Multiscale design and analysis of CO\textsubscript{2} capture, transport, and storage networks

Ahmed Alhajaj

A thesis submitted for the degree of
Doctor of philosophy of
Imperial College London

Centre for Process Systems Engineering
Department of Chemical Engineering and Chemical Technology
Imperial College London
London SW7 2AZ, United Kingdom
Declaration

I confirm that the work in this thesis is my own and that all else is appropriately referenced.
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Abstract

CO₂ capture, transport and storage (CCTS) is gaining a broad interest as a countermeasure to global warming. The systematic development of CCTS network infrastructure is a non-trivial activity that involves choosing the optimum design of the selected CO₂ capture plant technology and transportation mode, and identifying the key performance operating parameters and limiting uncertainties that need to be mitigated or optimized to ensure a safe cost-optimal network. This thesis focuses on developing a systematic multiscale modelling and optimization approach that integrates validated sub-process models of the MEA-based CO₂ capture plant, compression train and pipelines in which thermodynamic properties were calculated using SAFT-VR with the supply-chain CO₂ network model. A number of simulations were performed to analyse and identify the cost-optimal design and operating variables while considering different CO₂ prices, flue gas bypass option and uncertainty in transporting flow temperature and composition. A meta model that combines the results of the fine scale model was then used in the supply chain network model to successfully determine the cost-optimal CCTS network for a case study in Abu Dhabi. A key result of the thesis was that the cost-optimal degree of capture is a function of several site-specific factors, including exhaust gas characteristics, proximity to transportation networks, adequate geological storage capacity, CO₂ price, and the option to partially bypass flue gas. A higher CO₂ price had a clear impact on encouraging higher degree of capture. The flue gas bypass option was seen to be an optimal option for lower than 60% degree of capture. It was also observed that transportation companies should levy a charge to discourage transporting flow from low CO₂ content sources. This thesis serves to underscore the need to comprehend the science governing the behaviour at different scales and the importance of a whole-system analysis of potential CCTS networks.
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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_c$</td>
<td>Cross sectional area ($m^2$)</td>
</tr>
<tr>
<td>a</td>
<td>Interfacial dry mass transfer area per volume of packed bed ($m^2 m^{-3}$)</td>
</tr>
<tr>
<td>$a'$</td>
<td>Interfacial wet mass transfer area per volume of packed bed ($m^2 m^{-3}$)</td>
</tr>
<tr>
<td>c</td>
<td>Number of components</td>
</tr>
<tr>
<td>$CAPEX$</td>
<td>Capital expenditures</td>
</tr>
<tr>
<td>$CCC$</td>
<td>Commission on climate change</td>
</tr>
<tr>
<td>$CCTS$</td>
<td>Carbon capture, transport and storage</td>
</tr>
<tr>
<td>$CER$</td>
<td>Certified emission reduction</td>
</tr>
<tr>
<td>$CF$</td>
<td>Capacity factor</td>
</tr>
<tr>
<td>$CP$</td>
<td>Carbon price</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity ($kJ kg^{-1} K^{-1}$)</td>
</tr>
<tr>
<td>$Cr$</td>
<td>Compression ratio</td>
</tr>
<tr>
<td>$CRF$</td>
<td>Capacity recovery factor</td>
</tr>
<tr>
<td>$CS$</td>
<td>Carbon steel</td>
</tr>
<tr>
<td>$D$</td>
<td>Diameter ($m$)</td>
</tr>
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<td>$DCC$</td>
<td>Direct contact cooler</td>
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<tr>
<td>$DEC$</td>
<td>Direct equipment cost</td>
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<tr>
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<td>$DOF$</td>
<td>Degree of freedom</td>
</tr>
<tr>
<td>$E$</td>
<td>Weld joint factor</td>
</tr>
<tr>
<td>$EOR$</td>
<td>Enhanced oil recovery</td>
</tr>
<tr>
<td>$EU~ETS$</td>
<td>European union emission trading scheme</td>
</tr>
<tr>
<td>$F$</td>
<td>Basic design factor</td>
</tr>
<tr>
<td>$F_E$</td>
<td>Equipment multiplying factor</td>
</tr>
<tr>
<td>$F_I$</td>
<td>Instrument multiplying factor</td>
</tr>
<tr>
<td>FOM</td>
<td>Fixed operation and maintenance</td>
</tr>
</tbody>
</table>
$f$ Friction-factor

$FCC$ Facility capital cost ($\$\$)

$FFR$ Flue gas feed fraction ratio

$G$ Gas molar flow rate ($mol \ s^{-1}$)

$g$ Gravitational acceleration ($m \ s^{-2}$)

$GIS$ Geographical information system

$h$ Molar specific enthalpy ($J \ mol^{-1}$)

$H$ Packed bed height of a stage ($m$)

$he$ Elevation ($m$)

$HETP$ Height equivalent to a theoretical plate ($m$)

$HP$ Horse power

$HTU$ Height of transfer unit ($m$)

$H_{og}$ Overall height of transfer unit ($m$)

$IEA$ International energy agency

$IPCC$ Intergovernmental panel of climate change

$ISBL$ Inside battery limit

$KPIs$ Key performance indicators

$KOPs$ Key operating parameters

$k_g$ Mass transfer coefficient for gas phase ($m \ s^{-1}$)

$k_l$ Mass transfer coefficient for liquid phase ($m \ s^{-1}$)

$K_{og}$ Overall mass transfer coefficient ($mol \ m^{-2} \ s^{-1}$)

$L$ Liquid molar flow rate ($mol \ s^{-1}$)

$LCA$ Life cycle assessment

$Le$ Length ($m$)

$M$ Molecular weight ($kg \ kmol^{-1}$)

$MARKAL$ Market allocation

$m$ Slope of equilibrium line

$MILP$ Mixed integer linear programming
MINLP  Mixed integer nonlinear programming

mm  Millimetres

\(\dot{m}\)  Mass flow rate \((kg\ s^{-1})\)

\(N\)  Number of stages

NLP  Nonlinear programming

NPS  Nominal pipeline size

\(NTU_{dc}\)  Number of transfer units for direct contact cooling

\(OD\)  Outer diameter \((m)\)

OPEX  Operating expenditures

\(P\)  Pressure \((Pa)\)

PCC  Pipeline capital cost \((\$)\)

PSA  Pressure swing adsorption

\(PUI\)  Process unit investment \((\$)\)

\(Q\)  Cooling or heating duty \((W)\)

\(R\)  Universal gas constant \((Pa\ m^3\ mol^{-1}\ K^{-1})\)

\(Re\)  Reynolds number

\(ROW\)  Right of way

\(S\)  Molar specific entropy \((J\ mol^{-1})\)

SMYS  Specified minimum yield strength \((Pa)\)

SQP  Sequential quadratic programming

\(SS\)  Stainless steel

\(T\)  Temperature \((K)\)

\(TC\)  Total capital \((\$)\)

\(t\)  Thickness \((m)\)

\(TCCC\)  Total capture and compression cost \((\$/tCO_2)\)

\(TCTC\)  Total compression and transportation cost \((\$/tCO_2)\)

\(TIMES\)  The integrated MARKAL-EFOM system

\(TPCC\)  Total pipeline capital cost \((\$)\)
TSA Temperature swing adsorption

$U$ Overall heat transfer coefficient ($W \, m^{-2}K^{-1}$)

$u$ Velocity ($m \, s^{-1}$)

$V$ Molar specific volume ($m^3 \, mol^{-1}$)

$VC$ Variable cost ($$/tCO_2$)

$W$ Power of rotary equipment ($W$)

$WC$ Working capital ($$)

$x$ Liquid molar composition

$y$ Gas molar composition

$Z$ Compressibility factor

**Greek symbols**

$\Lambda$ Ratio of the slopes of operating and equilibrium line

$\epsilon$ Internal surface roughness of the pipe ($m$)

$\mu$ Viscosity ($Pa \, s^{-1}$)

$\mu^g_{(i,out)}$ Outlet gas chemical potential of component $i$ ($J \, mol^{-1}$)

$\mu^l_{(i,out)}$ Outlet liquid chemical potential of component $i$ ($J \, mol^{-1}$)

$\eta_{mec}$ Mechanical efficiency

$\eta_{isn}$ Isentropic efficiency

$\rho$ Density ($kg \, m^{-3}$)

$\theta_{lean}$ Lean loading of solvent at the inlet of the absorber ($x_{(CO_2,in)} / x_{(MEA,in)}$)

$\theta_{rich}$ Rich loading of solvent at the outlet of the absorber ($x_{(CO_2, out)} / x_{(MEA, out)}$)

$\Delta \theta$ Net solvent loading ($\theta_{rich} - \theta_{lean}$)

**Subscripts and superscripts**

$ave$ Average

$c$ Compressor

$cap$ Captured
cut  Cut-off pressure of the multi-stage compression

cw  Cooling water

E   Equipment

f   Factors: Materials; Labor; Right of Way (ROW); Miscellaneous

fg  Flue gas

g   Gas phase

I   Instrument

i   Components: 1 = H₂O; 2 = MEA;
    3 = CO₂; 4 = N₂

in  Inlet

j   Stage

l   Liquid phase

LM  Log mean

ls  Lean solvent

out Outlet

p   Pump

pip Pipe

ven Vented

*   Outlet assuming isentropic path
1 INTRODUCTION

There is a general consensus within the scientific community and all the UN member governments who signed the IPCC Fourth Assessment Report that global-warming is occurring, and that increased concentration of anthropogenic CO$_2$ emissions due to fossil fuels consumption is the major cause. This climate change might lead to deleterious effects such as rising sea levels, increased water and food shortages, droughts and floods. There are no simple solutions to this problem, however. Population and economic growth are predicted to lead to a 40% rise in world energy demand by 2035 under current policies (IEA, 2011). Current estimates suggest that despite the immense effort which is being invested in the development of alternative energy sources, majority of this increase will still be met by fossil fuels (IEA, 2011). The limited ability of new energy technologies to replace fossil fuels within the short or medium term is due to a number of factors. It will take time for some of these technologies to become efficient enough to rival fossil fuels in cost effectiveness and infrastructure availability. Biofuels must compete with food production for available land. Wind turbines face technical problems due to intermittency of supply. The nuclear option must cope with public acceptance issues and the challenge of waste disposal, which will require decades of monitoring. All in all, it is clear that if economic growth is not severely curtailed, the world will continue consuming fossil fuels for a considerable period of time yet.

One remedial measure, which can be implemented in the short to medium term, is to separate CO$_2$ from flue gas mixtures exiting large combustion sources and transport it to a geological site that will ensure long-term isolation from the atmosphere. The implementation of CO$_2$ capture, transport, and storage (CCTS) technology will allow us to consume fossil fuels, such as coal and gas, with minimum environmental impact. It will also pave the way towards a smooth transition to renewable energy in the long term. In fact, most of the technologies involved in CCTS are developed at full scale. CO$_2$ is routinely separated during natural gas production. The concept of using CO$_2$ as a displacement agent in EOR has been implemented
in the Permian Basin of Western Texas, where large quantities of CO$_2$ gas have been available in nearby underground deposits at a reasonable cost since the 1960s. The lack of such readily available CO$_2$ is the reason that this technology has not been significantly implemented elsewhere. The extensive usage of EOR in that region has resulted in more than 3100 km of CO$_2$ pipelines (Metz et al., 2005).

