Propane	Propane	Propane	Propane	Propane	Propane
i-Butane	i-Butane	i-Butane	i-Butane	i-Butane	i-Butane	i-Butane
n-Butane	n-Butane	n-Butane	n-Butane	n-Butane	n-Butane	n-Butane
i-Pentane	i-Pentane	i-Pentane	i-Pentane	i-Pentane	i-Pentane	i-Pentane
n-Pentane	n-Pentane	n-Pentane	n-Pentane	n-Pentane	n-Pentane	n-Pentane
n-Hexane	n-Hexane	n-Hexane	n-Hexane	n-Hexane	n-Hexane	n-Hexane
n-Heptane	Mcyclopentan	Mcyclopentan	n-Heptane	Mcyclopentan	n-Heptane	n-Heptane
n-Octane	Benzene	Benzene	n-Octane	Benzene	n-Octane	C10-C12*
	Cyclohexane	Cyclohexane	n-Nonane	Cyclohexane	n-Nonane	C13-C14*
	Mcyclohexane	Mcyclohexane	Mcyclopentan	Mcyclohexane	C10-C12*	C15-C16*
	Toluene	Toluene	Benzene	Toluene	C13-C14*	C17-C19*
	E-Benzene	E-Benzene	Cyclohexane	E-Benzene	C15-C16*	C20-C22*
	p-Xylene	p-Xylene	Mcyclohexane	p-Xylene	C17-C19*	C23-C26*
	135-MBenzene	135-MBenzene	Toluene	135-MBenzene	C20-C22*	C27-C32*
	n-Heptane	n-Heptane	E-Benzene	n-Heptane	C23-C26*	C33-C40*
	n-Octane	n-Octane	m-Xylene	n-Octane	C27-C32*	C41-C80*
	n-Nonane	n-Nonane	o-Xylene	n-Nonane	C33-C40*	
		n-Decane	124-MBenzene	C10-C12*	C41-C80*	
		n-C11	C10+*	C13-C14*		
		n-C12		C15-C16*		
		n-C13		C17-C19*		
		n-C14		C20-C22*		
		n-C15		C23-C26*		
		n-C16		C27-C32*		
		n-C17		C33-C40*		
		n-C18		C41-C80*		
		n-C19				
		n-C20				

in Excel VBA. Altogether, it was giving a total of 1757 different cases. For each case, the molar fraction is used as input for the flash algorithm therefore for every component the molar fraction was generated in the range between 0 and 1. Temperatures were generated in the range from 235K to 653K and pressures were in the range from 1x10^5 Pa to 95x10^5 Pa. Selected ranges of temperatures and pressures cover values which are supported in the real world by separator vessels.

The vapour-feed ratio is used to compare the proposed flash algorithm and AspenTech HYSYS. For that reason, all random generated test cases were calculated in AspenTech HYSYS and an implementation of our algorithm in Excel VBA. A summary of these results is given in Table 3.2. In addition, detailed information for each case is given in Figure 3.5a

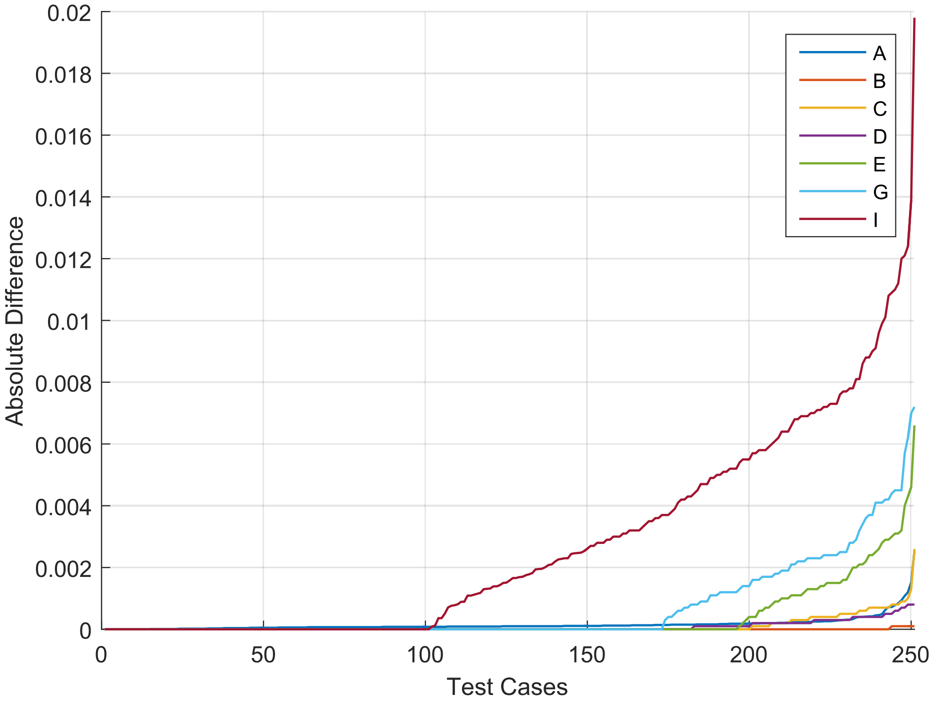
Table 3.2 Comparison of vapour-feed ratios between our proposed flash calculation algorithm and Aspen HYSYS results

Mixture	Count $\|\varepsilon\| < 0.001$	Count $\|\varepsilon\| > 0.001$	Max $\|\varepsilon\|$	Mean	Standard Deviation
Absolute Difference					
A	247	4	0.00254	0.00015	0.00024
B	251	0	0.00012	0.00001	0.00002
C	249	2	0.00256	0.00010	0.00027
D	251	0	0.00085	0.00008	0.00016
E	210	41	0.00659	0.00039	0.00093
G	187	64	0.00724	0.00071	0.00135
I	112	139	0.01979	0.00277	0.00337
Percentage Difference					
A	251	0	0.347%	0.02182%	0.03757%
B	251	0	0.337%	0.00721%	0.03310%
C	228	23	33.197%	0.46042%	2.42311%
D	231	20	14.415%	0.43083%	1.55047%
E	214	37	100%	1.70244%	8.31030%
G	196	55	100%	2.28488%	8.74536%
I	145	106	100%	7.45412%	19.20285%

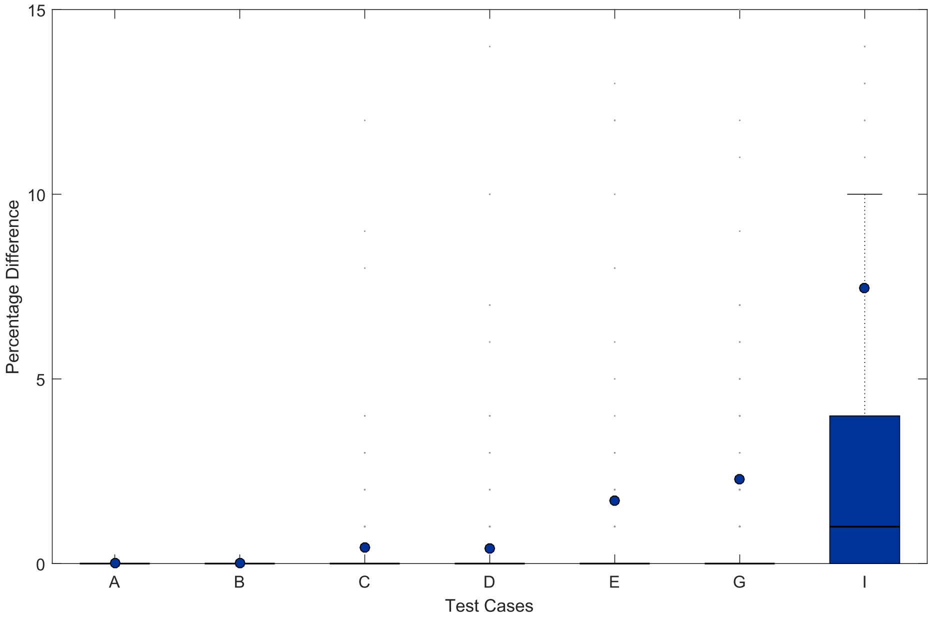
and Figure 3.5b. These figures show the absolute difference (ε) and percentage difference (δ), respectively, in the vapour-feed ratio between the AspenTech HYSYS results and those produced by our proposed algorithm. In both figures, the cases are sorted in ascending order of absolute difference.

As can be seen from Table 3.2 and Figure 3.5, for mixtures A and B, our flash algorithm reproduces the HYSYS results almost exactly. However, for other mixture from Table 3.2 there are cases where the percentage difference is higher than 1%. Our analysis of provided results shows that there are two reasons why in some cases a big percentage difference occurs.

The first main reason for high percentage difference between the proposed algorithm and HYSYS is that a little difference between close small numbers results in a large percentage error. A good example of this is mixture C, there are cases with the percentage difference between vapour-feed ratio of our algorithm and HYSYS higher than 1%. Analysis of these cases shows that this is because two very small numbers are being compared, so that even with a very small difference, such as 0.0001, a significant percentage difference can result. For example, the case of mixture C where $|\delta| = 33.197\%$, shows that HYSYS calculated the vapour-feed ratio as 0.00132 while our algorithm calculated it as 0.00088. The same happens for mixtures D, E, G and I where pseudo-components are included. Even where the percentage difference is 100% (i.e. either the vapour-feed ratio calculated by our proposed flash calculation algorithm or by AspenTech HYSYS is zero), the absolute numbers – and



(a) Absolute difference of vapour-feed ratio sorted by increasing error



(b) Percentage difference of vapour-feed ratio (box-plot)

Fig. 3.5 Detailed differences between AspenTech HYSYS and flash algorithm hence the absolute differences – involved are small. Furthermore, these differences are occurring under extreme conditions which can arise during the iterative search but not practically in a vessel. Also, in these circumstances AspenTech HYSYS may also be making some unpublished corrections to avoid mathematical irregularities so direct comparison may not be particularly meaningful.

The Second reason for the high percentage difference is the proportion a count of pure and pseudo-components used in our mixtures. Obtained results on mixture D (with only one pseudo-component) are good because there are no cases with absolute difference higher than 0.001. However, there are cases with absolute difference higher than 0.001 for mixtures E, G and I which have different number of pure component and fixed count of the same 9 pseudo-components. Our analysis of those cases shows that count of cases with high percentage difference increases when the number of pure component decreases while the number of pseudo-component increases and when the temperature and pressure conditions are close to dew or bubble point. Hence, AspenTech HYSYS may have some hidden features which maintain situation with high number of pseudo-components at temperature and pressure conditions close to dew or bubble point. So, as was mentioned above direct comparison with AspenTech HYSYS may not be particularly meaningful.

Nevertheless, our comparison with HYSYS (Table 3.2) shows that the biggest absolute difference between vapour-feed ratio of HYSYS and our algorithm is 0.0197. In this worse case, our algorithm calculated the vapour-feed ratio as 0.01474 while HYSYS calculated it as 0.03452. There are two circumstances which explain why a such difference is possible. Firstly, we do not have a special procedure for handling pseudo-components in our algorithm. Secondly, programming implementation of HYSYS and our algorithm (which was implemented in Excel VBA) handle small mathematical numbers with different truncation over to all calculations. Therefore, it is possible to have such difference between our algorithm and HYSYS. Moreover, it is very difficult to obtain the same agreement of in the relative differences after the floating point.

Chapter 4

Optimization of Offshore Oil and Gas Separation Processes

This chapter provides a literature review about the optimisation of oil separation system to produce hydrocarbons in the most valuable for by varying separator system control parameters. It also presentes the basic information about population-based algorithms and two of them are described in detail: differential evolution (DE) and adaptive differential evolution (JADE) algorithm. The second part of this chapter gives a formulation of the optimisation problem of the offshore oil separation process. Finally, the experimental setup and the results obtained by applying DE and JADE algorithms are presented.

4.1 Review of Literature

Today, optimisation of production processes of offshore oil platforms is highly desirable in the oil and gas industry, especially in UK waters, where the cost of exploration and production is relatively high [9]. Furthermore, optimisation of production processes of offshore oil platforms is a complex decision problem which is characterised by uncertain and incomplete information. There are reasons which make this problem dynamic. First of all, oil and gas prices change continually, sometimes dramatically such as in the late nineties and nowadays. The variation in gas price also results in changes of utility costs. Secondly, reservoir properties and composition vary over the lifetime of an oil field, and therefore maintaining a high efficiency of the processing plant over this lifetime is challenging. Finally, during the design of an offshore platform, engineers will incorporate some operating margin to accommodate uncertainties in anticipated production. So, after construction of the offshore platform there may be opportunities to exploit these margins in the operating conditions to optimise production [40].

In this research, by the operating conditions we mean the pressures and temperatures of oil and gas separation facilities (separators and scrubbers). Furthermore, the operating conditions have direct influence over the quantities and the quality of export oil and gas production. Also, there are other factors such as gas and liquid flow rates of wells, physical properties of the crude oil, presence of impurities, etc. which have an impact upon the export production. While these fluids properties are related with nature of the wells and very complicated to control, operating pressures and temperatures can be easily controlled in order to increase the profit of the offshore oil platform.

Despite the potential importance of optimization of separation systems there are not many public research materials about the optimization of operating conditions of offshore oil platforms. However, one of the first exploration of the optimization of separation pressure was done by Whinery and Campbell [41] in 1956. In this work, the authors introduce a simple method for determining the optimum second stage separation pressures in the three stage separation. The introduced method is based on an empirical correlation which avoids complex calculations such as flash calculations. Nonetheless, this method is applicable only for three stage separation system and optimises only the pressure of the second separator.

Bahadori et al. [42] presents methodology for optimization of pressures of multistage separation system where the optimum pressures corresponds to a maximum value of the stock tank API gravity [43] and a minimum value of the total gas-oil ratio (GOR)[44]. According to the results presented by the authors, the selection of operating pressures increase the profit in range of 3000-3600 dollars per day without installing any additional equipment or added cost.

Kylling [45] reports in his Masters thesis a flash algorithm for modeling and a brute force algorithm for pressure optimization of multistage separation system. According to the presented results, even the application of simple brute force optimization of pressure of separators allows to increase the profit with a rough estimation of two million US dollars per year.

Recently, Kim et al. [46] report that the most important variables for production optimisation are the temperatures and pressures of the separation process. The authors use Aspen HYSYS for simulation of separation processes and apply the convergence matrix adaptation evolution strategy (CMA-ES) to optimise temperature and pressure values. Moreover, the authors have employed their optimization for test cases with different numbers of separation stages, with and without recycle streams. According to the presented results, three and four stage separation systems after applied optimization show potential variations in profit from

18024 dollars per day to 58898 dollars per day. However, proposed assumptions for calculation of utility costs are unrealistic for offshore separator systems to justify this research. This is because, the used prices of utilities are based on data from January 2014 while utility costs are changed with the price of exported oil and gas production. Therefore, more clear mathematical definition of utility costs is required for this research.

As can be seen from presented review of literature, the application of algorithms for optimisation of temperatures and pressures increases significantly the quantities of produced oil and gas. Hence, the profit of an offshore oil platform also can be increased.

4.2 Population-Based Optimization

Many real world optimisation problems, such as optimisation of separation processes, are large scale combinatorial and highly non-linear optimization problems. Furthermore, the search space of those problems increases exponentially with the problem size and can have many local maxima/minima. Therefore, the used algorithms have to guarantee that they will not easily get trapped in sub-optima and will explore the search space in a relatively short time [47].

Nowadays, population-based algorithms have been proposed and developed to tackle challenging real complex optimisation problems. Population-based algorithms are nature-inspired optimization methods that can be used as general solver for wide range of optimization problems. These algorithms are not problem or domain specific, and they are capable of locating good quality solutions in a relatively short time, compared to traditional optimization techniques [48] [49].

In the last few decades, a variety of population-based algorithms have been developed. Among the most widely used are differential evolution [50], adaptive differential evolution [51], genetic algorithm [52] and particle swarm optimisation [53]. Those algorithms have shown excellent search abilities but usually their performance may vary considerably according to the optimisation problem and their configuration settings. Furthermore, algorithm selection is even more challenging when needs to address it to multiple problems, such as a separation configuration which varied over the offshore oil platforms [54]. Therefore, selection of the most appropriate algorithm for our optimisation problem needs considerable time and required application of proposed above algorithms with the aim to compare their performance and results.

Differential evolution and adaptive differential evolution are part of population-based searching techniques. These algorithms process a population of individuals with the aim to search a problem domain. Here, each individual of the population represents a potential solution and the term generation represents an iteration of the search in which new solutions are produced and evaluated. Both algorithms maintain and successively improve solutions until some stopping condition is met. At the beginning, individuals are initialized randomly, and are improved iteratively at each generation. The quality of individuals is measured by a fitness function. Moreover, the quality of the solution returned by both algorithms over generations should improve monotonically. So, the fitness of the solution at time $t+1$ should be no worse than the fitness at time t [55]. The general procedure of both algorithms is given in Algorithm 1. More detailed information about the algorithms is provided in the following sections.

Algorithm 1 General procedure of differential evolution

```
Generate random solutions
Initialize all individuals in the population
Evaluate all initialized individuals
while the stopping criteria is not met do
    for all individuals in the population do
        Reproduce individuals for a new population
        Evaluate the fitness of each solution
        Select solutions with better fitness values
        Save improving solution in next population
    end for
end while
```

4.2.1 Differential Evolution Algorithm

Differential evolution (DE) was proposed by Storn and Price [50]. This is a simple and efficient population-based optimisation algorithm for global optimization over continuous spaces [50]. It has found increasing applications in a number of electrical engineering, economic and finance fields [56], [57], [58]. The main reason for the popularity of DE is because of easy applicability for many real problems where objective function is non-differentiable, non-linear, have many local minima/maxima, etc. Problems like these are difficult or even impossible to solve analytically. Therefore, DE is widely used to find the solution of such problems.

For a given an objective function $f(x)$, DE attempts to find the vector $X^* = (x_1, x_2, ..., x_D)$ for which $f(x)$ has minimum (or maximum) value over the D-dimensional space of real numbers $\Re^D$. So, DE constructs a population P_t with N_P individuals:

$$x_j{}^i = [x_{j1}{}^i, x_{j2}{}^i, ..., x_{jD}{}^i] \tag{4.1}$$

where $j = 1, 2, ..., N_p$ and j indicates the number of the individuals.

The main stages of DE are initialisation, mutation, crossover, selection and termination Figure 4.1. Firstly, over the initialisation P_O generation is formulated. After that in order to find the global optima a loop executes in sequence mutation, crossover and selection operations until termination condition is achieved. Each run of the loop generated new generation P_{i+1} based on old generation P_i. Termination conditions can be objective met, maximum number of evaluations or some other problem specific criteria. However, more often as a termination condition for real problems with unknown optimum is used a given maximum number of evolutions. For detailed information about mutation, crossover and selection operations is provided below.

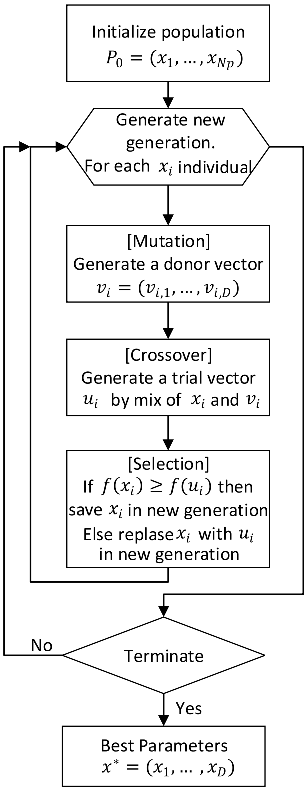


Fig. 4.1 Main stages of a differential evolution algorithm

Initialization

Initialization generates an initial population P_i, where $i = 0$, with N_p individuals. It begins with a uniform randomly initiated population of D-dimensional real-valued parameter vectors Equation 4.1 where for each parameter x^i_{jk} can be define lower and upper bounds:

$x_{k,low}, x_{k,upp}, k \in 1, ..., D$. The bounds are specified according to physical aspects of the problem. For example, the separator/scrubbers has a range of temperature and pressure which is permissible. So, there is no reason to generate temperatures which in the real life is impossible to be set due to the physical constraints of the equipment.

Mutation

According to the biology, mutation is the permanent alteration of the gene characteristics of a chromosome. In the context of the evolutionary optimisation, mutation is a perturbation with a random element and it allows to explore the search space.

Nowadays, various differential mutation strategies are proposed [59],[60]. The notation of mutation strategies used for DE is DE/x/y/z where x indicates the mutation base, y is the number of vector difference, and z indicates a type of the crossover [61]. Information about possible types of crossover is given in the following section. Although, there are a variety of mutation strategies there is no strategy which is the best for all optimisation problems. Some of the mutation strategies proposed by Storn and Price [62] are:

- *DE/rand/1/z*:
$$v_j{}^i = x_{r_1}{}^i + F(x_{r_2}{}^i - x_{r_3}{}^i) \tag{4.2}$$
- *DE/rand/2/z*:
$$v_j{}^i = x_{r_1}{}^i + F(x_{r_2}{}^i - x_{r_3}{}^i) + F(x_{r_4}{}^i - x_{r_5}{}^i) \tag{4.3}$$
- *DE/best/1/z*:
$$v_j{}^i = x_{best}{}^i + F(x_{r_1}{}^i - x_{r_2}{}^i) \tag{4.4}$$
- *DE/best/2/z*:
$$v_j{}^i = x_{best}{}^i + F(x_{r_1}{}^i - x_{r_2}{}^i) + F(x_{r_3}{}^i - x_{r_4}{}^i) \tag{4.5}$$
- *DE/target-to-best/1/z*:
$$v_j{}^i = x_j{}^i + F(x_{best}{}^i - x_j{}^i) + F(x_{r_1}{}^i - x_{r_2}{}^i) \tag{4.6}$$
- *DE/rand-to-best/1/z*:
$$v_j{}^i = x_{r1}{}^i + F(x_{r_2}{}^i - x_{r_3}{}^i) + F(x_{best}{}^i - x_{r_1}{}^i) \tag{4.7}$$

where $r_1, r_2, r_3, r_4, r_5 \in [1, 2, ..., N_p]$ are selected randomly for each donor vector, $v_j{}^i$, and the condition is met $r_1 \neq r_2 \neq r_3 \neq r_4 \neq r_5 \neq j$. The scaling factor F is a positive control parameter for scaling the difference vectors. ${x_{best}}^i$ is the best individual vector with the best fitness in the population P_i.

The classical DE proposed by Storn and Price [50] uses DE/rand/1/bin mutation strategy. In this strategy (Figure 4.2), for each target vector ${x_j}^i$, a donor vector ${v_j}^i$ is generated according to the following:

$${v_j}^i = {x_{r1}}^i + F * ({x_{r2}}^i - {x_{r3}}^i) \tag{4.8}$$

where $r_1, r_2, r_3 \in 1, 2, ..., N_p$ are selected randomly and the condition is met $r_1 \neq r_2 \neq r_3 \neq j$. Here, parameter F is a scalar factor, which is number used to control the length of the difference vector $({x_{r2}}^i - {x_{r3}}^i)$. According to Storn and Price [62], the range of F can be in a interval of [0,2] but strictly $F > 0$. However, in more recent work of Rönkkönen et al. [63] is suggested to use for F a positive real number that is typically less than 1.0.