Although the technologies involved in CCTS have been proven individually, the remaining challenge facing governments and industries is to implement the whole system safely and at a minimum cost on a large scale that makes a material effect on global warming mitigation. This requires detailed analysis of all the CCTS network components in an integrated fashion and understanding of several site-specific factors that must be considered when applying this technology on a scale that minimizes the environmental impact of global warming: for instance, the proximity of the sources to appropriate geological storage sites and the ability of the storage sites to accommodate these emissions at a certain rate per year and for the lifetime of the project.

The remainder of this chapter is organized as follows: It starts by giving a background of the applicable CO$_2$ capture approaches, separation technologies, transportation modes and storage options. Then, it briefly summarizes the attempts in the literature on formulating the integrated CCTS design problem, which is reviewed in detail in chapter 2. This chapter concludes with aim and objectives, and an outline of the thesis.
1.1 Background

In this section, CO₂ capture approaches, separation technologies, transportation modes and storage option are briefly outlined to highlight their technical challenges.

1.1.1 CO₂ capture approaches and separation technologies

1.1.1.1 CO₂ capture approaches

The four main approaches for capturing CO₂, based on the position of capturing unit in the overall fuel-utilisation process are: Post-combustion, Pre-combustion, Oxyfuel and Industrial processes.

1.1.1.1.1 Post-combustion

Stack flue gas containing CO₂ from combustion of fossil fuels (i.e., coal, natural gas, oil, or biomass) is passed through a separation unit. MEA based post combustion capture plant is an example of this approach. The main challenge in this approach is the large volume of flue gas that needs to be processed in order to separate the small proportion of CO₂ present (i.e., 3-15% by volume). This approach can be retrofitted to both power plants and industrial processes. However, integration will require steam extraction from the power plant or industrial source that will reduce its production capacity and increase cost. Although this technology does exist at a small scale, there is a challenge in deploying this technology at a large scale.

1.1.1.1.2 Pre-combustion

Fossil fuels are reformed in this process by reaction with oxygen/air and steam or solely steam to produce syngas, consisting of hydrogen and carbon monoxide. This then reacts with steam in a catalyst reactor to produce CO₂ and more hydrogen. The high CO₂ content produced in this process can be separated by absorption or adsorption in addition to novel technologies such as liquefaction and membranes. The hydrogen produced in this process can be used in hydro-treating to produce cleaner fuels. Further, power turbines and fuel cells can
use the hydrogen to produce electricity while emissions with a high CO₂ content are separated and captured. Integrated Gasification Combined Cycle (IGCC) is an example of such a system. This system may provide an opportunity to decarbonise the transportation system once fuel-cell cars are widely developed. The technologies for the pre-combustion process are commercially used at industrial scale in oil refineries and ammonia production while using natural gas reforming. The critical challenge is that this process is more complex than the post-combustion technology and harder to retrofit.

1.1.1.3 Oxyfuel-combustion

In this approach, an air separation unit produces oxygen, which is used instead of air for the combustion of fossil fuel and results in flue gas that is mostly H₂O and CO₂. CO₂ is then recycled into the combustor to moderate the excess heat and high temperatures arising from burning fossil fuel with pure oxygen. The main drawback of this technology is the need for oxygen, which is relatively expensive to produce from air, whether by adsorption or cryogenic means. Nevertheless, lower levels of NOx in the flue gas can ease the process of capture, especially in view of the high content of CO₂ (Nie et al., 2011).

1.1.1.2 Industrial processes

This system consists of CO₂ produced from industrial processes other than that produced from power and/or heat generation plants. An example of this is ammonia production, which is a promising area of application due to the presence of high CO₂ concentrations.

1.1.2 Separation Technologies

In this section, the major separation technologies (i.e., absorption, adsorption, membrane separation and cryogenic separation) are reviewed to examine their current limitations, and operational problems.
1.1.2.1 Physical absorption processes

This is an alternative technique for the natural gas and chemical industries. Meisen and Shuai (1997) identified the classic physical solvents as methanol, N-methyl-2-pyrrolidone, polyethylene glycol dimethylether, propylene carbonate and sulfolane. The amount of CO$_2$ dissolved in these solvents increases with pressure following Henry’s law. Thus, the energy required to capture the gas is halved if the pressure of CO$_2$ is doubled. This makes the process more suitable for high CO$_2$ content plants such as integrated gasification combined cycle (IGCC). The main challenge in applying this technology to low-pressure CO$_2$ sources such as NGCC is the cost of compressing flue gas, which is required to produce high operating pressure.

1.1.2.2 Adsorption

The adsorption process can be classified into physical adsorption and chemical adsorption. The physisorption processes are associated with intermolecular (van der Waals) forces between gas and the surface of solid materials, such as molecular sieves or activated carbon, leading to a layer of gas adhering to the surface. The chemisorption processes are associated with reaction of CO$_2$ with the sorbent to form a stable compound at one set of operating conditions. The adsorbed gas can then be separated using many regeneration methods, such as pressure swing adsorption (PSA) or temperature swing adsorption (TSA). Alternatively the trapped gas can be released by washing or by applying electricity (Shackley and Gough, 2006). Because of TSA’s high-energy requirement and slow regeneration, PSA is usually regarded as the best choice. The capacity and CO$_2$ selectivity of current adsorbents is low and this seems to be the main drawback in the implementation of this technique for large-scale CO$_2$ capture from flue gas.

However, there is growing interest in finding materials that have a better reaction rate, capacity, and ability to withstand operating temperature and the environment of the flue gas. Drage (2012) classified the developed materials meeting some of the above mentioned targets and that can be operated at the low temperature envelope (i.e., 40-110 °C) into supported
amine (Drage et al., 2008; Xu et al., 2002; Xu et al., 2003), immobilized amine (Harlick and Sayari, 2006; Serna-Guerrero et al., 2008), activated carbon (Arenillas et al., 2005; Drage et al., 2007; Pevida et al., 2008), zeolites (Xiao et al., 2008), Metallic Organic Framework (MOFs) (Han et al., 2012b; Torrisi et al., 2010) and hydrotalcites (Park et al., 2005; Walspurger et al., 2008). An example of this is the immobilized amine consisting of a sorbent with a mixture of amines that increases its reactivity and capacity combined with the advantages of avoiding the presence of water comprising most of the chemical solvent. This has the potential of reducing the energy penalty associated with TSA.

Another promising adsorbent that is designed to operate at very high temperature (i.e., 600-950°C) is calcium oxide (CaO), which can be derived from limestone. It is cycled in a fluidized bed between two columns as shown in Figure 1.1 resulting in carbonation (i.e., reaction of calcium oxide with CO₂), followed by calcination (i.e., the stripping of CO₂ and the recycle of calcium oxide) (Abanades et al., 2005; Anthony, 2008; Blamey et al., 2010; Li and Fan, 2008; Shimizu et al., 1999; Stanmore and Gilot, 2005). The operation of the columns at very high temperatures enables the recuperation of the heat generated from all the streams to produce steam used in useful work making the process more efficient from the thermodynamic point of view. The main drawback is that the recycled sorbent absorbability reduces with the number of cycles, which makes the lime (CaO) exhausted. Thus, this requires fresh CaCO₃ to be fed into the system. Nevertheless, the exhausted lime (CaO) can be sold as feedstock for cement production and thus reducing the overall cost of the process (Bosoaga et al., 2009; Rodriguez et al., 2009).
1.1.2.3 Gas separation membranes

The use of porous membranes, which can separate a mixture gases, governed by selectivity and permeability is another potential technique. The rate of flow through the membrane depends on the pressure difference across it. This technology has been successfully used to separate CO\textsubscript{2} from the light hydrocarbons in the petroleum industry (Baker and Lokhandwala, 2008; Meisen and Shuai, 1997). The findings of studies examining the use of membrane separation to capture CO\textsubscript{2} from flue gas have been mixed. Studies by Favre (2007), Feron et al. (1992) and Van Der Sluijs et al. (1992) discarded the use of single module membrane systems to capture CO\textsubscript{2} from low CO\textsubscript{2} content flue gas (i.e., <10 mol.%). This is due to the large number of component gases involved in the process, and the need for energy intensive and expensive flue gas compression. However, studies by Bounaceur et al. (2006), Czyperek et al. (2010), Hussain and Hägg (2010) and Zhao et al. (2010) found the membrane permeation processes to be competitive through developing innovative process flow configurations (e.g., cascade of membranes) and operating conditions that have the potential to lower the parasitic load associating with running the compressors and vacuum pumps.

\textbf{Figure 1.1:} Post-combustion calcium looping (Shimizu et al., 1999)
1.1.2.4 Membrane gas absorption

In this process, flue gas is passed through a tube bundle of a porous solid membrane while amine solution is passed through the shell side. CO$_2$ is selectively passed through the membrane that blocks other impurities, followed by CO$_2$ being absorbed by the solvent. This reduces the scrubbing plant size considerably, and hence the capital cost. This process has many advantages, such as minimizing entrainment, flooding, channelling and foaming. It is considered to be the most promising technique by many researchers (Belaissaoui et al., 2012; Bounaceur et al., 2012; Bram et al., 2011; Chabanon et al., 2013; Favre, 2007; Favre and Svendsen, 2012; Klaassen et al., 2005; Merkel et al., 2010; Yan et al., 2008); however, more research is still needed to minimize membrane plugging problems.

1.1.2.5 Cryogenic separation

In this technique, pressurization and refrigeration are used in a cryogenic cycle to physically separate CO$_2$ from other gases. This process is inherently expensive because of the high-energy requirement. Furthermore, flue gas streams that contain Nox, Sox, or H$_2$O may interfere with the cooling regime and cause corrosion, fouling and plugging. Nevertheless, it is commercially used for purification of gas with higher than 90% CO$_2$ content (Shackley and Gough, 2006).

1.1.2.6 Chemical absorption processes

The chemisorption technique is based on CO$_2$ reacting with chemical solvents such as mono-, di- or tri-ethanol amines, di-isopropanol amine, sodium hydroxide, sodium carbonate or potassium carbonate to form an intermediate compound with a weak bond that can be broken down by heat to release the captured CO$_2$ (Meisen and Shuai, 1997).

The post-combustion amine based CO$_2$ capture system consists of two packed columns as shown in Figure 1.2. The absorber is used to absorb CO$_2$ while the desorber is used to regenerate the solvent. The lean solvent enters the top of the absorber column and comes in direct contact with flue gas in a packed counter-current column that ensures sufficient driving
force. This solvent absorbs CO\textsubscript{2} while moving towards the bottom of the column and exiting it being rich solvent (higher CO\textsubscript{2} content). This stream is then regenerated in a packed column with a reboiler at the bottom and a condenser at the top. The reboiler is used to provide the heat required to shift the reaction towards the regeneration of solvent, to provide the vapour stream needed to drive the regeneration force, and to provide the sensible heat needed to increase the temperature in the heat exchanger. The condenser at the top of the desorber is used to ensure a higher CO\textsubscript{2} content gas, avoid water and amine loss and to provide a reflux stream.