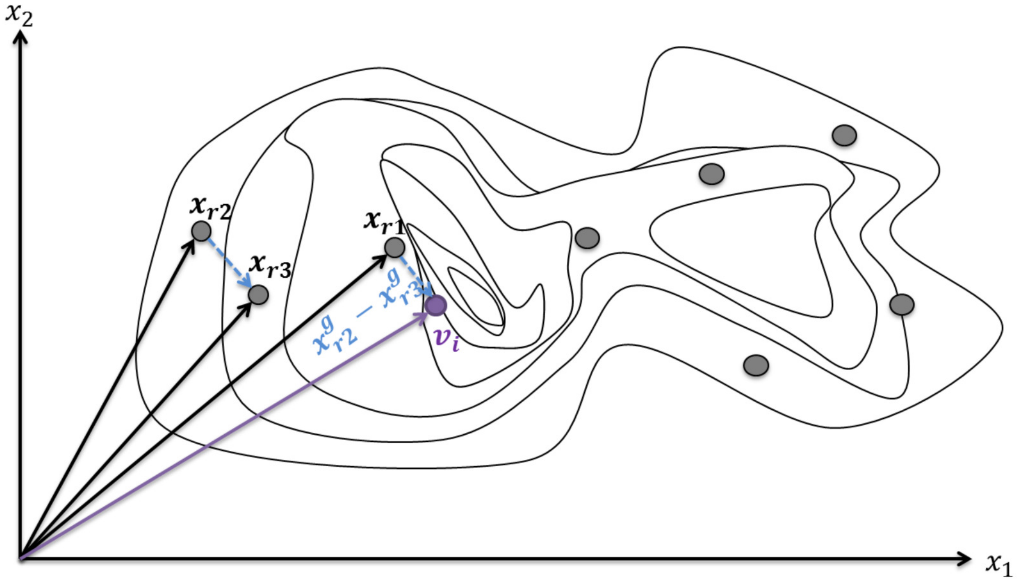


Fig. 4.2 Example of search space with differential mutation scheme of DE

Crossover

Crossover or recombination allows to incorporate successful individuals from the previous generation. DE has two main types of crossover, binomial (z=bin) and exponential crossover (z=exp).

In the binomial crossover, the target vector is mixed with the donor vector, using the following scheme, in order to obtain the trial vector ${u_j}^i$:

$$u_{jk}{}^{i} = \begin{cases} v_{jk}{}^{i}, & \text{if }, rand_{jk} \leq CR \text{ or } k = I_{rand} \\ x_{jk}{}^{i}, & \text{if }, rand_{jk} > CR \text{ and } k \neq I_{rand} \end{cases} \tag{4.9}$$

where $j = [1,2,...,N_p]$, $k = [1,2,...,D]$, $rand_{jk} \sim U[0,1]$ and I_{rand} is random integer from $[1,2,...,D]$. Here, I_{rand} ensure that $v_j{}^i \neq x_j{}^k$. Algorithm 2 presents pseudo-code of the binomial crossover. The crossover rate (CR) is set by the user and controls which and how many components are mutated in each element of the current population.

Algorithm 2 Binomial Crossover

```
$I_{rand}$ = rand(D)
$k = 0$
while $k < D$ do
    if $rand(0,1) \leq Cr$ or $k = I_{rand}$ then
        $u_{j,k} = v_{j,k}$
    else
        $u_{j,k} = x_{j,k}$
    end if
    $k = k+1$
end while
```

In exponential crossover (Algorithm 3), firstly the starting position of crossover is chosen randomly from $1,...,D$ and after that L successive elements are taken from the donor vector, u_j. Probability of replacing the k-th element in the sequence 1, 2, . . . ,L, $L \leq d$, decreases exponentially with increasing k [64].

Algorithm 3 Exponential Crossover

```
$u_j{}^i = x_j{}^i$, $k$ is randomly selected from [1, D], L = 1;
while rand[0,1) < CR and L < D do
    $u_{j,k}{}^i = v_{j,k}{}^i$
    $k = (k+1)$ modulo $D$
    $L = L+1$
end while
```

Selection

DE apply a greedy selection scheme which mimics survival-of-the-fittest. Here, calculation of the fitness function for vector $u_j{}^i$ is performed firstly. After that, if the fitness value $f(u_j{}^i)$ is better than the fitness value of $f(x_j{}^i)$, then $u_j{}^i$ is set to $x_j{}^{i+1}$. Otherwise, the old vector $x_j{}^i$ is set to $x_j{}^{i+1}$, i.e. the old vector is saved in new generation.

$$x_j{}^{i+1} = \begin{cases} u_j{}^i, & \text{if } , f(u_j{}^i) \leq f(x_j{}^i) \\ x_j{}^i, & \text{Otherwise} \end{cases} \tag{4.10}$$

4.2.2 Adaptive Differential Evolution Algorithm (JADE)

Differential evolution has been developed as a simple, fast and easy to use algorithm for wide range of real world optimisation problems. One the one hand, there are only a few parameters which have to be set (the population size (N_p), mutation strategy, crossover type, scalar factor F and crossover rate CR) but on the other hand, the efficiency and results of DE are very sensitive to these parameters [65]. According to Tvrdik [64], the most valuable parameters for the DE are the scalar factor F and the crossover rate CR. Unfortunately, the finding of an appropriate set of DE control parameters required a trial-error tuning for each particular problem which is time consuming and not adapted to problem with dynamic features.

Nowadays, adaptive and self-adaptive DE algorithms are developed with the aim dynamically to find the control parameters without prior knowledge of the problem and exclude the trial-error tuning of control parameters. A brief summary of the key features of some adaptive DE algorithms (SaDE [66],SaNSDE [67], jDE [68] and JADE [51]) is provided in Table 4.1 [69].

Table 4.1 Summary of key features of different adaptive DE algorithms

Algorithm	Features
SaDE	Mutation strategies: DE/rand/1 & DE/current-to-best/2 F: Gaussian randomization CR: Gaussian randomization & parameter adaptation
SaNSDE	Mutation strategies: DE/rand/1 & DE/current-to-best/2 F: Gaussian & Cauchy randomization CR: Gaussian randomization & parameter adaptation
jDE	Mutation strategy: DE/rand/1 F: Uniform randomization & adaptation CR: Uniform randomization & parameter adaptation
JADE	Mutation strategy: Archive-assisted DE/current-to-pbest/1 or DE/rand-to-pbest/ F: Cauchy randomization & adaptation CR: Gaussian randomization & parameter adaptation

According to Zhang and Sanderson [51] and their results, JADE has been tested on a set of classic benchmark functions and shows better optimisation performance compared to other adaptive algorithms and even the canonical PSO algorithm. Therefore, for the purpose of this research as a initial stage of evaluating adaptive DE algorithms, it has been decided to try the JADE algorithm for optimisation of offshore separation systems.

The stages and sequence of JADE are the same as for the classic DE (Figure 4.1). The main difference between DE and JADE is in the way of how the control parameters F and CR are found and entered. These parameters in the DE are determined by trial-error tuning and entered by the user while in JADE they are controlled by the adaptive parameters μ_F and μ_{CR}. However, JADE introduces two new parameters c and p. According to Zhang and Sanderson [51] JADE parameter c is used to determinate the adaptation rates of μ_F and μ_{CR} while p determines the greediness of the mutation strategy.

According to the authors, the adaptation of μ_F is based on the principle that better control parameter values tend to generate individuals that are more likely to survive and thus these values should be propagated to the following generations. Therefore, the operation used for adaptation of μ_F is to record recent successful crossover probabilities and use them to guide the generation of new CR_i. At the same time, the authors use two other principles of adaptation of μ_F. Firstly, F_i are generated according to a truncated Cauchy distribution which is is more helpful to diversify the mutation factors and thus avoid premature convergence. Secondly, the adaptation of μ_F places more weight in larger successful mutation factors by using the Lehmer mean which improves the progress rate. Here, it is important to note that if constant $c = 0$ there is no parameter adaptation. Otherwise, the life span of a successful CR_i or F_i is roughly $1/c$ generations. That means that after $1/c$ generations, the old values of μ_F or μ_{CR} is reduced. Parameters c and p are problem insensitive according to their roles in JADE. However, authors mention that it is still interesting to find a range of these parameters which is appropriate for different problems. In their paper, authors expect that a small value of $1/c$ or p may lead to less satisfactory results in some cases. However, suggested value for c and p are $c = 0.1$ and $p = 0.05$.

Additionally, JADE introduces a new strategy (DE/current-to-pbest/1) with two modifications. The first one (equation 4.11) is used when the archive option of JADE is not employed while the second strategy is used (equation 4.12) when the archive option is employed.

$$v_i{}^G = x_i{}^G + F_i * (x_{p,best}{}^G - x_i{}^G) + F_i * (x_{r1}{}^G - x_{r2}{}^G) \tag{4.11}$$

where $x_{p,best}{}^G$ is randomly chosen as one of the top $100p\%$ individuals in population G.

$$v_i{}^G = x_i{}^G + F_i * (x_{p,best}{}^G - x_i{}^G) + F_i * (x_{r1}{}^G - \hat{x_{r2}}{}^G) \tag{4.12}$$

where all parameters are the same as in equation 4.11 except the parameter $\hat{x_{r2}}^G$ which is randomly chosen from the union $P \cup A$. Here, P denotes the current population while A denotes archive of the parent individuals which are failed in the selection operation.

The scalar factor F_i, for both modification of DE/current-to-pbest/1, is associated with individual x_i and it is calculated in accordance with a Cauchy distribution with parameter μ_F and scale parameter 0.1 and then truncated to $[0,1]$ (equations 4.13 and 4.14).

$$F_i = rand_{ci}(\mu_F, 0.1) \tag{4.13}$$

where adaptive parameter μ of the Cauchy distribution is initialized to be 0.5 and then updated at the end of each generation (equation 4.14).

$$\mu_F = (1-c) * \mu_F + c * mean_L(S_F) \tag{4.14}$$

where $mean_L(S_F)$ is the Lehmer mean of S_F (equation 4.15) which is the set of all successful mutation factors in generation G.

$$mean_L(S_F) = \frac{\sum_{F \in S_F} F^2}{\sum_{F \in S_F} F} \tag{4.15}$$

Finally, JADE provides equations 4.16 and 4.17 for calculation of the crossover rate CR. Here, each calculated crossover rate CR_i for each individual x_i is independently generated in accordance with a normal distribution of mean μ_{CR} and standard deviation 0.1 and then truncated to $[0,1]$.

$$CR_i = rand_{ci}(\mu_{CR}, 0.1) \tag{4.16}$$

$$\mu_{CR} = (1-c) * \mu_{CR} + c * mean_L(S_{CR}) \tag{4.17}$$

where $mean_L(S_{CR})$ is the Lehmer mean of S_{CR} (similar to equation 4.15) which is the set of all successful crossover rates in generation G.

4.3 Formulation of the optimisation problem

Offshore oil platform separation processes typically consist of a network of m vessels organised in two sequences of l separators $S = (s_1, ..., s_l)$ and k scrubbers $Scrub = (scrub_1, ..., scrub_k)$. Those vessels are linked together by pipes and the hydrocarbons flow through the system of vessels eventually (Figure 2.1). The vessels essentially split the hydrocarbon feed into two phases (oil and gas) and may decant free water also as a second liquid phase. Because of the limitations of weight and size of equipment used in offshore oil platforms typically two-stage (Figure 4.3a), three-stage (Figure 4.3b) or four-stage (Figure 4.3c) separation processes are used, the number of stages corresponding to the number of separators. The $m = l + k$ vessels operates at given temperatures $T = (t_1, ..., t_m), T \in \Re^m$ and pressure $P = (p_1, ..., p_m), P \in \Re^m$.

Separation simulations generally use flash calculation [11] which, for each vessel and given feed streams of n hydrocarbon components $Z = (z_1, ..., z_n)$ determines the resulting gas (or vapour) $V = (v_1, ..., v_n)$ and oil (or liquid) $L = (l_1, ..., l_n)$ which would be achieved at specific temperature and pressure conditions.

4.3.1 Objective function

The above-mentioned industrial process of offshore oil and gas separation can be formulated as an optimisation problem where the objective is to maximise the profitability of the platform and the decision variables are the temperature and pressure of the separation vessels.

A separation problem is defined by:

- A separator diagram (Figures 4.3a, 4.3b, 4.3c): which defines the network of m separators and scrubbers, the feed streams from wells, the oil and gas export stream and the connections and recycle streams between each separators.
- The composition of the input mixtures from each well.
- The market value of each components:
  - $V_O = (v_{O1}, ..., v_{On})$ is the price of each hydrocarbon in \$/tonne
  - $CV_G = (cv_{G1}, ..., cv_{Gn})$ is the calorific energy of each hydrocarbon in GJ/tonne
  - E_{GAS} is the gas price in \$/GJ

The decision variables as described above are:

$$x = \{x_1, ..., x_i, ..., x_m, ..., x_{m+i}, ..., x_{2m}\} \tag{4.18}$$

The temperature and pressure of each separator and scrubber i is then defined by $(t_i, p_i) = (x_i, x_{m+i})$

Given a problem definition, the object is to maximise the profitability of the platform by maximising the market values of the export oil and gas and minimising the operating costs of the offshore separation process.

Market value maximisation

From the composition of the feed streams from wells and the value of each component in each phase, it is possible to calculate the *maximum theoretical value* (MTV). It is obtained by calculating the value of each component feed in the system in its most valuable form.

The first objective is thus to minimise the market loss:

$$L(x) = MTV - (S_{oil}(x) + S_{gas}(x)) \tag{4.19}$$

where, given the output oil $O = (o_1, ..., o_n)$ and gas $G = (g_1, ..., g_n)$ tonnages obtained in conditions x, $S_{oil}(x) = \sum_{i=1}^{n} v_{Oi} o_i$ and $S_{gas}(x) = \sum_{i=1}^{n} cv_{Gi} g_i E_{GAS}$

Utility cost minimisation

The second objective is to minimise the utility costs (C) as the sum of compressors (C_{comp}), heaters (C_{heat}) and coolers (C_{cool}) costs:

$$C(x) = C_{comp}(x) + C_{heat}(x) + C_{cool}(x) \tag{4.20}$$

The calculations of utility costs (or operation costs) for offshore [70] and onshore [71] oil production are different.

Utility cost for all r compressors, in USD per day, can be calculated as an expression of mass, in tonne, of gas fuel ($FGm_{comp,i}$) which is used by compressor i per day.

$$C_{comp}(x) = E_{GAS} \times \sum_{i=1}^{r} FGm_{comp,i}(x) \tag{4.21}$$

$$FGm_{comp,i}(x) = 9.79 \times 10^{-3} M_{gas} T \left(\left(\frac{P_{out}}{P_{in}} \right)^{0.28} - 1 \right) \tag{4.22}$$

where

- M_{gas} - mass [tonne/day] of the stream which is passed by the compressor i
- T - temperature [K] of the stream which is passed by the compressor i
- P_{in} - pressure [Pa] of the stream before to enter into the compressor i
- P_{out} - pressure [Pa] of the stream after the compressor i

Utility cost for all h heaters, in USD per day, can be calculated as an expression of mass, in tonne, of gas fuel ($FGm_{heat,i}$) which is used by heater i per day.

$$C_{heat}(x) = E_{GAS} \times \sum_{i=1}^{h} FGm_{heat,i}(x) \tag{4.23}$$

$$FGm_{heat,i}(x) = 6.5372 \times 10^{-3} M_{gas}(T_{out} - T_{in}) \tag{4.24}$$

where:

- M_{gas} - mass [tonne/day] of the stream which is passed by the heater i
- T_{in} - temperature [K] of the stream before to enter into the heater i
- T_{out} - temperature [K] of the stream after the heater i

Utility cost for all s coolers, in USD per day, can be calculated as an expression of mass, in tonne, of gas fuel ($FGm_{cool,i}$) which is used by cooler i per day.

$$C_{cool}(x) = E_{GAS} \times \sum_{i=1}^{s} FGm_{cool,i}(x) \tag{4.25}$$

$$FGm_{cool,i}(x) = 6.94833 \times 10^{-5} M_{gas}(T_{in} - T_{out}) \tag{4.26}$$

where

- M_{gas} - mass [tonne/day] of the stream which is passed by the cooler i
- T_{in} - temperature [K] of the stream before to enter into the cooler i
- T_{out} - temperature [K] of the stream after the cooler i

As both objectives aim at maximising the profit, we formulate this problem as a single objective optimisation problem:

$$\min_{x} F(x) = L(x) + C(x) \tag{4.27}$$

It corresponds to the difference between the theoretical value of the extracted hydrocarbon and the actual profit that is generated from the separation process.

4.3.2 Constraints

Constraints in this work are separated into two categories: pre-simulation constraints, which can be tested before running the simulation (the most computationally expensive part of an evaluation) and post-simulation constraints.

Pre-simulation constraints

The design variables for optimisation of separation processes are temperatures and pressures of separators and scrubbers. All provided constraints here are related with the values that can be used for these variables. These are physical constraints that correspond to infeasible conditions. There are not any constraints for the search space of temperatures and the amount of the temperature value. However, in order to reduce the search space of temperatures we have used values ranging from 273K to 363K. This range is used because those temperatures are supported by the most types of separators and scrubbers and there is no reason to search for temperatures which are not supported by separation systems. However, there are more constraints for the different pressure values applied to the separators and scrubbers:

- The pressure of a separator whose input stream is a well must be inferior to the pressure of the well.
- The pressure between two separators i and j can only drop ($p_i > p_j$) if separator i is the direct predecessor of separator j. Likewise, the difference between those two separators cannot be more than $\Delta = 0.2 \times 10^5 Pa$, $p_i - p_j > \Delta$.
- Pressure between two scrubbers i and j can only rise ($p_i < p_j$) if scrubber i is a direct predecessor of scrubber j. Likewise, the difference between those two scrubbers cannot be more than $\theta = 3.5$ times, $\theta p_i < p_j$.
- The pressure of the export gas, which is given by the pressure of the last scrubbers in the line must be superior or equal to the gas export pressure (GEP).
- There are no constraints related to the value of the pressure. However, there is no a reason to search for pressure's value which physically is not supports by the separators or scrubbers. Therefore, in our constraints we have used values ranging from 14.50 to 2300 psia for pressures. This range is used with the aim to reduce the search space of pressures. Nevertheless, the range can be change if there is a separator/scrubber which supports lower or higher pressures.

Post-simulation constraints

Check true vapor pressure (TVP [43]) which guarantees that exported oil production for given exported temperature and pressure ensures only liquid phase of exported production. That means that quantity of exported oil will not change during transportation. In order to check TVP it is necessary to run the flash algorithm with exported oil production for a given exported temperature and pressure. If the flash algorithm calculates a vapour-feed ratio which equals to 0, then the TVP criteria is met. Otherwise, TVP criteria is not met and post-simulation constraints are broken. Check true vapor pressure (TVP [43]) which guarantees that exported oil production for given exported temperature and pressure ensures only liquid phase of exported production. That means that quantity of exported oil will not change during transportation. In order to check TVP it is necessary to run the flash algorithm with exported oil production for given exported temperature and pressure. If the flash algorithm calculates vapour-feed ratio equal to 0, then the TVP criteria is met. Otherwise, TVP criteria is not met and post-simulation constraints are broken.

Constraint handling

In order to avoid the simulation of infeasible solutions, we first check if the pre-simulation constraints are broken. If they are, they are automatically discarded.

Post-simulation constrains can be check only after completion of the whole simulation. This is because in order to validate TVP criteria is required to know the quantity of exported oil production which is a result of the simulation.

4.4 Experimental setup

In this section, we explain the method used to tackle this problem. First we describe the representation used to encode the temperature and pressures of each separator. We then describe the Differential Evolution algorithms and its components used. Finally, we present the test cases used for the experiments.

4.4.1 Representations

As most of the constraints are related to the pressure relations between subsequent separators and scrubbers, our representation encodes the pressure difference between a separator and the pressures of its predecessors in the network. To do so, the pressure values or set one after the other according to the pressures of its inlet streams following the rules dictated by the constraints. Therefore, in order to represent the temperatures (T) and pressures (P) of each separator, we use constructive representation where a solution is represented by $x = (x_1, x_2, ... x_{2m})$ (equation 4.18) where $x_i \in [0,1]$ and $t_i = x_i(T_{max} - T_{min}) + T_{min}$ and $p_i = x_{(m+i)}(P_{max\_allowed} - P_{min\_allowed}) + P_{min\_allowed}$. Here, the minimum, $P_{min\_allowed}$, and the maximum, $P_{max\_allowed}$, allowed pressures are calculated according to the constraints defined in the previous section. The values of the minimum, T_{min}, and the maximum, T_{max}, temperature are defined for all separators and scrubbers.

The idea of the constructive representation is to prevent the pre-simulation constraints to be broken and encode directly in the solution the effect of the compressors (increasing the pressure) and valves (decreasing the pressure).

4.4.2 Application of Differential Evolution

To tackle this problem, in our work, we use the original version of the algorithm proposed by Storn et Al [62]. There are a few main reasons for our choice to use the original version of DE instead of more recent works. First of all, DE is one the most popular metaheuristic for solving single objective global optimisation problems [72]. Its efficiency has been proven in several work. Secondly, the original version of DE is well described and easy and fast for software implementation. Moreover, considering that the scope of this research is to formulate optimisation problem for offshore separation processes and investigate application of population based algorithms for the formulated problem, the classical version of DE is an ideal candidate for it. The general DE algorithm we use is described in Algorithm 4.

The initialization has been slightly modified in order to ensure that the initial population is only composed of feasible solutions.

The parameters scale factor F and crossover rate Cr are generated for each individual with a normal distribution $N(\mu_F, \sigma_F)$ and $N(\mu_{Cr}, \sigma_{Cr})$. In our experiments, all pairs with combinations of values $\mu_F = (0.1, 0.5, 0.9)$ and $\mu_{Cr} = (0.1, 0.5, 0.9)$ are tested. Also, in our tests the following parameters are fixed: $N_p = 20$ (population size), $\sigma_F = 0.3$ and $\sigma_{Cr} = 0.1$.

We assess here five different mutation strategies DE/rand/1/bin (equation 4.2), DE/rand/2/bin (equation 4.3), DE/best/1/bin (equation 4.4), DE/best/2/bin (equation 4.5) and DE/target-to-best/1/bin (equation 4.6).

The former encourage exploration of the search space while the latter forces the population to converge towards the best solution.

4.4.3 Application of Adaptive Differential Evolution (JADE)

To tackle this problem, we use JADE adaptive differential evolution. In our work, we use the original version of JADE proposed by Zhang and Sanderson [51]. The general JADE algorithm we use is described in Algorithm 5.

The initialization for JADE is as for DE, i.e. it is modified in order to ensure that the initial population is only composed of feasible solutions.

The parameters $c = 0.1$, $p_{best} = [0.05, 0.1, 0.2]$ and mutation strategy JADE/current-to-pbest/1/bin(equation 4.11) are used based on recommendation provided for JADE [51]. Here, as in the case of DE the population size is N_p=20.

Algorithm 4 Pseudo-code for Differential Evolution on the separation optimisation problem

```
$POP = \emptyset$
while $|POP| < NP$ do
    Generate random solution $x$
    if $F(x) \neq +\infty$ (no broken constraints) then
        $POP = POP \cup x$
    end if
end while
while not reached max number of simulation do
    for each individual $x_i$ POP do
        $F_i = N(\mu_F, \sigma_F)$
        Generate mutation vector $v_i$ with $F_i$
        $Cr = N(\mu_{Cr}, \sigma_{Cr})$
        binomial crossover : $u_{i,j} = v_{i,j}$ if $rand(0,1) < Cr$
        if $F(u_i) < F(x)$ then
            $x_i = u_i$
        end if
    end for
end while
```

Algorithm 5 Pseudo-code for JADE on the separation optimisation problem

```
$POP = \emptyset$
$\mu_{CR} = 0.5$ and $\mu_F = 0.5$
while $|POP| < NP$ do
    Generate random solution $x$
    if $F(x) \neq +\infty$ (no broken constraints) then
        $POP = POP \cup x$
    end if
end while
while not reached max number of simulation do
    $S_F = \emptyset$ and $S_{CR} = \emptyset$
    for each individual $x_i$ POP do
        $CR_i = randn_i(\mu_{CR}, 0.1)$ and $F_i = randc_i(\mu_F, 0.1)$
        Generate mutation vector $v_i$ with $F_i$
        binomial crossover : $u_{i,j} = v_{i,j}$ if $rand(0,1) < Cr$
        if $F(u_i) < F(x)$ then
            $x_i = u_i$ and $CR_i \rightarrow S_{CR}$ and $F_i \rightarrow S_F$
        end if
    end for
    $\mu_{CR} = (1-c) * \mu_{CR} + c * mean_A(S_{CR})$ and $\mu_F = (1-c) * \mu_F + c * mean_L(S_F)$
end while
```