**Figure 1.2:** Simplified flow sheet of amine based CO\textsubscript{2} capture process
There are a number of technical challenges with the implementation of chemical absorption processes. The first technical challenge is the extensive capital expenditures associated with the large volume of packing required. Thus, there have been many innovative designs suggested in the literature to reduce the column size. For example, researches suggested the use of rotating packed bed columns leading to an enhanced centrifugal acceleration that results in intensified mass transfer driving force and hence reduced column size (Cheng and Tan, 2011; Jassim et al., 2007; Joel et al., 2014; Ramshaw and Mallinson, 1981; Reay, 2008). Further, many authors also investigated the use of a hybrid system that couples oxygen-enriched combustion with chemical absorption plant (Doukelis et al., 2009; Huang et al., 2012; Zanganeh et al., 2009). The results obtained highlighted a massive reduction in the required packed volume (Doukelis et al., 2009; Huang et al., 2012). However, further investigation with regard to solvent degradation in the presence of oxygen is needed.

The second technical challenge is the high operating cost associated with large parasitic energy demands of the solvent generation and CO₂ compression system. Therefore, there have been many attempts in the literature to minimize this energy penalty through developing innovative solvents and configurations of the CO₂ capture plant (Amrollahi et al., 2011; Amrollahi et al., 2012; Darde et al., 2012; Freeman et al., 2010; Karimi et al., 2011; Oyenekan, 2007).

The third technical challenge is the presence of oxygen, and acidic components such as, Nox and Sox mixed with the CO₂ in the flue gas. Oxygen can cause degradation of amine and its presence at high concentrations can lead to massive corrosion of the internal parts of the absorber. Acidic components reacting with the amine results in the formation of salts, which causes loss of the solvent and reduction in the absorption capacity. Further, acidic components reacting with the amine can also result in the formation of nitrosamine, which poses a health risk to humans as it enters the atmosphere and undergoes further atmospheric degradation. Thus, there are specifications for amine tolerance. Those reported by IEA require that the processed gas should be no more than 90 ppm O₂, 10 ppm SO₂ and 20 ppm Nox (IEA, 2004). A separate unit to remove the impurities in the flue gas is therefore needed.
before using post combustion amine scrubbing. Alternatively, prevention methodologies that minimize slippage of amine and its degradation products to the atmosphere can be applied. The core technology is to use a water wash system installed at the top of the absorber to cool the flue gas to a temperature that minimizes its vaporization. Other promising technologies such as acid water removal, filters and demisters in addition to utilizing UV-light minimize the slippage and reverse the degradation products (i.e., nitrosamine and nitramine) back to amine (Kolderup et al., 2011). These all can be applied once a well-defined amine emission standard is defined (e.g., 0.2ppmv).

1.1.3 \( \text{CO}_2 \) TRANSPORTATION MODES

There are various means of \( \text{CO}_2 \) transport including pipelines, rail, road and ship. Analysis with respect to costs, capacity, distance and means of storage has shown the limited ability of rail and road to compete due to the lack of capacity and high cost (Metz et al., 2005; Skovholt, 1993; Svensson et al., 2004). Therefore, \( \text{CO}_2 \) pipelines are considered the best means of transport onshore. Offshore, pipelines and tankers are equally feasible modes of \( \text{CO}_2 \) transport due to their similarity in cost per ton of \( \text{CO}_2 \) transported (Metz et al., 2005; Svensson et al., 2004). Although millions of tonnes of \( \text{CO}_2 \) has already been transported from natural underground deposits via pipelines for EOR projects since the 1960s, there are a number of technical challenges involved with transporting \( \text{CO}_2 \) from CCTS projects.

The first technical challenge is the presence of impurities that affect the physical properties of the flow such as density and compressibility, which in turn affect the capacity and the safety of the pipeline (Mohitpour et al., 2008). Further, the variability in seasonal temperature between the summer and winter affects the physical properties of the flow in pipelines and hence changing the operating capacity of the pipeline.

The second technical challenge is a risk of leakage especially as most of future \( \text{CO}_2 \) pipelines might be crossing populated areas. Thus, standardised guidelines should be enhanced with safety features, which prevent pipeline ductile fracture and minimize the risk of leakage.
1.1.4 CO₂ STORAGE OPTIONS AND ISSUES

In principle, CO₂ can be stored in many places, including, in the ocean at great depth, in deep saline formations, in unminable coal beds, and in oil / gas reservoirs. The last of these (especially for EOR) has great potential to push the CCTS down the learning curve. In fact, more than 30 million tons of CO₂ is injected yearly for EOR worldwide and increasing this could add economic benefits to the implementation of CCTS. The process consists of mixing CO₂ with oil in the reservoir, resulting in a lowering of the viscosity of the trapped oil and its displacement toward the production well.

There are a number of issues involves with CO₂ storage in geological formations. The biggest hurdle is the risk of leakage, which affects public acceptance. Thus, a standardised risk assessment, management and communication framework such as OSPAR (OSPAR, 2007) and EU directive for CO₂ storage (EC, 2009), directive should be implemented for the whole lifetime of the project. Further, public acceptance should be raised by building an understanding of the characteristics of CO₂ stored in this way. When CO₂ is injected into a porous rock formation, it displaces the fluid, which is already there (e.g., oil in EOR). Since the CO₂ needs to be at a temperature and pressure consistent with dense or supercritical phase, the reservoir should ideally be at a depth of more than 800 m. This will also mean that the density of the CO₂ is 50 to 80% of the density of water (Metz et al., 2005). There are two trapping mechanisms for the retained fraction of CO₂, namely physical and geochemical. The stratigraphic and structural (physical) trapping mechanism works by blocking upward migration of CO₂, which is provided by an impermeable layer known as “cap rock”. Added to that, capillary forces can provide physical trapping by retaining CO₂ in the pore space of the formation. The geochemical trapping mechanism occurs when the CO₂ dissolves in the formation fluid and then reacts with the cap rock minerals, which takes thousands of years to occur, forming solid carbonate minerals (Metz et al., 2005).

The second technical challenge is the difficulty in estimating capacity and injectivity of each potential storage site. This is a data intensive characterization approach that requires an understanding of geoscience and reservoir engineering. It involves seismic surveys, core
sampling, lab work and model simulations. Although EOR storage sites have been extensively characterized, the data that determines the capacity and injectivity of the reservoir such as porosity and relative permeability is not disclosed in the open literature.

1.2 CCTS network design problem

The CCTS network design problem involves formulating the problem using different methods to identify appropriate values of some of the following decision variables: sources to be included in the network; degree of capture from each selected source; network topology including pipeline sizes, capacity and flow rate; sinks to be included in the network. Previous work formulated the design of CCTS network problem using the following approaches (see chapter 2): a simplified approach in which the potential CCTS networks were obtained by limiting the distance between attractive CO₂ sources and sinks; scenario based approaches in which different scenarios are manually assessed using cost and benefits of deploying CCTS networks at varying scales as performance indicators while having different market structures and incentives; heuristic approaches in which the problem is formulated and solved using generic algorithms; systematic approaches in which performance objective functions presented in mathematical form are used to find the optimum layout of the CCTS network.

The CCTS network design problem is best dealt with using systems modelling and optimization. It is characterised by a set of mathematical equations representing performance objective functions that assess alternative decisions of the system and a set of equality constraints that represents the behaviour of the system in addition to inequality constraints that limit the solutions to a feasible region only. The optimization-based model comprises parameters (e.g., CO₂ reduction target) and decision variables that can be binary (e.g., establish capture plant or not) or continuous (e.g., amount of CO₂ transported along a particular link). The solution obtained while maximizing or minimizing the objective function (e.g., cost, environmental impact) and incorporating the constrained equations that limit the
feasible region (e.g., capacity of pipelines) is the global optimum, if it is formulated as mixed integer linear programming (MILP) problem or other convex model. Thus, this makes optimisation-based network design ideal for decision makers. This type of model can be classified according to how uncertainties of the parameters are handled and the level of detail incorporated, leading to: deterministic; stochastic; and multiscale models. The first two approaches were used in the literature to find the cost optimum CCTS network while utilizing single-scale models in which cost and physical models of many components were simplified or overlooked (see chapter 2).

On the other hand, there have been limited attempts in developing multiscale modelling approaches in which the complex CCTS system that exhibits behaviours across different length and time scales is described using a series of interacting scale-specific models. This ensures that the science governing the behaviour of the components is taken into consideration while making non-trivial strategic decisions. There is only one group in the USA developing multiscale CCTS model in which storage site models that range from the pore scale to the reservoir and site scales are coupled with network models (Keating et al., 2010; Middleton et al., 2012a; Middleton et al., 2012b). However, the details of the capture plant and compression train models were overlooked. Given the fact that the main economic barrier that needs to be overcome is the cost incurred with establishing capture plants and compression trains, there is a need to include detailed models of these components with the CO₂ network model.

1.3 Aim and objectives

The aim of the thesis is to fill this gap through the development of a multiscale modelling and optimization approach that integrates all the components of CCTS to enable us to provide decision makers with a systematic tool which will help them find and analyse the cost optimal deployment of CCTS infrastructure meeting reduction mandates at the national or regional level.
The main objectives are as follows:

- Develop detailed sub-process models of an MEA-based post-combustion capture plant, compression train and pipelines in gPROMS™.
- Validate these sub-process models to ensure a reliable prediction of the behaviour of the system across the integrated scales.
- Analyse the effects of key operating parameters on the performance of the MEA-based post-combustion capture plant and compression train coupled with a potential CO₂ source using selected non-monetized key economic and environmental performance indicators.
- Develop an optimization-oriented model of the MEA-based capture plant, compression train and pipelines in gPROMS™.
- Identify the key performance operating parameters and limiting uncertainties in the MEA-based capture plant and transportation system that need to be mitigated or optimised to ensure a safe cost-optimal network.
- Develop a multiscale supply chain network model in GAMS to design the cost-optimal network linking CO₂ sources (e.g., power stations) with potential sinks (e.g., depleted oil reservoirs) while utilizing a meta-model, which summarises the results obtained by the fine scale models.

1.4 Outline of the thesis

The remainder of this thesis is structured as follows:

- In chapter 2, the methods used on developing integrated CCTS systems in the literature have been reviewed while giving attention to: problem definition and how successful the solution was; objective function of the problem; topology of network; incorporation of details of CCTS components; taking into account economies of scale.
• In chapter 3, an equilibrium-stage model of an MEA-based CO₂ capture plant and CO₂ compression train was developed and implemented in gPROMS™. The proposed model was validated using data from the CASTOR project. The performance of the CO₂ capture process and compression coupled with a combined cycle gas turbine (CCGT) power plant was described using selected non-monetized key economic and environmental performance indicators. The effects of solvent lean loading, rate of CO₂ capture in addition to the temperature of the lean solvent and flue gas were examined. The regional impact of the effect of cooling water temperature on the compression duty was also examined.

• In Chapter 4, a detailed optimization-orientated model of an MEA-based CO₂ capture plant and compression train was proposed and implemented in gPROMS™. The model was applied to an exhaust gas typical of a gas-fired combined cycle power plant. This integrated model was used to determine the cost optimal control and design variables including capture bypass ratio at different degree of capture (DOC). The effects of varying carbon prices on the levelized cost of CO₂ capture and compression were also studied.

• In Chapter 5, a detailed optimization-based model of the whole CO₂ transport system including compression train, booster pump and pipeline was developed and implemented in gPROMS™ and was then successfully used to simultaneously find the cost optimal design considering a case study under variability in seasonal temperature and uncertainty in composition. The decision variables obtained included pipeline diameter in addition to design and control variables (i.e., compressor output pressure and rating power, pipeline operating velocity, compressibility and pressure drop) that were overlooked or assumed to be at constant values in the literature.
• In Chapter 6, an integrated whole-system model of a CO₂ capture, transport and storage (CCTS) network was developed in order to design the cost-optimum network linking CO₂ sources (e.g., power stations) with potential sinks (e.g., depleted oil reservoirs). This model was then used to determine the optimum location and operating conditions of each CO₂ capture process while giving full consideration to the whole-system behaviour.

• In Chapter 7, a conclusion of the thesis and possible directions for further work in the area of CCTS are presented.
2 LITERATURE REVIEW

The first design of an integrated CCTS network started by Krickenberger and Lubore (1981) with the aim of supplying CO\textsubscript{2} for EOR. This approach is being revisited again with the aim of mitigating climate change with a prospective of large-scale CCTS infrastructures that need to be built within the coming decades to curtail CO\textsubscript{2} emissions.

The development of such integrated CCTS systems has to find answers to the following questions:

(1) Where to build capture plants, what technology to use and how much to capture?
(2) How to transport CO\textsubscript{2} and to which CO\textsubscript{2} sinks?
(3) What is the CO\textsubscript{2} network topology (i.e., single-source single-sink, hub-spoke and complex network shown in Figure 2.1).

![Figure 2.1: CO\textsubscript{2} network topology](image)

(4) How will the network evolve with future expansion (e.g. due to national reduction targets being implemented in phases)?
(5) How to deal with the uncertainties that affect the performance of CCTS components?
(6) How to deal with the transient behaviour of CCTS components (e.g., power plant running in sporadic way)?
(7) How to design safe, controllable and operable networks?
(8) What are the important details of the CCTS components that need to be captured in order to find realistic solutions?
(9) What are the key performance indicators (e.g., cost, environmental impact)?

There is abundant research that deals with the above-mentioned questions independently. In contrast, there are limited efforts being made to answer some combination of the network design questions simultaneously. This comprehensive review will examine the following components:

- The problem definition and how successful the solution was
- Objective function of the problem
- Topology of network
- Incorporation of details of CCTS components
- Taking into account economies of scale

The layout of the literature review is presented according to the approach used to develop integrated CCTS network designs. The approaches are classified into the following:

1. Simplified approaches;
2. Scenario based approaches;
3. Heuristic approaches;
4. Systematic “optimization based” approaches.

A summary of the literature examined in this chapter is shown in Figure 2.2 in which a further classification (e.g., static, temporal, stochastic) is explained in section 2.4. Outlines of the gaps in developing systematic based approaches for the optimum design of CCTS network are analysed.
Figure 2.2: Integrated CCTS network literature review

20
2.1 Simplified approaches

These studies consider the whole system but neglect to give sufficient weight to certain factors. For instance, Van-Bergen et al. (2004) highlights the economic benefit of CCTS, namely enhanced oil recovery (EOR) and coal bed methane recovery, but they assume that the distance between storage and high CO$_2$ content sources is an important cost factor and so recommend that this should not exceed 100 km. However, the benefits of revenue realized from EOR projects might exceed the marginal cost of longer pipelines. A similar limitation is evident in the work of Bradshaw et al. (2004). They applied a bottom-up approach, utilizing more storage site details such as risks, capacity, and injection depth to ensure better matching with the sources and hence better utilization of the CCS infrastructure. This study has estimated Australia’s storage potential to be 110-115 Mt CO$_2$/year. However, once again, they limit the distance between appropriate storage sites and emission sources to less than 300 km.

2.2 Scenario-based approaches

This approach is used mostly by governments and consultant companies with the aim to assess the cost and benefits of deploying CCTS networks at varying scales while having different market structures and incentives (e.g., CO$_2$ emission credits, reduction targets, value for EOR and utilization). For example, the Poyry Energy (2007) study examined the cost and opportunity of having varying scales of CCTS infrastructure in the UK. Each component of the CCTS system in the region is looked at separately in order to find the cost optimal choice for each one, considering IPCC report cost data for the capture plant, the IEA GHG cost models for the pipelines (IEA GHG, 2009a) and the British Geological Survey data for storage. The connections between these CO$_2$ sources and sinks are based on manually picking different network topologies (e.g., direct connect and hub-spoke) and assessing their value chain. The latter topology was shown to have a lower cost for CO$_2$ transportation to existing gas pipelines, which is then used to transport CO$_2$ back to the reservoirs. The costs of the
whole CCTS systems were obtained by aggregating the optimum cost for each component in addition to accounting for uncertainties in fuel prices and carbon credits.

Similarly, the cost assessments of having a cluster of \( \text{CO}_2 \) networks in the Yorkshire and Humber region that transport \( \text{CO}_2 \) emitted from distinct sources with a common trunk line to geological storage were analysed for a period spanning from 2012-2030 (Yorkshire Forward, 2008). The study classified the \( \text{CO}_2 \) sources according to the amount of \( \text{CO}_2 \) emitted and focused more on the network development for 3 scenarios that represent the scale of CCTS deployment. Details of the \( \text{CO}_2 \) capture plants and storage plants were not incorporated in this study. Further, re-using existing gas pipelines was not included in this study. The network topology used in this study was based on a hub- spoke approach despite the fact that it was presented as a tree shape solution. The effect of impurities on the \( \text{CO}_2 \) transportation and the need for common entry specifications were highlighted in this study as it was focused more on the transportation side.

On the other hand, (Brunsvold et al., 2011; Jakobsen and Brunsvold, 2011; Jakobsen et al., 2011; Jakobsen et al., 2008; Røkke et al., 2009) standardize the scenario-based approach through defining common module parameters that are common for all the components of the CCTS system (e.g., capital cost, operating cost, energy usage) and global parameters that demonstrate the uncertainties associated with the market conditions such as fuel price and carbon credits. The net present value is used as the aggregated level common parameter to analyse the cost and benefit of the network considering the lifetime of the project. This value-chain approach was used to assess the effects of different technology improvements, markets and regulations on the cost and profits of CCTS for EOR or storage in saline aquifers. These studies shed light upon the importance of having common module parameters across the whole CCTS components that help assessing the performance of the whole network while taking account of uncertainties.
2.3 Heuristic approaches

Krickenberger and Lubore (1981) designed the first integrated CCTS network in order to supply the CO$_2$ for EOR. The objective of the study was to find the minimum cost of a CO$_2$ network connecting hypothetical coal gasification plants to reservoirs amenable to CO$_2$ for EOR. The problem was formulated as a set of nodes representing both gasification plants “sources” which emit certain amounts of high CO$_2$ content gas and oil reservoirs “sinks” having a specific capacity per day. The connection between each source and sink is allowed in one direction though an arc representing a 0.507 m (20 inch) pipeline with specific capacity. This connection comprises a cost representing pipeline construction, compression in addition to operating and maintenance. The network topology was based on single source single sink (e.g., large basin) matching. The cost of the capture plant was not included in this study because it was based on gasification plants being built in the future with specified capacity. The least cost network that defines which route to pick and how much CO$_2$ to transport and to which geological storage was obtained through the out of kilter algorithm (i.e., heuristic greedy algorithm) (Fulkerson, 1961). The main drawback of this formulation is the neglect of economies of scale that can be obtained from combining CO$_2$ sources into a common trunk line. Further, the obtained solution is not guaranteed to be the optimum one.

Turk et al. (1987) expanded the previous CCTS network model and added complexity into it. The problem was formulated as having a number of prospective coal plants that can be modified with an oxy-fuel combustion and then transport this CO$_2$ (i.e., gathering system) to existing gas pipelines (i.e., mainlines) within a range of 100 miles. Then, these mainlines move the CO$_2$ in the reverse direction to a prospective oil reservoir through a pipeline (i.e., feeder line) constructed between the mainline and the reservoir. A developed model based on the knapsack problem tries to find the combination of CO$_2$ sources, existing pipelines and CO$_2$ storage sites for EOR that maximize the profit obtained from selling CO$_2$ for EOR projects in addition to acid rain credits. The following data are used in the model: (1) Power plant CO$_2$ emissions, cost of retrofitting a capture plant and building a gathering system from source to mainline, and credits obtained from avoiding acid rain; (2) Mainline capacity and
cost of utilization; (3) Oil fields feeder line cost, demand of CO\textsubscript{2} and value of utilization obtained from the reservoir development model of the National Petroleum Council. The mathematical formulation was solved using a logical solution algorithm based on a greedy heuristic approach that was believed to be a more efficient solver at that time especially when considering a larger size problem. The main drawback of this approach is that it assumes a direct link for the feeder line and the gather line, which might limit the benefits of economies of scale. However, this model showed the benefit of reusing existing gas pipelines in the CCTS deployment.

These heuristic approaches have not been used recently for designing CCTS networks because the solution obtained is not the optimum one. However, Fimbres Weihs and Wiley (2012) revisited this approach because of the flexibility on formulating the problem while incorporating non-linear aspects of the CCTS network. They developed a heuristic based approach using a generic algorithm to design the near cost-optimal solution of the steady state CCTS network topology. This method represents the CO\textsubscript{2} source and CO\textsubscript{2} storage as nodes where one or more operations (e.g., emission, capture, compression, mixing, splitting, injection and storage) may take place. The physical connections between these nodes are allowed through “links” that represent the pipelines and any booster stations. This model objective was to find the near optimal minimum network cost per ton of CO\textsubscript{2} avoided considering the cost of a capture plant associated with 90\% degree of capture, the transportation pipelines with booster station and the number of wells drilled for storage. Despite the flexibility of this model in setting the pipeline pressure at each node, there are many drawbacks within this methodology. This model formulation requires a large amount of input data from the users to find the solution and hence increases the size of the problem. Further, the solution obtained is not the global optimum. Thus, this method is a practical option for complex problems in the absence of a realistic rigorous approach.
2.4 Systematic “optimization-based” approaches

Another important approach to design the CCTS network is through modeling the problem in a mathematical formulation that has a standardized set of common key performance indicators for the whole chain (e.g., net present value, environmental impact). It comprises parameters (e.g., CO₂ reduction target) and decision variables that can be binary (e.g., establish capture plant or not) or continuous (e.g., amount of CO₂ transported). The solution obtained while maximizing or minimizing the objective function (e.g., cost, environmental impact) and incorporating the constrained equations that limits the feasible region (e.g., capacity of pipelines) is the global optimum. Thus, this makes it ideal for decision makers. This type of model can be classified according to how parameter uncertainty is handled and the level of details incorporated, leading to: deterministic; stochastic; and multiscale models. All of these can have some parameters that remain steady or change in a predictable way with time (e.g., known reduction targets at different time). This can further classify the approaches into static “single-period” and temporal “multi-period”.