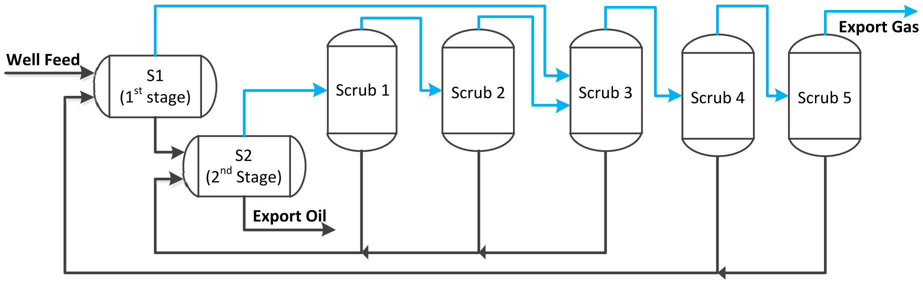
Table 4.2 Hydrocarbon mixtures and molar fractions for each wells

Two-stage separation		Three-stage separation					Four-stage separation	
Hydrocarbon	Well	Hydrocarbon	Well A1	Well A2	Well B	Well C	Hydrocarbon	Well
Nitrogen	8.95E-4	Nitrogen	0.00E+0	1.87E-3	1.24E-3	1.42E-3	Nitrogen	1.65E-3
CO2	1.01E-3	CO2	0.00E+0	7.04E-3	1.02E-2	5.36E-3	CO2	1.91E-2
Methane	3.06E-2	Methane	3.57E-2	3.38E-2	1.24E-1	9.04E-2	Methane	1.01E-1
Ethane	8.82E-3	Ethane	1.67E-2	1.84E-2	3.69E-2	3.21E-2	Ethane	2.60E-2
Propane	2.65E-2	Propane	2.45E-2	2.17E-2	3.50E-2	2.86E-2	Propane	3.39E-2
i-Butane	8.27E-3	i-Butane	0.00E+0	3.87E-3	8.56E-3	7.88E-3	i-Butane	8.54E-3
n-Butane	3.10E-2	n-Butane	2.15E-2	1.63E-2	2.39E-2	1.95E-2	n-Butane	2.50E-2
i-Pentane	1.39E-2	i-Pentane	1.34E-2	7.69E-3	1.18E-2	1.02E-2	i-Pentane	1.38E-2
n-Pentane	2.17E-2	n-Pentane	1.34E-2	1.35E-2	1.65E-2	1.61E-2	n-Pentane	1.51E-2
n-Hexane	2.41E-2	n-Hexane	1.60E-2	2.30E-2	2.47E-2	2.88E-2	C6*	2.65E-2
Mcyclopentane	8.61E-3	n-Heptane	3.71E-2	3.87E-2	2.13E-2	3.33E-2	C7*	4.08E-2
Benzene	9.40E-4	n-Octane	4.23E-2	4.41E-2	2.60E-2	3.71E-2	C8*	5.02E-2
Cyclohexane	9.93E-3	n-Nonane	4.75E-2	3.76E-2	2.41E-2	3.22E-2	C9*	4.43E-2
Mcyclohexane	1.77E-2	Mcyclopentan	0.00E+0	0.00E+0	4.96E-3	0.00E+0	C10-14*	1.63E-1
Toluene	5.45E-3	Benzene	0.00E+0	0.00E+0	2.81E-3	4.53E-3	C15-20*	1.52E-1
E-Benzene	3.13E-3	Cyclohexane	0.00E+0	0.00E+0	6.75E-3	1.74E-2	C21-29*	1.51E-1
p-Xylene	1.11E-2	Mcyclohexane	0.00E+0	0.00E+0	1.06E-2	0.00E+0	C30+*	1.28E-1
135-MBenzene	4.19E-3	Toluene	0.00E+0	0.00E+0	4.53E-3	6.74E-3		
n-Heptane	2.28E-2	E-Benzene	0.00E+0	0.00E+0	1.74E-3	0.00E+0		
n-Octane	2.59E-2	m-Xylene	0.00E+0	0.00E+0	5.21E-3	0.00E+0		
n-Nonane	2.11E-2	o-Xylene	0.00E+0	0.00E+0	2.09E-3	0.00E+0		
C10-C12*	1.20E-1	124-MBenzene	0.00E+0	0.00E+0	2.36E-3	0.00E+0		
C13-C14*	4.85E-2	C10+*	7.32E-1	7.32E-1	5.94E-1	6.28E-1		
C15-C16*	9.12E-2							
C17-C19*	6.47E-2							
C20-C22*	9.15E-2							
C23-C26*	7.08E-2							
C27-C32*	7.41E-2							
C33-C40*	7.41E-2							
C41-C80*	6.73E-2							

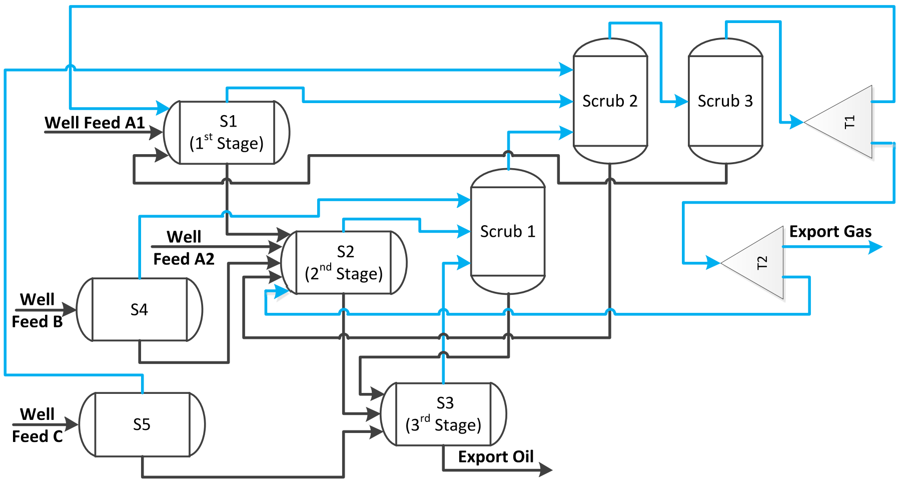
4.4.4 Test cases

For the purpose of this research three case studies are used. Those cases are typical systems in offshore oil and gas platforms. The two and three stages systems (Figure 4.3a and 4.3b) are provided by Accord-ESL and the four-stage system (Figure 4.3c) was taken from [46]. It is important to note, that the number of stages in a separation process relates to the number of separator on which action can be taken. Therefore, the last test case is a four-stage system although there are five separators. In addition, all provided cases have recycle streams which improve oil recovery.

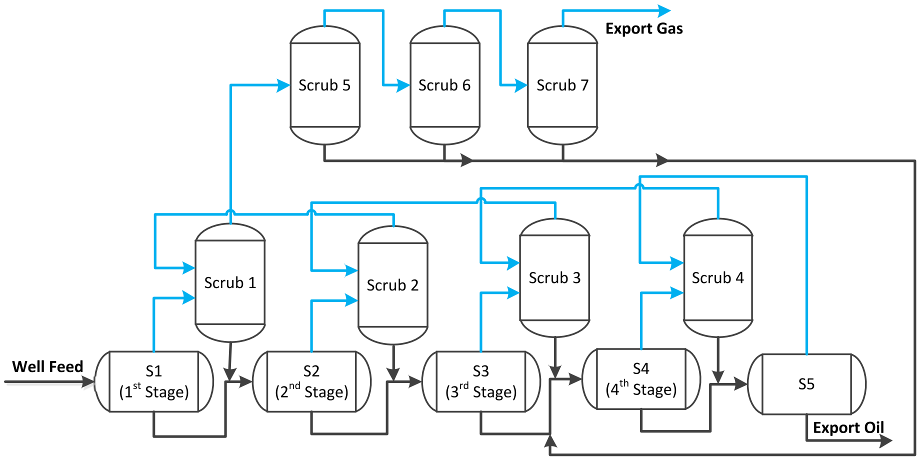
All study cases are real systems with their own specific hydrocarbon mixture. Hydrocarbon components and their molar fractions which are used in each of study cases are given in Table 4.2.



(a) Two-stage separation diagram



(b) Three-stage separation diagram



(c) Four-stage separation diagram

Fig. 4.3 Separation diagrams

Additionally, each of those cases has its own requirements for the temperature and pressure of exported production which is given in Table 4.3. For instance, as oil is transported by pipelines, three-stage separation process requires pressure of exported oil to be around 3.8×10^6 Pa.

We assume that every separator and scrubber is equipped with all the supporting equipment necessary to control their parameters. Separators are equipped with valves to decrease the pressure and scrubbers are equipped with a compressor to increase pressure. The temperature of all vessels is controlled by coolers and heaters.

4.5 Results

In this section, we present the results obtained by application of DE and JADE. We analyse the influence of each settings of these algorithms and the financial impact of the optimisation. All results showed here are the average over 25 independent runs.

4.5.1 Comparison of DE configuration settings

Here we compare the average final fitness for each test case and each set of configuration settings for DE algorithm. The results of two-stage separation are shown in Table 4.4, three-stage separation in Table 4.6 and four-stage separation Table 4.8. As can be seen from the tables, the best settings for each test case from Section 4.4.4 are the following:

- Two-stage separation - DE/rand/2/bin, $F = 0.5$ and $CR = 0.9$.
- Three-stage separation - DE/rand/2/bin, $F = 0.5$ and $CR = 0.9$.
- Four-stage separation - DE/best/2/bin, $F = 0.5$ and $CR = 0.5$.

Independent-samples t-test is used in order to determine whether there is a statistically significant difference between the means of the configuration settings of DE. Defined for the t-test a null hypothesis is that there is no difference between the compared configuration settings. Also, the Bonferroni-Holm method is used to counteract the problem of multiple comparisons.

Table 4.3 Export oil and gas requirements

Parameter	Two-stage	Three-stage	Four-stage
Oil Export Pressure	101325 Pa	380325 Pa	117210 Pa
Oil Export Temperature	288.15 K	288.15 K	288.15 K
Gas Export Pressure	6617531 Pa	5423325 Pa	18857161. Pa

The results from all t-tests and employed Bonferroni-Holm method are presented in Table 4.5 for two-stage, Table 4.7 for three-stage and Table 4.9 for four-stage separation.

As can be seen from Table 4.5 for two-stage separation, t-tests for all DE configurations reject the null hypothesis. However, for three-stage (Table 4.7) and four-stage separation (Table 4.9) there are a few DE configurations for which we fail to reject the null hypothesis. So, for those cases our data does not provide statistically significant evidence in the difference of the means. On the cases where statistical significance was not reached, the standard deviation was very high in comparison with other cases. So, there are some DE configurations that correlates with a high variation in results.

4.5.2 Comparison of JADE configuration settings

Here we compare the average final fitness for each test case after application of JADE. Here, only the adaptive parameter p is tuned. The results of two-stage separation are shown in Table 4.10, three-stage separation in Table 4.12 and four-stage separation Table 4.14. As can be seen from the tables, the best settings for each test case from Chapter 4.4.4 are following:

- Two-stage separation - DE/target-to-pbest/1/bin and $p = 0,1$.
- Three-stage separation - DE/target-to-pbest/1/bin and $p = 0.1$.
- Four-stage separation - DE/target-to-pbest/1/bin and $p = 0.05$.

Independent-samples t-test and Bonferroni-Holm method are applied to the different configuration settings of JADE. Here, the null hypothesis is the same as for DE. The obtained results are presented in Table 4.11 for two-stage, Table 4.13 for three-stage and Table 4.15 for four-stage separation.

As can be seen from provided tables we fail to reject the null hypothesis for two, three and four-stage separation system. So, for those cases our data does not provide statistically significant evidence in the difference of the means. One of the reason to fail the null hypothesis is the sample size which is 25.

4.5.3 Comparison and Impact of DE and JADE for Offshore Oil Optimisation

The comparison of the best configuration setting of DE and JADE, for each test case from Section 4.4.4), is provided on Table 4.16 and Figures 4.4 (Two-stage separation), 4.5 (Three-stage separation) and 4.6 (Four-stage separation). Also, the results are plotted with the

Table 4.4 DE optimisation results for two-stage separation

Strategy	F	Cr	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
rand2	0.5	0.9	41433.902	618.6244519	10109024.63	29623.71
target-to-best1	0.9	0.9	42360.572	1159.572161	10108097.96	30276.51
best2	0.5	0.5	42592.660	900.7612022	10107865.87	30624.81
rand1	0.9	0.9	42643.146	1181.627672	10107815.38	30654.22
target-to-best1	0.5	0.5	42825.181	1165.119942	10107633.35	30754.83
best2	0.5	0.9	43145.831	1726.597041	10107312.70	31209.71
best1	0.9	0.5	43300.355	913.4587521	10107158.18	31032.14
target-to-best1	0.9	0.5	43402.631	961.5176361	10107055.90	31377.67
rand1	0.5	0.5	43614.570	957.0601582	10106843.96	31443.08
best1	0.5	0.5	44094.449	1827.037853	10106364.08	31757.42
best1	0.9	0.9	44663.980	2386.261403	10105794.55	32145.70
rand2	0.5	0.5	44788.227	607.125588	10105670.30	32632.05
rand1	0.5	0.9	44798.843	1458.196444	10105659.69	32197.41
target-to-best1	0.5	0.1	44907.579	1058.114793	10105550.95	32518.66
best2	0.9	0.9	44973.570	1184.499241	10105484.96	32644.64
best1	0.5	0.1	45017.922	988.2611632	10105440.61	32754.59
rand1	0.9	0.5	45090.768	895.5988612	10105367.76	33135.10
best2	0.5	0.1	45293.921	1060.797699	10105164.61	33204.49
best1	0.9	0.1	45364.429	1280.051549	10105094.10	33429.89
best2	0.9	0.5	45447.394	758.6967885	10105011.14	33369.46
best1	0.5	0.9	45468.943	2229.969994	10104989.59	32983.41
target-to-best1	0.9	0.1	45585.816	1278.551337	10104872.72	33598.85
rand2	0.1	0.1	45695.566	892.1108466	10104762.97	33084.57
rand1	0.1	0.1	45729.482	868.8127295	10104729.05	33028.86
rand1	0.5	0.1	45741.228	1201.858327	10104717.30	33334.79
rand2	0.5	0.1	45749.460	1058.368049	10104709.07	33864.05
rand1	0.9	0.1	45786.918	1008.332824	10104671.61	33462.79
rand2	0.9	0.1	46029.592	1109.428511	10104428.94	33827.35
best2	0.9	0.1	46296.989	1542.179962	10104161.54	34047.73
best2	0.1	0.1	46452.688	2018.613469	10104005.84	33452.28
rand2	0.1	0.5	46714.329	1709.202661	10103744.20	33048.25
rand2	0.9	0.5	47024.193	1162.915926	10103434.34	35069.93
rand1	0.1	0.5	47155.238	1616.307178	10103303.29	33071.70
best1	0.1	0.1	47199.518	1938.121159	10103259.01	33612.80
rand2	0.9	0.9	47215.407	1192.310124	10103243.12	35158.13
target-to-best1	0.1	0.1	47644.159	1508.384335	10102814.37	33710.33
target-to-best1	0.5	0.9	48494.090	1786.778836	10101964.44	34434.88
target-to-best1	0.1	0.5	49167.364	1653.493472	10101291.17	35115.50
best2	0.1	0.5	49174.622	2956.627603	10101283.91	34750.89
best1	0.1	0.5	50567.911	2992.099287	10099890.62	36227.62
target-to-best1	0.1	0.9	53208.029	3069.494987	10097250.50	38432.32
rand2	0.1	0.9	53442.594	3222.653024	10097015.94	38399.68
best2	0.1	0.9	54164.597	3470.672852	10096293.93	39016.08
rand1	0.1	0.9	55167.753	3295.973229	10095290.78	39538.90
best1	0.1	0.9	55400.951	4451.056104	10095057.58	40531.81

Table 4.5 DE decision for the null hypothesis of two-stage separation

The Best Configuration (Reference) - rand2 F=0.5 Cr=0.9						
DE Configuration			T-Test		Bonferroni-Holm	
Strategy	F	Cr	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
target-to-best1	0.9	0.9	TRUE	0.00116	TRUE	0.00116
best2	0.5	0.5	TRUE	0.00000	TRUE	0.00002
rand1	0.9	0.9	TRUE	0.00005	TRUE	0.00010
target-to-best1	0.5	0.5	TRUE	0.00000	TRUE	0.00002
best2	0.5	0.9	TRUE	0.00003	TRUE	0.00010
best1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.5	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.9	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
best2	0.5	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.5	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000

Table 4.6 DE optimisation results for three-stage separation

Strategy	F	Cr	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
rand2	0.5	0.9	19024.313	9.866568784	1728808.72	11767.38
best2	0.5	0.5	19068.918	44.8428636	1728764.11	11862.09
target-to-best1	0.9	0.5	19087.783	34.40063386	1728745.25	11885.22
rand1	0.5	0.5	19097.565	49.84276975	1728735.46	11882.50
rand1	0.9	0.9	19101.294	189.2092816	1728731.74	11907.10
best2	0.5	0.9	19129.706	387.8856682	1728703.32	11833.99
best1	0.9	0.5	19132.832	109.1204373	1728700.20	11834.72
target-to-best1	0.9	0.9	19160.405	570.0652435	1728672.62	11861.50
rand2	0.5	0.5	19172.258	60.65007044	1728660.77	12015.44
rand1	0.9	0.5	19223.150	68.86191689	1728609.88	12042.56
best1	0.9	0.9	19284.691	595.7499436	1728548.34	11931.93
best2	0.9	0.5	19301.468	92.96109779	1728531.56	12119.34
best1	0.5	0.5	19347.775	371.7509517	1728485.25	12081.59
best2	0.9	0.9	19423.161	867.4594294	1728409.87	12148.08
target-to-best1	0.5	0.5	19496.183	396.4808082	1728336.85	12344.42
rand2	0.9	0.5	19571.672	195.5478231	1728261.36	12522.59
rand1	0.5	0.9	19575.907	530.4553785	1728257.12	12436.15
best2	0.5	0.1	19646.257	258.663631	1728186.77	12582.02
target-to-best1	0.9	0.1	19663.242	234.7941543	1728169.79	12579.67
best1	0.9	0.1	19704.904	317.8975462	1728128.13	12630.59
rand2	0.9	0.9	19710.264	184.5805873	1728122.77	12643.16
best2	0.9	0.1	19799.298	258.0200266	1728033.73	12716.28
best1	0.5	0.1	19869.412	494.9440182	1727963.62	12817.85
rand1	0.9	0.1	19877.679	294.3887616	1727955.35	12820.75
rand2	0.5	0.1	19910.568	414.3236758	1727922.46	12966.29
target-to-best1	0.5	0.1	19913.196	426.7510117	1727919.83	12930.28
rand2	0.9	0.1	19991.693	320.3887736	1727841.34	13020.04
rand1	0.5	0.1	20034.617	340.7094944	1727798.41	13107.70
best1	0.5	0.9	20227.051	937.3568382	1727605.98	12948.53
rand2	0.1	0.1	20561.033	486.0115196	1727272.00	13489.67
best2	0.1	0.1	20562.806	605.025892	1727270.22	13132.30
rand1	0.1	0.1	20686.087	631.7708891	1727146.94	13422.11
best1	0.1	0.1	20855.225	552.6392978	1726977.80	13446.03
rand2	0.1	0.5	21097.067	789.8751643	1726735.96	13525.63
rand1	0.1	0.5	21286.002	840.3257903	1726547.03	13814.34
target-to-best1	0.1	0.1	21579.059	477.0705699	1726253.97	14091.52
best1	0.1	0.5	22459.625	749.2574698	1725373.40	15419.75
target-to-best1	0.5	0.9	22549.281	1280.221032	1725283.75	15479.63
best2	0.1	0.5	22560.172	1094.32686	1725272.86	15349.51
target-to-best1	0.1	0.5	24219.891	1034.605875	1723613.14	17169.86
rand2	0.1	0.9	24468.175	1252.113029	1723364.85	17117.78
rand1	0.1	0.9	24525.824	1155.388665	1723307.21	17301.95
best1	0.1	0.9	24868.144	1463.316278	1722964.89	17399.70
best2	0.1	0.9	24926.682	1429.683675	1722906.35	17690.94
target-to-best1	0.1	0.9	25653.512	1180.704368	1722179.52	18323.05

Table 4.7 DE decision for the null hypothesis of three-stage separation

The Best Configuration (Reference) - rand2 F=0.5 Cr=0.9						
DE Configuration			T-Test		Bonferroni-Holm	
Strategy	F	Cr	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
best2	0.5	0.5	TRUE	0.00002	TRUE	0.00013
target-to-best1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.9	FALSE	0.05225	FALSE	0.15675
best2	0.5	0.9	FALSE	0.18958	FALSE	0.37916
best1	0.9	0.5	TRUE	0.00001	TRUE	0.00011
target-to-best1	0.9	0.9	FALSE	0.24803	FALSE	0.37916
rand2	0.5	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.9	TRUE	0.03739	FALSE	0.14957
best2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.5	TRUE	0.00009	TRUE	0.00057
best2	0.9	0.9	TRUE	0.02891	FALSE	0.14455
target-to-best1	0.5	0.5	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.9	TRUE	0.00001	TRUE	0.00005
best2	0.5	0.1	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.5	0.1	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000

Table 4.8 DE optimisation results for four-stage separation

Strategy	F	Cr	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
best2	0.5	0.5	57725.066	544.3544957	6749417.60	45061.60
rand1	0.5	0.5	57860.935	644.1807921	6749281.74	44914.61
rand2	0.5	0.9	58092.008	837.2172364	6749050.66	44911.47
best1	0.9	0.5	58163.960	740.9477751	6748978.71	45179.38
target-to-best1	0.5	0.1	58363.716	605.1876774	6748778.95	45096.15
best2	0.5	0.1	58405.030	432.8963505	6748737.64	45054.65
target-to-best1	0.9	0.5	58418.239	484.8500528	6748724.43	45388.80
best1	0.5	0.1	58563.597	988.4542952	6748579.07	45539.24
target-to-best1	0.9	0.9	58752.509	1641.868877	6748390.16	45433.15
target-to-best1	0.9	0.1	58758.720	564.970805	6748383.95	44778.09
rand1	0.5	0.1	58782.162	499.1574323	6748360.51	45323.40
best1	0.9	0.1	58798.318	612.8348272	6748344.35	44930.88
rand1	0.9	0.9	58926.214	745.9561857	6748216.46	45468.90
rand2	0.5	0.5	59089.735	718.5787173	6748052.93	45236.83
best1	0.5	0.5	59389.393	1627.724548	6747753.28	45859.69
rand2	0.5	0.1	59413.183	777.3742778	6747729.49	45484.51
best2	0.5	0.9	59417.423	1483.562317	6747725.25	45899.03
rand2	0.1	0.1	59456.778	877.4137189	6747685.89	45858.45
rand1	0.9	0.1	59794.498	615.7652542	6747348.17	45842.12
rand1	0.5	0.9	60037.498	1969.095853	6747105.17	46412.81
rand1	0.1	0.1	60235.898	1016.16696	6746906.77	46643.04
target-to-best1	0.5	0.5	60343.488	1236.836207	6746799.18	46463.93
best2	0.9	0.1	60461.315	1128.934472	6746681.36	45812.17
best2	0.1	0.1	60639.104	1064.108745	6746503.57	46971.54
rand2	0.9	0.1	61058.252	962.719599	6746084.42	46506.85
rand1	0.9	0.5	61230.774	1399.764276	6745911.90	46031.40
best1	0.9	0.9	61289.309	3723.722793	6745853.36	47726.21
best1	0.1	0.1	61901.114	1893.360898	6745241.56	47747.59
rand2	0.1	0.5	64025.710	2396.968915	6743116.96	49857.36
best1	0.5	0.9	64275.275	2631.689539	6742867.40	49429.27
target-to-best1	0.1	0.1	64294.632	1358.729748	6742848.04	47688.74
best2	0.9	0.9	64570.636	1772.677024	6742572.03	49061.95
best2	0.9	0.5	64930.850	2647.816245	6742211.82	49728.27
rand1	0.1	0.5	65163.718	2417.819302	6741978.95	50175.91
best2	0.1	0.5	67863.508	3395.486902	6739279.16	51693.14
target-to-best1	0.1	0.5	67948.771	1681.871744	6739193.90	49582.73
rand2	0.9	0.5	68597.219	3026.791318	6738545.45	53338.54
target-to-best1	0.5	0.9	68998.992	2743.71611	6738143.68	51543.28
rand2	0.9	0.9	69910.288	1984.687309	6737232.38	54303.69
best1	0.1	0.5	70297.638	3653.084334	6736845.03	53257.56
target-to-best1	0.1	0.9	71023.505	2863.645027	6736119.17	52021.33
rand2	0.1	0.9	75925.276	3970.610053	6731217.39	57734.01
rand1	0.1	0.9	78299.408	4850.85036	6728843.26	60086.29
best2	0.1	0.9	78581.851	5624.631192	6728560.82	59826.34
best1	0.1	0.9	80783.292	6135.102657	6726359.38	61678.77