2.4.1 Deterministic “optimization-based” approach

Akimoto et al. (2004) designed the CCTS network while utilizing an optimization based model (i.e., Mixed Integer Linear Programming Model (MILP)). The objective function was to minimize the total cost of energy and CCTS in Japan in parallel with other mitigation options that meet energy demand, and a reduction target of 0.5% per year between the years 2000 to 2050. Thus, the CCTS aspect was embedded in this model as a carbon mitigation plan. They divided Japan into 20 onshore and 20 offshore regions. Their mathematical model is designed to inform decision-making on when, where and how much CO₂ sequestration will be implemented in addition to fuel and energy mix variations in Japan. The network topology used in the study is based on a hub-spoke network as it only considers transportation between regions. The economy of scale in transportation was neglected in this study because a linear cost correlation of pipelines that depends only on distance was assumed regardless of the diameter of the pipeline. Further, there are many cost components of the CCTS chain
neglected in this study such as compression and liquefaction in addition to loading facilities needed for CO₂ liquid transportation in tankers. CO₂ sequestration in aquifers and the deep ocean were considered in this study. It is suggested that Japan will economically be a suitable place for the development of CCTS by 2020. The results show that more CO₂ will be sequestered in the ocean than the aquifers, which might be as a result of the limited capacity of the aquifers in Japan or because of the neglect of many cost intensive components such as CO₂ liquefaction. This highlights the importance of incorporating details of the CCTS in finding a realistic CCTS network. It is noteworthy that delay of CCTS deployment in Japan is because most of the emissions reductions in the first two decades will come from switching to a lower CO₂ content fuel.

On the other hand, Bakken and von Streng Velken (2008) have developed a Linear Programming (LP) model for CCTS network that was consistent with their developed infrastructure models for gas, electricity and heat. This model was used as a systematic tool to compare different design options such as the location, size and timing of the investment in fossil fuel power plants and CCTS networks while considering the net present value, which includes investment cost, emission taxes and usage of CO₂ for EOR, as a performance indicator. The usage of an LP method in this study has limited the model potential in defining discrete choices such as the location of a new power plant and the diameter of the pipeline that might be used. Thus, this model has limited usage for detailed design of CCTS networks.

As part of an early work, a single scale, snapshot model for the CO₂ supply-chain network in Abu Dhabi has been developed (Alhajaj, 2008). It was formulated as Mixed Integer Linear Programming (MILP) optimisation model that minimizes the Net Present Cost (NPC). It has to decide which CO₂ source to include, and how much of this CO₂ will be transported to a specific oil reservoir amenable to CO₂ flooding, while using a pipeline with a specific diameter. The network topology in this work was based on complex networks where pipelines can be merged into a trunk line to exploit economies of scale. The model was used to link three major CO₂ sources with three major CO₂ sinks while satisfying different portions
of demand for EOR activities. The main limitation of this study is that it assumed linear cost of capture correlations obtained from commercial plants in the literature.

Middleton and Bielicki (2009) and Middleton et al. (2011) have developed a similar steady state MILP model (i.e., SimCCS) and demonstrate it using 37 CO$_2$ sources and 14 sinks in California in addition to a case study of capturing CO$_2$ from oil refineries to supply the potential market of CO$_2$ for EOR activities in the US Gulf region. The objective was to minimize the total cost that meets varying reduction targets or demand for EOR sites. This model was also used to find the optimum reduction target and CCTS network layout while having a fixed CO$_2$ price (Kuby et al., 2011a). The SimCCS model takes into account the economies of scale while using pipelines (Kuby et al., 2011b). It also utilises ArcGIS as a useful tool that helps find feasible routes for the pipelines. It comprises a number of cells that have 1 km$^2$ size and an aggregation weight of the obstacles (i.e., slope, protected area such as parks and crossing railway, road and highways) that might be encountered. This weight forms a multiplying factor for the pipeline crossing a particular cell. The network topology comprises of a number of sources and sinks represented by nodes and potential arcs that connect these nodes (i.e., source-source, sink-sink and source-sink). The raster paths are defined by choosing the cells with minimum weight factor, which are then converted into discrete vectors with respective cost. This can further be refined through removing redundancy and simplification (i.e., emerge nodes, collapse and cut side of triangles) that does not significantly change the cost (Middleton et al., 2012c). The limitation of this model is that it considers the simplified published cost of the IPCC (2005) report, which does not take into account any site specific factors such as local flue gas compositions and availability of cooling water.

In order to design a CCTS network that takes into account the parameter changes along the time of utilizing CO$_2$ for EOR projects, Klokk et al. (2010) developed an MILP temporal optimization model. The temporal aspects of this system are due to the changes of CO$_2$ demand with time and the benefits of producing extra barrels of oil for each ton of CO$_2$ injected (i.e., EOR ratio). For example, in the first one to two years, there is a large demand
for CO₂ without any EOR ratio obtained. Then, there is growing demand for CO₂ while the EOR ratio is increasing at a similar rate until it reaches a peak. In the last period, the demand of CO₂ decreased massively due to the availability of recycled CO₂ and the decline of the EOR ratio. Therefore, sequencing the development of CCTS network is an important factor in EOR projects. This work takes into account a case study of Norway where there are few potential CO₂ sources (e.g., few gas fired power plants because 90% of electricity generation is from hydro) with a known cost of capture. There are also many oil reservoirs amenable to CO₂ flooding for EOR in addition to the benefits of acquiring EU ETS (i.e., European Union emission trading schemes) credits while storing CO₂ in aquifers. The objective function was to maximize the NPV of the value chain of designing CCTS network for the whole time period with the above mentioned benefits. The decisions include when and where to build the capture plant and the transportation pipelines with different sizes in addition to which oil reservoir to pick and how much to inject each time. The network topology in this work was based on a hub-spoke model including regions where neighbouring sources and sinks are grouped into one. This study was very successful in highlighting the benefits of using a temporal approach for defining the optimum CCTS network for EOR projects.

Similarly, (Kemp and Sola Kasim, 2010) developed a temporal linear model that finds the CCTS network layout for a UK case study. The temporal aspects considered in this study are limited to the varying CO₂ emissions at selected sources in specific locations in addition to the changeable CO₂ storage capacity (i.e., 28njectivity) with time in active oil reservoirs for EOR and/or permanent storage sites such as depleted gas and oil reservoirs and saline aquifers. This study did not take into account any dynamic reservoir response for EOR obtained in the earlier study and assumed a constant CO₂ demand for the whole time period. However, the consideration of exploiting oil reservoirs as permanent storage sites once they reach cessation of oil production is an important element highlighted in this study. The objective function was to minimize the total pipeline cost needed to facilitate a certain reduction target that was defined by different scenarios such as accelerating CO₂- EOR start date with a specified minimum CO₂ injection in reservoirs per year. Although the location of
CO₂ sources and emissions were incorporated in this study, the cost of CO₂ capture was neglected. The topology of the network considered was based on single source single sink matching while utilizing a pipeline with a single diameter. This is due to the formulation of the model as a linear programming model, which limited the model capability in using pipelines with different sizes. Further, it avoided the consideration of building a larger pipeline initially that will accommodate future expansion. This model was not a successful approach because of the overflow obtained in a few of the sinks while meeting variable scenarios. This is due to the LP 29njectivi and topology used, in which flexibilities are limited, and hence it limits finding a realistic solution such as those obtained from MILP formulations and complex topology.

In contrast, there have been many attempts to integrate the design of CCTS infrastructure with the development of a cost optimal low carbon energy system at both national and regional levels. The CCTS systems is embedded in a MARKAL model (i.e., a linear optimization model for energy allocation developed by the IEA) as a carbon mitigation option that can be used in parallel with other low carbon technologies such as renewable energy and nuclear. Van den Broek et al. (2009; 2010) developed a stepwise methodology that aims to design the cost optimum CCTS network. The first step was to build an inventory of the CO₂ sources (i.e., power plants and industrial plants) within the region of the Netherlands. Then a database of the CO₂ sinks with a ranking option considering their capacity and 29njectivity were obtained. After that, these CO₂ sources and sinks are clustered into regions in which the centre was decided based on a weighting factor for each source, e.g., higher weight for a larger source. Utilizing the ArcGIS (a geographical information system) and the hub-spoke topology, the possible least-cost routes for the trunk lines that connect source and sink regions were identified considering land-use. This developed database is then fed into a MARKAL model in order to find the cost optimal technical configuration of energy systems and CO₂ infrastructure for the period of 2012-2050 while considering a specific carbon price. The mathematical model used to solve the CCTS network problem was formulated as a MILP model that takes into account the temporal
aspect (i.e., phase in development with time). The results highlighted a reduction in the cost of the pipeline in 2050 due to the investments that were made in the early stages. It also highlighted the benefit of capturing the CO$_2$ from industrial sources that have been overlooked by policy makers. However, the use of a hub-spoke approach has limited the model in finding complex CO$_2$ networks that could be more cost-effective.

A similar stepwise approach was used to design optimum trans-European CO$_2$ networks. The CO$_2$ sources (i.e., power plants) and sinks (mainly offshore storage because of public acceptance) were aggregated into clusters represented by nodes that have a radius of 50 Km of coverage zone from the centre of the node. The purpose of the work was to map the network evolution while considering the temporal aspects of the problem for the duration of 2015-2050. The cost optimal trans-Europe CCTS network that would be required to transport all the CO$_2$ from deployed capture plants according to exogenous scenario based on PRIMES model was obtained from running the MILP formulation. This study predicted the need to build an oversized pipeline at the initial stages that will meet the expanded CCTS projects in the future. Thus, it is important to incorporate a policy that supports such an early higher investment that will be more cost effective for future expansions (Morbee et al., 2010; Morbee et al., 2012).

In order to analyse the effects of planning CCTS networks at the national and global level in exploiting common storage sites, Strachan et al. (2011) examined the consequence of optimizing energy system models (e.g. MARKAL and TIMES) at alternative scales in the potential of storing CO$_2$ in Utsira formation. This is a common storage site that will be shared among the countries in the North Sea region (i.e., Norway, UK, Denmark, Netherlands and Germany). The model was formulated using the stepwise methodology similar to van den Broek et al. (2009; 2010) while harmonizing the data in the energy models developed for different scales. The inputs of the models were the CO$_2$ emission reduction targets obtained from the Times PanEu-27 and the amount of electricity consumed and imported. The results of modelling at the regional and local scales highlighted discrepancies in exploiting Utsira formation as a common storage site. This was a result of varying CCTS deployment projected
by the MARKAL and TIME models in which different policies and technical assumptions were embedded.

The successful implementation of the previous approach encouraged other energy modellers to use the model for different regions. For example, Boavida et al. (2011) proposed a research plan of developing an integrated CCTS infrastructure in the West Mediterranean Countries (i.e., Portugal, Spain and Morocco). The objective was also similar to design the cost-optimal CCTS infrastructure at the regional level, while using similar approaches of gathering the CO₂ sources and sinks into hubs. They consider all the transportation options including rail, ship, and pipelines. The cost minimum routes are found while utilizing ArcGIS. These routes will then be investigated with deep analysis with regard to their potential considering different scenarios, techno-economic evolution and public acceptance to find the optimal solution.

Most of the above mentioned studies focused on minimizing the cost of the CCTS network; however, Han and Lee (2011a) developed an MILP mathematical model with the objective of finding the optimum CO₂ capture, transport, storage and utilization (CCTSU) network that maximize the profit generated from CO₂ utilization in the chemical industry (i.e., butanol from algae and green polymers) while meeting a CO₂ reduction target. This model was applied to a case study of east Korea in which the CO₂ sources (i.e., power, steel, oil refinery and petrochemical plants) and sinks (e.g., chemical industry plant, reservoirs) were clustered into regions. The costs of capture from these different sources were obtained from the literature (e.g., cost of capture and capacity of the plant) and then by applying the six-tenths role to incorporate economies of scale. This work expanded the modes of transportation between regions to include trucks and rail in addition to ships and pipelines with different diameters. One of the advantages of this model is the incorporation of learning rates that reduce the cost of capture in 2020. A noteworthy limitation of this study, however, is that it overlooks the compression cost in the model. Further, CO₂ was assumed to be transported as a sub-cooled liquid phase through all modes of transportation including pipelines. This might add another challenge of maintaining a lower temperature pipelines especially in the summer.
Thus, considering these physical details of the CCTSU components are very important to ensure the compatibility of the optimum design obtained by high-level analysis.