Table 4.9 DE decision for the null hypothesis of four-stage separation

The Best Configuration (Reference) - best2 F=0.5 Cr=0.5						
DE Configuration			T-Test		Bonferroni-Holm	
Strategy	F	Cr	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
rand1	0.5	0.5	FALSE	0.43386	FALSE	0.43386
rand2	0.5	0.9	FALSE	0.07813	FALSE	0.15626
best1	0.9	0.5	TRUE	0.02357	FALSE	0.07071
target-to-best1	0.5	0.1	TRUE	0.00036	TRUE	0.00214
best2	0.5	0.1	TRUE	0.00002	TRUE	0.00016
target-to-best1	0.9	0.5	TRUE	0.00003	TRUE	0.00020
best1	0.5	0.1	TRUE	0.00067	TRUE	0.00333
target-to-best1	0.9	0.9	TRUE	0.00547	TRUE	0.02186
target-to-best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.1	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.5	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.5	TRUE	0.00002	TRUE	0.00017
rand2	0.5	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.5	0.9	TRUE	0.00000	TRUE	0.00004
rand2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.5	0.9	TRUE	0.00000	TRUE	0.00001
rand1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.5	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.1	TRUE	0.00000	TRUE	0.00000
rand1	0.9	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.9	0.9	TRUE	0.00003	TRUE	0.00020
best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.1	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.5	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.9	0.9	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.5	TRUE	0.00000	TRUE	0.00000
target-to-best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
rand2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
rand1	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best2	0.1	0.9	TRUE	0.00000	TRUE	0.00000
best1	0.1	0.9	TRUE	0.00000	TRUE	0.00000

Table 4.10 JADE optimisation results for two-stage separation

Strategy	p_{best}	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
current-to-pbest1	0.1	43186.03	1372.79	10107272.50	31125.30
current-to-pbest1	0.2	43867.53	1874.26	10106591.00	31645.14
current-to-pbest1	0.05	43904.14	1400.75	10106554.39	31787.59

Table 4.11 JADE decision for the null hypothesis of two-stage separation

The Best Configuration (Reference) - current-to-pbest1 p_best=0.1					
JADE Configuration		T-Test		Bonferroni-Holm	
Strategy	p_{best}	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
current-to-pbest1	0.2	FALSE	0.15718	FALSE	0.15831
current-to-pbest1	0.05	FALSE	0.07916	FALSE	0.15831

Table 4.12 JADE optimisation results for three-stage separation

Strategy	p_{best}	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
current-to-pbest1	0.1	19205.73	173.66	1728627.30	11968.20
current-to-pbest1	0.2	19227.90	236.26	1728605.13	11988.68
current-to-pbest1	0.05	19389.51	611.78	1728443.51	12128.66

Table 4.13 JADE decision for the null hypothesis of three-stage separation

The Best Configuration (Reference) - current-to-pbest1 p_best=0.1					
JADE Configuration		T-Test		Bonferroni-Holm	
Strategy	p_{best}	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
current-to-pbest1	0.2	FALSE	0.71267	FALSE	0.71267
current-to-pbest1	0.05	FALSE	0.16330	FALSE	0.32659

Table 4.14 JADE optimisation results for four-stage separation

Strategy	p_{best}	Average Fitness	Standard Deviation	Average Payoff ($/day)	Average Utility Cost ($/day)
current-to-pbest1	0.05	58213.68	1168.88	6748928.99	45213.24
current-to-pbest1	0.2	58617.09	1227.49	6748525.58	45626.03
current-to-pbest1	0.1	58663.57	1095.29	6748479.10	45350.01

Table 4.15 JADE decision for the null hypothesis of four-stage separation

The Best Configuration (Reference) - current-to-pbest1 p_best=0.05					
JADE Configuration		T-Test		Bonferroni-Holm	
Strategy	p_{best}	Reject Null Hypothesis	P-value	Reject Null Hypothesis	Adjusted P-value
current-to-pbest1	0.2	FALSE	0.24033	FALSE	0.33216
current-to-pbest1	0.1	FALSE	0.16608	FALSE	0.33216

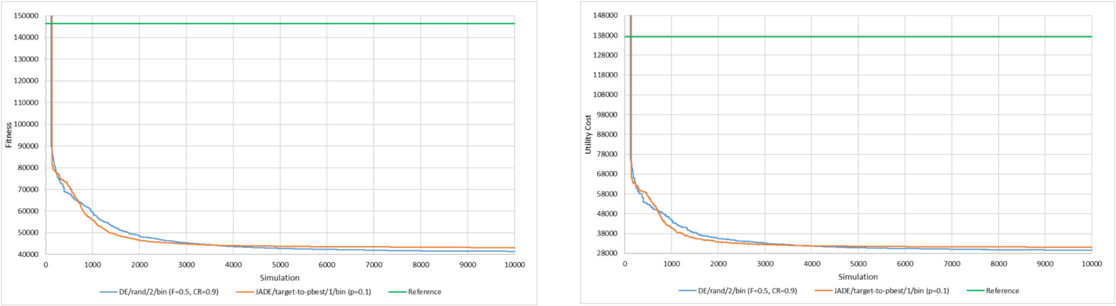
performances of the system with the reference temperatures and pressures. Those parameters are the ones used by the offshore operators. In addition, t-tests are performed between the best configurations of DE and JADE (Table 4.17). As can be seen from provided table of t-test, the null hypothesis is rejected.

Table 4.16 Performance comparison between the best settings of DE and JADE

Avg Fitness after Simulation Run	1000	2000	3000	4000	5000	6000	7000	8000	9000	10000	Final StDev for simulation 10000
Two-Stage Separation											
DE/rand2/F=0.5/Cr=0.9	59455.7	48522.9	45372.6	43652.1	42789.1	42299.7	41947.6	41649.75	41509.3	41433.9	618.6
JADE/curr-to-pbest1/c=0.1/p=0.1	55807.9	46562.9	44840.6	44090.8	43782.0	43530.4	43451.3	43328.1	43237.6	43186.0	1372.8
Three-Stage Separation											
DE/rand2/F=0.5/Cr=0.9	20871.7	19667.5	19275.0	19139.5	19080.6	19053.3	19039.7	19031.7	19026.7	19024.3	9.9
JADE/curr-to-pbest1/c=0.1/p=0.1	20108.6	19476.0	19356.4	19295.4	19261.3	19240.4	19225.0	19217.6	19210.6	19205.7	173.7
Four-Stage Separation											
DE/best2/F=0.5/Cr=0.5	73568.0	64780.9	60980.4	59390.6	58844.0	58426.5	58229.2	58022.8	57847.8	57725.1	544.4
JADE/curr-to-pbest1/c=0.1/p=0.05	67065.6	61215.8	59801.5	59098.5	58817.5	58612.6	58443.0	58329.1	58258.4	58213.7	1168.9

Table 4.17 T-test between the best DE and JADE configurations

Algorithm	Reject Hypothesis	P-Value
Two-Stage Separation		
DE/rand2/F=0.5/Cr=0.9	TRUE	7.163E-07
JADE/current-to-pbest1/c=0.1/p=0.1		
Three-Stage Separation		
DE/rand2/F=0.5/Cr=0.9	TRUE	5.543E-06
JADE/current-to-pbest1/c=0.1/p=0.1		
Four-Stage Separation		
DE/best2/F=0.5/Cr=0.5	TRUE	0.043
JADE/current-to-pbest1/c=0.1/p=0.05		

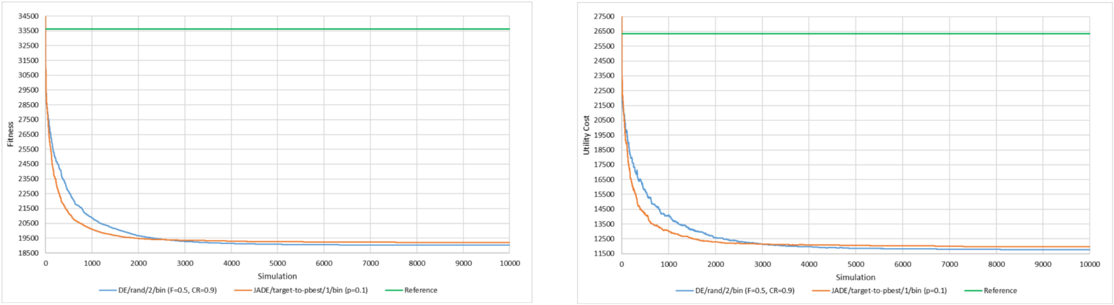


(a) Fitness

(b) Utility Cost

Fig. 4.4 Two-Stage Separation - DE vs JADE

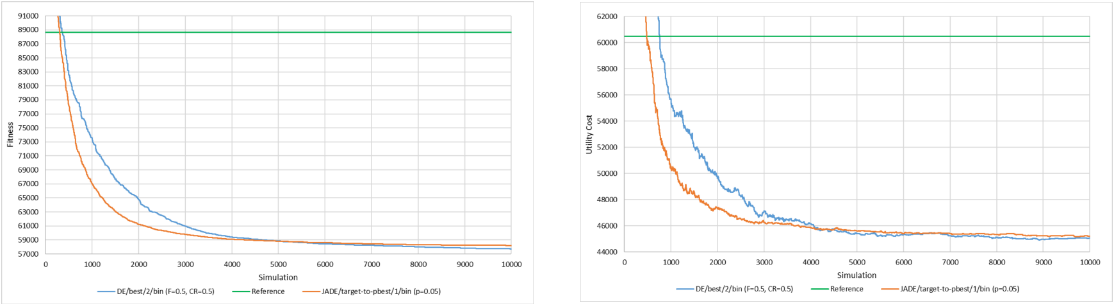
It is interesting to note that in first 4000 simulations for each test case and for both objectives (fitness and utility cost) JADE performs better optimisation results than DE. However, there is an exactly opposite situation after 4000 simulations, i.e. the results of DE become better than JADE. Therefore, when our termination criteria is met (10000 simulations) DE shows better results than JADE. Also, as can be seen from Table 4.16 and graphics application of any of the algorithms, DE and JADE, allows an increases of the profit and a reduction of the utility cost compared to reference values.



(a) Fitness

(b) Utility Cost

Fig. 4.5 Three-Stage Separation - DE vs JADE



(a) Fitness

(b) Utility Cost

Fig. 4.6 Four-Stage Separation - DE vs JADE

The financial impact of the optimisation is presented in Table 4.18. Depending on the production, the optimised settings increases the profits from 10,000USD to 100,000USD per day.

Table 4.18 Profit variation between reference settings and settings obtained by mean of optimisation (all figures are in USD/day)

	Two-stage		Three-stage		Four-stage	
	Obtained	Reference	Obtained	Reference	Obtained	Reference
MTV	10,150,459	10,150,459	1,747,833	1,747,833	6,807,143	6,807,143
Fitness	41,434	146,460	19,024	33,631	57,725	88,664
Overall profit ($/day)	10,109,024	10,003,999	1,728,809	1,714,202	6,749,418	6,718,479
Utility Cost ($/day)	29,624	137,193	11,767	26,341	45,061	60,463
Profit variation ($/day)	**103,526**		**14,529**		**30,574**	

Chapter 5

Conclusions and Future Work

This final chapter provides an overview of the contributions made in this thesis. Also, the chapter presents some potential directions for future work.

5.1 Summary of Contributions

This thesis makes contributions to the oil and gas industry in general and offshore oil industry in particular. The thesis presents novel solutions for simulation of any type separation systems and optimisation of offshore oil platforms. The main contributions can be summarized as follows:

- **A novel approach for simulation of separation systems**: In Chapter 3 a novel approach for simulation of oil separation systems based on the flash algorithm is presented. The first and main advantage of this approach is that it can be used for both offshore and onshore separation system. Likewise, this approach can be used not only for the simulation but also for hydrocarbon allocation which is highly important for cases when suppliers have a shared separation system. The applicability of the proposed method is demonstrated in a commercial simulation software package CHARM [1], which incorporates the idea developed during my KTP project between RGU and ACCORD-ESL.
- **The improved flash algorithm**: The flash algorithm takes a key place into the simulation of separation systems because it models separation processes into the separator/scrubber and its results of the whole simulation are based on the flash algorithm calculations. Therefore, analysis and investigation of instabilities in the flash algorithm

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[1] Compact Hydrocarbon Allocation Reference Model (CHARM), web-site: https://charm.accord-esl.com/

have been done in this research (see Section 3.3). Sources of these instabilities include a poor estimation of K-factors, an incorrect and/or slow solution of the cubic equation of state and the use of invalid compressibility factors. Respectively, those instabilities have been solved which allows to increase the speed, accuracy and efficiency of the flash algorithm. The proposed improvements are validated with different real world hydrocarbon mixtures for a wide range of temperatures and pressures. Finally, it is highly important to mention that the flash is one of the major and most valuable algorithms in the oil industry because it is widely used by chemical engineers for many tasks, such as separator design, separation modelling, etc. So, the proposed improved flash algorithm has high contribution value not only for this research but also for the wider community of application.

- **Mathematical formulation of the optimisation problem for offshore oil platforms**: Despite the importance of the optimisation of offshore oil platfroms with the aim to increase the profit, without additional costs for new equipment, our literature review shows that there are a limited number of public sources in this area. Moreover, a clear mathematical formulation of this problem there is missing. In Section 4.3 the mathematical formulation of the optimisation problem where define decision variable with their limitations and constraints, and the fitness function are introduced. Additionally, formulas for calculations of utility costs for offshore oil platforms are formulated and described. A key advantage of defined fitness function and utility cost calculations is that their results are in USD and this is the best quality parameter for measure of the best solution.

- **The increased profit of the offshore oil platform by application of DE and JADE**: In Section 4.4 pseudo code of the applied DE and JADE algorithms for search of the best settings parameters (temperatures and pressures) for three real world test cases (two-stage, three-stage and four-stage) are provided. As can be seen from the results provided in Table 4.18, the application of optimisation algorithms discovers solutions with the potential to increase the profit of the offshore oil platform between 10,000 and 100,000 USD/day.

- **The best configuration settings of DE and JADE**: Due to this research many runs are performed with a wide range of configuration settings for DE and JADE in order to find which configuration settings of these algorithms provide the best solutions. According to the obtained results, for DE the best configuration settings are $F = 0.5$, $Cr = [0.5, 0.9]$ and the strategy is $DE/rand/2/bin$ or $DE/best/2/bin$. With the case of JADE there is only one parameter which is investigated and this is p which has to be 0.1 or 0.05.

5.2 Future work

5.2.1 Validation of the Optimisation of Offshore Oil Platforms

The proposed simulation and applied DE and JADE optimisation algorithms are validated on three real-life offshore oil platforms with real hydrocarbon compositions. Moreover, the test cases cover the most common offshore oil platforms where the number of stages is two, three or four. However, it is possible to have different numbers and configuration of scrubbers. Therefore, testing over a large set of benchmark examples it might be possible to discover a relationship between particular configuration features and optimal parameter settings of DE and JADE.

Analysis of the time necessary for meeting of some optimisation target is also required on the future. Here, it is interesting to note, at the beginning of the optimisation procedure, during to the first 5000 runs, the JADE shows better optimisation results than DE (see Figures 4.4, 4.5, 4.6). However, this situation changes after the 5000 runs, i.e. DE shows better results than JADE.

In addition, application of other population-based algorithms such as Genetic Algorithm (GA) and Particle Swarm Optimisation (PSO) may also be explored. The performance and results generated by the GA and PSO have to be compared with DE and JADE in order to find one optimisation algorithm which can have a relatively small time to met given optimisation target.

5.2.2 Multiobjective Optimisation and Hydrocarbon Allocation

Nowadays, as was mentioned in Section 2.3, the collaboration in the offshore area is crucial for the future of oil and gas companies. Furthermore, there are a lot of important reasons for collaboration. First of all, technical and institutional challenges occurring in hostile environments, extreme reservoirs and building of transportation oil and gas networks. Secondly, sharing the cost and risks related with the building and exploitation of an offshore oil platform. In addition, collaboration can be needed even in friendly environment for profit maximisation. For instance, two oil and gas companies want to produce oil and gas production with required API gravity. To achieve that crude oil from underground reservoirs of these companies is mixed with the aim to produce export oil with required API gravity [73].

The importance and vital role of collaboration required it to be taken into account during the development of optimisation framework for offshore oil platforms. Collaboration in the exploitation of a shared offshore oil and gas platform means that:

- Several oil companies/suppliers use the same offshore oil platform for extraction and producing of transportable oil and gas production.
- Each company/supplier has underground reservoir(s).
- Each company/supplier has different number of wells into their reservoir(s).
- Composition of crude oil from different reservoirs varied.
- Each company/supplier has its own commercial interests based on signed contracts with clients. From these contracts, information about how much oil and/or gas production have to be delivered until a certain date has to be taken into account during an optimisation.
- Each company/supplier saves in secret their contracts and usually not share it even with collaborating companies.
- Quantities of export oil and gas production for one company/supplier can vary for the same quantity of their crude oil. This happens for two reasons. Firstly, under different sets of pressures and temperatures their crude oil can become more in vapour phase (export gas) instead of liquid phase (export oil) or vice versa. Secondly, if the composition of the mixed crude oil is changed then for the same set of temperatures and pressures the quantities of export oil and gas will be changed.
- Software for modelling and hydrocarbon allocation has to be used in order to determine the quantities of exported oil and gas products between the companies/suppliers.

Taking into account these facts, it is possible to have two different scenarios for optimisation of offshore oil platforms.

- For the first scenario, we assume that *collaborating companies have a single common objective* to *increase the total profit and decrease the utility cost* of the shared offshore oil platform. This case has been reviewed, investigated and described into this thesis (see Chapter 4). So, for the optimisation of this scenario is necessary to find temperatures and pressures where total profit increases and utility cost decreases. Therefore, only a simulation software for separation processes is required (see Chapter 3). In addition, this scenario covers the case when there is only one owner of the oil platform which wants to optimise his offshore oil platform.

- For the second scenario, we assume that *collaborated oil companies have distinct commercial interests* [74]. Hence, *each company has its objective* and will advance its own strategy. So, the objectives of companies are competitive, and multiobjective optimisation is required. For instance, there are two companies which share the offshore oil platform. Likewise, the first company wants to produce more export oil while the second company wants to produce more export gas. So, the companies have competing objectives because of signed contracts with clients. As a result, the optimisation has to determine optimal temperatures and pressures without causing unfair detriment to either of the companies. Also, hydrocarbon allocation (see Section 2.3) has to be used in order to split exported oil and gas production between collaborating oil companies.

In this research we have investigated and described the first scenario. The second scenario has not been investigated due to complexity, uncertainties related to the domain and time limitation of the master of research. However, results from first scenario have solved many of the uncertainties, such as a calculation of the profit, utility cost, and they can be used as a strong base for future work under the second scenario. For this second scenario are required multiobjective optimisation algorithms, such as MOEA/D and NSGA-III that could be used to explore this topic.

5.3 In Conclusion

This thesis offers comprehensive solutions for simulation of separation systems and optimisation of offshore oil platforms.

The proposed novel approach for simulation of separation system is based on the flash algorithm which has been improved and validated with real world hydrocarbon mixture for wide range of temperatures and pressures. Furthermore, the proposed method is applicable for onshore and offshore separation system and allows hydrocarbon allocation.

The proposed optimisation for offshore oil platforms is based an application of population-based algorithms. Here is provided description of the separation process, the parameters it is controlled by and how to formulate it as an optimisation problem in order to maximise the overall profit of the production. This profit is affected by two factors, the quality of the separation between of the hydrocarbons and the utility costs involved by this process. Also, in the thesis all the constraints imposed by this system and included them in formulation of the problem are defined.

In this research a simple DE and JADE algorithm to optimise the settings of three different types of separators systems (two-stage, three-stage and four-stage) and different hydrocarbon mixture are applied.

The results show that optimising parameters of the system can generate substantial profit increase (10,000 to 100,000 USD/day).

Finally, a comprehensive program of further research has been proposed.

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Appendix A

Vieta's trigonometric formulas

Vieta's trigonometric formulas can be used for analytical solution of cubic equation (equation A.1).

$$x^3 + ax^2 + bx + c = 0 \tag{A.1}$$

Calculate Q (equation A.2) and R (equation A.3).

$$Q = \frac{a^2 - 3b}{9} \tag{A.2}$$

$$R = \frac{2a^3 - 9ab + 27c}{54} \tag{A.3}$$

Calculate discriminant S (equation A.4).

$$S = Q^3 - R^2 \tag{A.4}$$

If $S > 0$, then there are three real roots (equations A.5, A.6, A.7, A.8).

$$\varphi = \frac{1}{3} arccos\Big(\frac{R}{\sqrt{Q^3}}\Big) \tag{A.5}$$

$$x_1 = -2\sqrt{Q}\cos(\varphi) - \frac{a}{3} \tag{A.6}$$

$$x_2 = -2\sqrt{Q}\cos(\varphi + \frac{2}{3}\pi) - \frac{a}{3} \tag{A.7}$$

$$x_3 = -2\sqrt{Q}\cos(\varphi - \frac{2}{3}\pi) - \frac{a}{3} \tag{A.8}$$

If $S = 0$, then less than three real roots, multiple roots (equations A.9, A.10).

$$x_1 = -2sgn(R)\sqrt{Q} - \frac{a}{3} \tag{A.9}$$

$$x_{2,3} = sgn(R)\sqrt{Q} - \frac{a}{3} \tag{A.10}$$

If $S < 0$, then one real root and complex conjugate roots. So, in order to calculate root value of Q has to be taken into account.

If $S < 0$ and $Q > 0$, equations A.11,A.12,A.13 have to be used.

$$\varphi = \frac{1}{3}arch\Big(\frac{|R|}{\sqrt{Q^3}}\Big) \tag{A.11}$$

$$x_1 = -2sgn(R)\sqrt{Q}ch(\varphi) - \frac{a}{3} \tag{A.12}$$

$$x_{2,3} = sgn(R)\sqrt{Q}ch(\varphi) - \frac{a}{3} \pm i\sqrt{3}\sqrt{|Q|}sh(\varphi) \tag{A.13}$$

If $S < 0$ and $Q < 0$, equations A.14, A.15, A.16 have to be used.

$$\varphi = \frac{1}{3}arsh\Big(\frac{|R|}{\sqrt{|Q|^3}}\Big) \tag{A.14}$$

$$x_1 = -2sgn(R)\sqrt{|Q|}sh(\varphi) - \frac{a}{3} \tag{A.15}$$

$$x_{2,3} = sgn(R)\sqrt{|Q|}sh(\varphi) - \frac{a}{3} \pm i\sqrt{3}\sqrt{|Q|}ch(\varphi) \tag{A.16}$$

If $S < 0$ and $Q = 0$, equations A.17, A.18 have to be used.

$$x_1 = -\sqrt[3]{c - \frac{a^3}{27}} - \frac{a}{3} \tag{A.17}$$

$$x_{2,3} = -\frac{a + x_1}{2} \pm \frac{i}{2}\sqrt{|(a - 3x_1)(a + x_1) - 4b|} \tag{A.18}$$