This work was expanded to include temporal factors that change along the time of planning (i.e., 2011-2030) (Han et al., 2012a). The included varying parameters are the CO$_2$ emitted from different CO$_2$ sources, the different reduction targets, and the reservoirs capacity and availability with time. This study was successful in outlining the phasing in the development of the CCTS network while taking into account the economies of scale.

Recently, Middleton et al. (2012d) extended their previous SimCCS model to account for similar temporal effect of having varying reduction targets at different times of planning. This model examines the gradual evolvement of the network through building oversized pipelines that would meet future expansion. The topology of the network considered in this study was based on complex networks, which allow a more realistic forward planning of CO$_2$ networks routes that can be built with minimum cost. This model is important to help decision makers optimize when as well as how to deploy CCTS networks.

Most of the above work considered an optimum network using a single objective function that relates to the cost; however, Lee et al. (2012) developed an MILP model that considers finding the cost optimal CCTS network while minimizing the LCA (life cycle assessment) of the all of the CCTS components. This information is obtained from building the inventory of CCTS components (e.g., emissions, land use, extraction of fossil fuels) that help evaluate their impacts and damages value (e.g., MJ/ t CO$_2$, PDF (potentially disappearing fraction) m$^2$ yr/ t CO$_2$). These values are then standardized using a common weighting factor (i.e., point number) indicated by the Eco-indicator99 score. The mathematical formulation of the multi-objective problem was based on minimizing the NPV cost while meeting a specific reduction target in addition to the constrained minimum accepted environmental impact that was set up using the e-constraint method (i.e., Pareto approach). This modelling approach in which LCA was included as a KPI will help decision makers understand the tradeoffs between choosing different layouts of CCTS networks.
2.4.2 **Stochastic Model**

The objective of the stochastic model is to develop a robust optimization model that takes into account uncertainties in parameters. Han and Lee (2011b) extended their previous model to include the uncertainty of the mandated CO\textsubscript{2} reduction target. The objective function was modified with an equal probability of having three different scenarios (i.e., low, average and high). Mathematical equations that have variables that depend on the CO\textsubscript{2} reduction target were reformulated. The authors assumed a formulation based on two stage stochastic modelling in which the first stage decision variables reflect initial investments and the second stage variables are decided to minimize the penalty associated with first choices. This model was useful in simultaneously finding all the non-trivial decision variables that depend on all scenarios. However, the assumption of having uncertainty in carbon reduction targets while meeting a specified reduction target has limited the usage of the model. This is due to the fact that the model tries to satisfy the maximum reduction targets that were set by the problem while considering a steady state formulation. Recently, Han and Lee (2012) extended this model using a previously developed multi-period model. This study considered more applicable scenarios such as the uncertainty in product prices and operating cost in addition to the previously limited scenario of uncertainty in CO\textsubscript{2} reduction targets.

2.4.3 **Multiscale Models**

Most of the systematic paradigms used to develop an integrated CCTS design assume a simplified cost and physical model for the different CCTS components (e.g., capture plant cost, storage capacity and cost) that overlook many size specific factors. However, Keating et al. (2010) optimized the CCTS network needed to manage the CO\textsubscript{2} produced from the oil shale activities by integrating models of site scale geological performance (CO\textsubscript{2}-Pens), regional scale infrastructure design (SimCCS) and oil shale production simulator (CLEAR\textsubscript{off}). This later model accounts for CO\textsubscript{2} produced from the electricity production required to heat the oil in addition to the cleanup of the rotor gas coproduced with it. Two scenarios were considered in the study: (1) Production of electricity from NGCC both onshore and offshore;
(2) Production of electricity from NGCC onshore and IGCC offshore. The objective function was to minimize the cost of the total CCTS infrastructure that meets the reduction targets from the above-mentioned scenarios while considering explicit details of the storage site factors that affect its cost, capacity and injectivity. The detailed storage site model was used to define 9 storage sites while considering reservoir’s details such as the depth, the accessibility of the pore space while utilizing GIS that avoids regions that have slopes and water bodies. Further, the CO$_2$-Pens model was used to provide more information with regard to storage capacity and cost associated with building many wells in addition to a network of local pipeline distribution between these wells to inject certain amounts of CO$_2$ for the duration of 50 years. The main parameters that affect the storage capacity and its associated cost are the permeability, porosity and thickness. The first one affects the number of wells needed and hence cost and the latter variables define the capacity of the reservoirs. The average variables of cost and capacity obtained from 100 realization of the Monte Carlo simulation were fed into the SimCCS model to optimize the whole CCTS network considering one oil shale basin and 9 storage sites. This study took into account economies of scale obtained from the SimCCS model and modified the GIS weighting factor on it by taking into account the following geographical factors: land use; land ownership; population density and topography. The study sheds light upon the importance of incorporating explicit details of the storage in defining a more realistic design of CCTS network. For example, the model might result in favouring a distant site that is cheaper to exploit compared to the proximate sinks that have higher costs outweighing the benefits of shorter pipelines. This type of tradeoff is over looked in simple models that consider a simple storage cost for all reservoirs.

Recently, Middleton et al. (2012b) extended this model to account for uncertainties in the main parameters (i.e., permeability, porosity and thickness of reservoir) that affect the storage capacity and cost. These main variables were simulated with 100 runs of the Monte Carlo simulation that results in varying storage capacity and cost. A random selection of these variables were considered in the 1400 simulations of the SimCCS model finding the cost
optimum CCTS network design that meets 14 different reduction targets for a similar oil shale case study outlined in earlier study. The objective of the study was to highlight the commutative layout of networks that is robust against uncertainties in cost and storage estimations. The study was focused on highlighting the propagating issues that might arise from uncertainties in the storage sites in the whole CCTS network design. The work underscores the tradeoffs that decision makers need to make between investing in site characterization and handling uncertainty through investments on a flexible network.

Lately, Middleton et al. (2012a) expanded the previous models through incorporation of phenomena occurring at the pore and reservoir scale into the site and regional scale models (i.e., CO$_2$-Pens and SimCCS). Each model at specific scale will be able to capture a behaviour that propagates to the adjacent scale. For example, the Lattice Boltzmann method captures the interfacial tension at the pore scale, which influences the relative permeability predicted at the reservoir scale while using the Finite Element Heat and Mass (FEHM) transfer model. This will affect the number of wells and pipeline distribution and hence cost predicted by the site scale model (i.e., CO$_2$-PENS). Further, this model is integrated with the SimCCS model that finds the optimum local distribution of the CO$_2$ between wells in addition to the cost required to extract saline water and treat it. The obtained reservoir costs of exploitation obtained from the cross-scale models provide inputs to the regional scale model (i.e., SimCCS) that find the deployment of the cost optimum CCTS network. The study demonstrated the methodology through designing a CCTS network that met varying reduction targets while considering 64 coal-fired boilers and 6 reservoir sites. These results emphasize the need to comprehend the science and understanding of phenomena at different scales in order to successfully design cost-optimal and safe networks.
2.5 Summary

From the literature review, all of the systematic models that have been used for CCTS network design did not include the explicit details of the CO$_2$ capture plant and compression train as outlined in Table 2.1. This is considered to be the major cost component of the whole CCTS network and hence more fine-scale models describing the phenomena that happen at the capture plant are needed to find and optimize the decision variables that propagate to the whole CCTS network design. There are few studies in the literature that examine how amine-based post combustion capture plant can be optimised in terms of operability, efficiency and cost. For instance: Lawal et al. (2010; 2012; 2009) developed detailed dynamic model of the post combustion capture plant and coal fired power plant to assess the operability of the coupled system; Rao and Rubin (2005) and Abu-Zahra et al. (2007a; 2007b) examined the effect of degree of capture on the total cost of the capture plant. However, they did not consider the whole-system economics and performance of the CCTS network.

The objective of this work is to develop a multiscale model that incorporates a capture plant model comprising a molecular scale model (i.e., SAFT), film scale model (i.e., two film theory), unit scale model (i.e., mass and energy transfer) and cost model with a regional based model (i.e., MILP supply chain network).
### Table 2.1: Systematic CCTS network models gaps analysis

<table>
<thead>
<tr>
<th>Authors</th>
<th>Model type</th>
<th>Details of models incorporated</th>
<th>Objective function</th>
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<tbody>
<tr>
<td>Akimoto et al.(2004)</td>
<td>*</td>
<td></td>
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<tr>
<td>Alhajaj (2008)</td>
<td>*</td>
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<tr>
<td>Middleton and Bielicki (2009)</td>
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<tr>
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<td>*</td>
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<td>Profit</td>
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<tr>
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<td>Cost</td>
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<tr>
<td>Keating et al.(2010)</td>
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<td>Kuby et al.(2011b)</td>
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<td>Cost</td>
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<tr>
<td>Han and Lee (2011a)</td>
<td>*</td>
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<td>Profit</td>
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<tr>
<td>Middleton et al.(2011)</td>
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<td>Kuby et al.(2011a)</td>
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<td>Boavida et al.(2011)</td>
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<td>Morbee et al. (2012)</td>
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3 A TECHNO-ECONOMIC ANALYSIS OF POST-COMBUSTION CO₂ CAPTURE AND COMPRESSION APPLIED TO A CCGT: PART I. A PARAMETRIC STUDY OF THE KEY TECHNICAL PERFORMANCE INDICATORS

3.1 Introduction

Although there are several CO₂ capture technologies (e.g., absorption, adsorption, membrane separation and cryogenic separation) that can be applied to different CO₂ sources (Boot-Handford et al., 2013; Mac Dowell et al., 2010a; Rao and Rubin, 2002; Rubin et al., 2012), post-combustion capture using amine-based solvents is a promising choice owing to its technological maturity and commercial availability (Metz et al., 2005; Rao and Rubin, 2002; Rubin et al., 2012; Wang et al., 2011). There are, however, important drawbacks with the incorporation of post-combustion amine-based CO₂ capture in a power plant. In addition to the significant capital expenditure associated with these systems, the large parasitic energy demands of the solvent regeneration and CO₂ compression systems, and amine emissions to atmosphere are also of severe concern. This last point is of particular concern in hot countries, e.g., the Gulf Cooperation Council (GCC) countries, e.g., Qatar, UAE, Saudi Arabia.

The carbon capture plant is the most energy-intensive aspect of the CCTS value chain. Thus many studies focus on improving the performance and efficiency of the capture plant using various key performance indicators (KPIs). Reducing the energy penalty associated with solvent regeneration, increasing loading capacity and minimizing degradation were the main goals for designing innovative solvents in many studies (Darde et al., 2012; Freeman et al., 2010; Mangalapally and Hasse, 2011). Reducing energy penalty imposed on a power plant by the CO₂ capture plant (i.e., reboiler duty and electricity consumption) or minimizing cost of CO₂ avoided or improving exergy (i.e., available work) were suggested through innovative configurations of CO₂ capture system (i.e., absorber with inter coolers, stripper with vapour-compression and split flows to strippers with variable pressures) (Amrollahi et al., 2011;
Amrollahi et al., 2012; Karimi et al., 2011; Oyenekan, 2007). Further, minimizing energy penalty and cost of CO₂ avoided, and enhancing operating capacity were examined through considering different steam supply sources (i.e., natural gas auxiliary boiler (Romeo et al., 2008), internal steam flow from power plant (Lucquiaud and Gibbins, 2011; Romeo et al., 2008), auxiliary gas turbine (Romeo et al., 2008), solar collectors with thermal storage (Mokhtar et al., 2012)) in addition to storing rich solvent at peak hours and restoring it off-peak (Chalmers and Gibbins, 2007).

The effect of various degrees of capture and the option to allow a portion of the flue gas to bypass the capture process has been studied for the addition of an MEA-based CO₂ capture plant to a coal-fired power plant. It was evaluated according to the capital required per ton of CO₂ per hour and cost of CO₂ avoided. The results revealed the importance of variable degree of capture in reducing the cost of capture while having smaller units (Rao and Rubin, 2005). It has been observed that partial capture scenarios can appreciably reduce the capital and operating cost of decarbonising power plants (Hildebrand and Herzog, 2009; Mac Dowell and Shah, 2013; Rao and Rubin, 2006). This suggests that a phased deployment of CO₂ capture processes can be used to reduce “first-mover disincentive” (Hildebrand and Herzog, 2009). From a UK perspective, however, the UK Committee on Climate Change (CCC) recommends that from 2020 onwards, all newly installed power generation capacity needs to be “low carbon”, where low carbon is defined as having a CO₂ emission intensity of no more than 100 kg CO₂/MWhr, and no more than 50 kg CO₂/MWhr by 2030 (Committee on Climate Change, 2013). This recommendation would essentially rule out partial capture scenarios in the context of coal-fired power plants, in fact requiring greater than 90% DOC.

In order to determine the optimal value of selected key operating parameters (KOPs) (i.e., amine lean loading, degree of capture, stripper pressure and lean solvent temperature inlet to the absorber) of retrofitting an MEA-based post-combustion capture plant to a supercritical coal plant, reboiler duty, liquid circulation rate, cooling duty and cost were selected as KPIs (Abu-Zahra et al., 2007a; Abu-Zahra et al., 2007b). Others have cost-optimized similar KOPs of retrofitting a similar separation technology to supercritical coal plant while using
piperazine promoted calcium carbonate as the solvent (Oexmann et al., 2008). A recent study implemented in GAMS used a mixed integer nonlinear programming (MINLP) approach to find the cost-optimum operating parameters and dimension of the carbon capture and compression units attached to theoretical low CO₂ content exhaust gas that meet different degree of capture (DOC) (Mores et al., 2012a). Their results showed that the total cost varies linearly between 70-80 % DOC and exponentially at 80-95% DOC.

Previous studies have focused on determining the optimum design and operating parameters of CO₂ capture plants incorporated in fossil fuel fired power plants in Europe, where cooling water is readily available at a temperature in the range of 5-18°C. However, the majority of the economies of the GCC countries have extremely high CO₂ emissions per capita owing to the presence of energy intensive industry (Mac Dowell et al., 2011a). Further, these countries are gas-rich, and the majority of their energy is produced from the combustion of natural gas in combined cycle gas turbines (CCGT). It is therefore important, to assess the effects of attaching or retrofitting a capture plant with MEA to power plants (e.g., CCGT) in hot countries where the cooling water temperature reaches 33°C most of the year.

The objective of this chapter is to develop a mathematical model of an amine-based post-combustion CO₂ capture plant and CO₂ compression train, which can be used to help decision makers analyse the performance of such a system. This model is then used to identify the KOPs of the whole system. This model is used to evaluate the performance and efficiency of the capture plant while considering various KPIs. An important contribution of this work is the explicit consideration of the trade-offs between capital and operating costs, and environmental impacts through inclusion of indictors that represent the height of the columns, power consumptions and amine slippage. This required concurrent consideration of the design and operation of the entire CO₂ capture and compression system.
3.2 Methodology

3.2.1 Model Development

The proposed model of the CO$_2$ capture process and compression train was implemented in gPROMS$^\text{TM}$ and is illustrated in Figure 3.1. The model comprises a blower that receives a flue gas from a CCGT power plant and increases its pressure to overcome the pressure drop associated with the packed bed of the absorber column and direct contact cooler (DCC). This increases the temperature of the flue gas further, which then is cooled to 40-50 °C inside the DCC. This flue gas is then scrubbed using an MEA solvent in a packed column (i.e., the absorber). This rich solvent is regenerated in the stripper. A more detailed description of an amine-based CO$_2$ capture process was presented in section 1.1.2.6. The scrubber located at the top of absorber is used to remove excess water in the flue gas before venting it to the atmosphere. This is used to balance the water in the system. Following the capture plant, CO$_2$ is compressed in multi-stage compression train with intercoolers to the desired pipeline pressure (typically in the range of 10-15 Mpa).

---

Figure 3.1: Carbon capture plant with multi-stage compression process flow sheet modelled in gPROMS.
3.2.1.1 Stage model

One of the most complex aspects of the proposed model is the description of the phenomena of simultaneous heat and mass transfer with chemical reaction presented in the absorber column. There are a wide range of methods available for the description of these phenomena ranging from the relatively simple (equilibrium stages) to the more complex (rate based heat and mass transfer with chemical reaction kinetics) (Kenig et al., 2001). In the interest of simplicity, an equilibrium-based model has been implemented in this work. The packed height of the column is then obtained via the HETP concept (Mores et al., 2012b; Taylor and Krishna, 1993).

The SAFT-VR equation of state was used to describe the thermophysical properties and reaction equilibria in this work (Chapman et al., 1989; Chapman et al., 1990; Galindo et al., 1998; Gil-Villegas et al., 1997). The chemical reaction between the amine and the CO$_2$ is explicitly described in the thermodynamic model (Mac Dowell et al., 2010b; Mac Dowell et al., 2011b; Rodriguez et al., 2012). The description of the reactions at the level of the thermodynamic model appreciably simplifies the process model (Mac Dowell et al., 2010b; Mac Dowell et al., 2013). The governing mass transfer equations for all these columns and the junctions are the MESH equations (i.e., mass, energy, summation and heat) for the equilibrium stage outlined below (Taylor and Krishna, 1993):

Material balance

$$G_{in} \cdot y_{i,j}^{in} + L_{(in)} \cdot x_{i,j}^{in} = G_{out} \cdot y_{i,j}^{out} + L_{out} \cdot x_{i,j}^{out}. \quad \forall i = 1 \cdots c, \forall j = 1 \cdots N \quad (3.1)$$

Equilibrium relations

$$\mu_{i,\text{out}}^l (T_{out}^l, V_{out}^l, x_{i,j}^{out}) = \mu_{i,\text{out}}^g (T_{out}^g, V_{out}^g, y_{i,j}^{out}), \quad \forall i = 1 \cdots c, \forall j = 1 \cdots N, \quad (3.2)$$

$$p_{\text{out}}^g (T_{out}^g, V_{out}^g, y_{i,j}^{out}) = p_{\text{out}}^l (T_{out}^l, V_{out}^l, x_{i,j}^{out}), \quad \forall i = 1 \cdots c, \forall j = 1 \cdots N, \quad (3.3)$$
\[ P_{\text{in},j}^g - \Delta P = P_{\text{out},j}^g, \quad \forall j = 1 \ldots N, \]  

(3.4)

and

\[ T_{\text{out},j}^g = T_{\text{out},j}^l, \quad \forall j = 1 \ldots N. \]  

(3.5)

Summation equations

\[ \sum_{i=1}^{C} x_{i,j}^\text{out} = 1; \sum_{i=1}^{C} y_{i,j}^\text{out} = 1, \quad \forall i = 1 \ldots C, \forall j = 1 \ldots N. \]  

(3.6)

Heat balance equations

\[ G_{\text{in}} h_{\text{in}}^g (T_{\text{in}}^g, V_{\text{in}}^g, y_{i,j}^\text{in}) + L_{\text{in}} h_{\text{in}}^l (T_{\text{in}}^l, V_{\text{in}}^l, x_{i,j}^\text{in}) - \]

\[ G_{\text{out}} h_{\text{out}}^g (T_{\text{out}}^g, V_{\text{out}}^g, y_{i,j}^\text{out}) - L_{\text{out}} h_{\text{out}}^l (T_{\text{out}}^l, V_{\text{out}}^l, x_{i,j}^\text{out}) \]

\[ Q = 0. \quad \forall i = 1 \ldots C, \forall j = 1 \ldots N. \]  

(3.7)

### 3.2.1.2 Heat exchanger, reboiler and condenser models

#### 3.2.1.2.1 Heat exchanger model

All heat transfer equipment (i.e., coolers and heat exchangers) are modelled using conservation of mass and energy and hydraulic equilibrium represented in Equations. (3.1), (3.3), (3.4), (3.6) and (3.7).
3.2.1.2.2 **Reboiler model**

The governing equations for the reboiler are the MESH equations represented below:

**Material balance**

\[
L_{in}x_i^{in} = G_{out}y_i^{out} + L_{out}x_i^{out}. \quad \forall i = 1 \cdots c \quad (3.8)
\]

The same Equilibrium and Summation relations outlined in Equations. (3.2), (3.3), (3.4), (3.5), and (3.6) are used here.

**Energy balance**

\[
L_{in}h_{in}^l(T_{in}^l, V_{in}^l, x_i^{in}) - G_{out}h_{out}^g(T_{out}^g, V_{out}^g, y_i^{out}) - \\
L_{out}h_{out}^l(T_{out}^l, V_{out}^l, x_i^{out}) + Q = 0. \quad \forall i = 1 \cdots c. \quad (3.9)
\]

3.2.1.2.3 **Condenser model**

Similarly, the MESH equations governing the condenser are presented below:

**Material balance**

\[
G_{in}y_i^{in} = G_{out}y_i^{out} + L_{out}x_i^{out}. \quad \forall i = 1 \cdots c \quad (3.10)
\]

Equations. (3.2), (3.3), (3.4), (3.5), and (3.6), which represents the Summation and Equilibrium relations are also used here.

**Energy balance**

\[
G_{in}h_{in}^g(T_{in}^g, V_{in}^g, y_i^{in}) - G_{out}h_{out}^g(T_{out}^g, V_{out}^g, y_i^{out}) - \\
L_{out}h_{out}^l(T_{out}^l, V_{out}^l, x_i^{out}) - Q = 0. \quad \forall i = 1 \cdots c. \quad (3.11)
\]
3.2.1.3 Columns design

3.2.1.3.1 Absorber height

In the absorber assuming a fast reaction and a dilute solvent, the mass transfer rate of the CO\(_2\) to the solvent is expressed in Equation (12) (Graf, 2011). This accounts for diminishing driving force along the stage through the log mean difference of the mole fraction. The overall mass transfer coefficient presents the efficiency of the stage in the presence of enhanced mass transfer through chemical reaction.

\[
G_{in} \cdot y_{C_{O2},j}^{in} - G_{out} \cdot y_{C_{O2},j}^{out} = \left( y_{C_{O2},j}^{in} - y_{C_{O2},j}^{out} / \ln \left( y_{C_{O2},j}^{in} / y_{C_{O2},j}^{out} \right) \right) K_{og} \cdot a' \cdot A_c \cdot H.
\]

\( \forall j = 1 \cdots N \) \hspace{1cm} (3.12)

3.2.1.3.2 Stripper height

For the stripper column, the number of theoretical stages plays a role in the mass transfer of the CO\(_2\) from the liquid phase to the gas phase. Then the height equivalent to theoretical plate (HETP) is calculated from Equation (3.13)-(3.17) (Graf, 2011; Taylor and Krishna, 1993).

\[
HTU_g = \frac{u_g}{k_g a'} \hspace{1cm} (3.13)
\]

\[
HTU_l = \frac{u_l}{k_i a'} \hspace{1cm} (3.14)
\]

\[
H_{og} = HTU_g + \Delta HTU_l \hspace{1cm} (3.15)
\]
\[ \Lambda = m \frac{G_{in}}{L_{in}} \quad \text{(3.16)} \]

\[ \text{HETP} = H_{og} \frac{\ln \Lambda}{(\Lambda - 1)} \quad \text{(3.17)} \]

### 3.2.1.3.3 DCC and scrubber heights

DCC and scrubber heights are obtained from the number of transfer units needed to cool the flue gas temperature to the inlet temperature of the absorber or to a temperature that keep the water balanced in the case of the scrubber column. This is calculated from Equations (3.18) and (3.19) while the height of transfer unit is equal to 0.12-1.2 m for packed columns (Couper, 2010). This maximum value was used for the current study.

\[ NTU_{DC} = \frac{(T_{in}^g - T_{out}^g)}{\Delta T_{LM}} \quad \text{(3.18)} \]

\[ \Delta T_{LM} = \frac{\left( \frac{T_{in}^g - T_{out}^g}{\ln \left( \frac{T_{in}^g - T_{out}^g}{T_{in}^l - T_{out}^l} \right)} \right)}{\ln \left( \frac{T_{in}^g - T_{out}^g}{T_{in}^l - T_{out}^l} \right)} \quad \text{(3.19)} \]

### 3.2.1.3.4 Columns diameter

The diameters of the column were assumed to be at a larger size that would limit the requirement of the height of the column. Initial sizes of diameters were obtained from the empirical correlations used in earlier work (Chapel et al., 1999). It was also ensured that it would meet the pressure drop and the flooding limitations being functions of packing factor, which relates to liquid and gas flow rates and their densities (Kister, 1992).

### 3.2.1.3.5 Columns physical and transport properties

Physical and transport properties correlations and sources of data are summarized in Table 3.1.
Table 3.1: Physical and transport properties correlations and sources of data.

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Reference</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusivity of CO$_2$ in gas</td>
<td>$D_{co2,g}$</td>
<td>(Fuller et al., 1966)</td>
<td>Fuller Equation</td>
</tr>
<tr>
<td>Diffusivity of CO$_2$ in water</td>
<td>$D_{co2,water}$</td>
<td>(Versteeg et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Diffusivity of CO$_2$ in loaded amine solution</td>
<td>$D_{co2,l}$</td>
<td>(Snijder et al., 1993)</td>
<td>$D_{co2,l} = D_{co2,water} (\mu_{water}/\mu_l)^{0.6}$</td>
</tr>
<tr>
<td>Loaded amine viscosity</td>
<td>$\mu_l$</td>
<td>(Weiland et al., 1998)</td>
<td></td>
</tr>
<tr>
<td>Water viscosity</td>
<td>$\mu_{water}$</td>
<td>(Cheng et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Physical solubility of CO$_2$ in water</td>
<td>$H_{e_{CO2,water}}$</td>
<td>(Versteeg et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Physical solubility of N$_2$O in water</td>
<td>$H_{e_{N2O,water}}$</td>
<td>(Versteeg et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Physical solubility of N$_2$O in amine solution</td>
<td>$H_{e_{N2O,l}}$</td>
<td>(Wang et al., 1992)</td>
<td></td>
</tr>
<tr>
<td>Physical solubility of CO$_2$ in amine solution</td>
<td>$H_{e_{CO2,l}}$</td>
<td>(Versteeg et al., 1996)</td>
<td>$H_{e_{CO2,l}}/H_{e_{N2O,l}} = H_{e_{CO2,water}}/H_{e_{N2O,water}}$</td>
</tr>
<tr>
<td>Gas phase mass transfer coefficient</td>
<td>$k_g$</td>
<td>(Onda et al., 1968)</td>
<td></td>
</tr>
<tr>
<td>Liquid phase mass transfer coefficient</td>
<td>$k_l$</td>
<td>(Onda et al., 1968)</td>
<td></td>
</tr>
<tr>
<td>Gas viscosity</td>
<td>$\mu_g$</td>
<td>(Pedersen et al., 1989)</td>
<td>Pederson model</td>
</tr>
<tr>
<td>Enhancement Factor “Pseudo first order”</td>
<td>$En$</td>
<td>(Danckwerts, 1970)</td>
<td>$En = \sqrt{k_2 D_{co2,l}/k_l}$</td>
</tr>
<tr>
<td>Liquid surface tension</td>
<td>$\sigma$</td>
<td>(Vázquez et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Reaction rate constant</td>
<td>$k_2$</td>
<td>(Versteeg et al., 1996)</td>
<td></td>
</tr>
<tr>
<td>Specific wet area</td>
<td>$a$</td>
<td>(Onda et al., 1968)</td>
<td></td>
</tr>
</tbody>
</table>
3.2.1.4 Rotary equipment (pumps, blower and compressor)

In addition to the energy required for solvent regeneration, further important energy sinks are the blowers and compressors required to move the flue gas through the absorption unit and to compress the CO$_2$ for transport. The design procedure for a compression stage for both blowers and compressors is presented in Figure 3.2.
Figure 3.2: Steps to calculate power and cooling duty of compression stages. All thermophysical properties are calculated using the SAFT-VR equation of state.
The first step is to obtain the pressure output of the multi-stage compressor and the single-stage blower. In the case of the blower, this depends on the pressure drop in the absorber column, which in turn depends on its height and the type of packing used.

To decrease the parasitic power consumption and cost of CO$_2$ compression, a pump is considered to be more favourable in the last stage of pressurising the gas in the dense phase (Aspelund and Jordal, 2007; Skovholt, 1993). Thus, the outlet pressure of the compressor should be in the high density phase to facilitate this.

Assuming isothermal compression (see Figure 3.3), the pressure output of the compressor needed to reach this high density depends on the output temperature of the gas, which depends on the cooling water temperature available within specific region.

Figure 3.3 highlights the effect of the cooling water temperature in two different regions, one with a hot climate and the other one in a cold climate. Initially, the inlet pressures of the compressor in both regions are the same but the temperature is different. As we pressurise the CO$_2$ along the isothermal path (i.e., 20°C and 50°C), the density of the gas at the same output pressure in the hot countries is lower than that in cold countries. Thus, a higher output pressure is required in the hot countries to reach similar density obtained in cold countries at lower pressure. The discharge pressures in the dense phase are shown to be around 7 Mpa (i.e., 810 kg/m$^3$ density) in the cold environment (i.e., cooling flue gas to 20°C) and around 14 Mpa (i.e., 670 kg/m$^3$ density) in the hot climate (i.e., cooling flue gas to 50°C). In cold countries, booster pumps with lower energy consumptions and capital cost can be used to increase the pressure of the dense gas from 7-14 Mpa. This implies overall lower energy consumption and thus capital cost for CO$_2$ pressurizing to 14 Mpa in cold countries when compared to hot countries.
Figure 3.3: Cut-off pressures obtained from isothermal compressor paths; the dots present the path for cold environment and the stripped lines show the path in hot climate. Mollier chart adapted from GPA (1998)
The multi-stage compressor has a total of 5 stages; it consists of three low pressure stages (i.e., 1-18 bar) with an after cooler and a knock-out drum taking excess water and a two high pressure stages with an after cooler only. A dehydration unit should be included between the low and high compression stages in order to avoid hydrate formation and corrosion in carbon steel pipelines (Aspelund and Jordal, 2007; Zhang et al., 2006); however, as detailed pipeline design was not considered in this study, this unit was not included in the model.

The second step is to calculate the isentropic enthalpy through an isentropic compression path to a desired output pressure for each stage. Then, we correct the output enthalpy through incorporation of the isentropic efficiency, facilitating the calculation of the exit gas temperature. After which, the mechanical efficiency is applied to find the actual work of each stage. In the last step, we calculate the cooling water required and the amount of condensate by utilizing either a condenser that represents both cooler and a knock-out drum for low pressure compression stages or utilizing only a cooler only in the high pressure compression stages.

The power input of the pump \( (W_p) \) in watts is calculated using Equation (3.20). This is obtained from the effect of static head needed to raise the liquid to the height of the absorber, stripper, DCC, and Scrubber, and also to increase the pressure outlet of the rich solvent to meet the input pressure of the stripper.

\[
W_p = \frac{\rho_{\text{liq}} m_{\text{liq}} \left[ p_{\text{out}} - p_{\text{in}} \right]}{\eta_p \rho g \Delta z}
\]  

(3.20)

The \( \eta_p \) is the efficiency of the pump, \( \rho \) is the density of the solvent (kg/m\(^3\)), \( m_{\text{liq}} \) is the solvent flow rate (kg/s) and \( \Delta z \) is the elevation change (m). The frictional losses are neglected here and it is assumed that there is no change in the velocity.
3.2.1.5 Model degree of freedom analysis

In order to implement the model of the whole capture and compression system, degree of freedom (DOF) analysis was performed. This was calculated while considering flue gas compositions, flow rate, temperature and pressure, columns diameters and efficiencies of rotary equipment as inputs to the model. Table 3.2 lists number of equations, variables, DOF and assigned DOF for the units in capture plant and compression systems.

Table 3.2: DOF analysis for the units in capture plant and compression system

<table>
<thead>
<tr>
<th>Units</th>
<th>Number of equations</th>
<th>Number of variables</th>
<th>DOF</th>
<th>Assigned DOF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Columns</td>
<td>$(10 + 4c)N$</td>
<td>$(10 + 4c)N$</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Coolers</td>
<td>$5 + c$</td>
<td>$4 + c$</td>
<td>1</td>
<td>Output temperature</td>
</tr>
<tr>
<td>Compression stage</td>
<td>$12 + 2c$</td>
<td>$14 + 2c$</td>
<td>2</td>
<td>Cut off pressure and compression ratio or number of compression stages</td>
</tr>
<tr>
<td>Condenser</td>
<td>$10 + 4c$</td>
<td>$11 + 4c$</td>
<td></td>
<td>$\text{CO}_2$ mole fraction at output</td>
</tr>
<tr>
<td>Heat exchanger</td>
<td>$9 + 2c$</td>
<td>$10 + 2c$</td>
<td>1</td>
<td>Rich/lean temperature difference</td>
</tr>
<tr>
<td>Junctions</td>
<td>$10 + 2c$</td>
<td>$10 + c$</td>
<td>$c$</td>
<td>Degree of capture or liquid circulation rate and compositions</td>
</tr>
<tr>
<td>Pumps</td>
<td>$4 + c$</td>
<td>$3 + c$</td>
<td>1</td>
<td>Outlet pressure</td>
</tr>
<tr>
<td>Reboiler</td>
<td>$10 + 4c$</td>
<td>$12 + 4c$</td>
<td>2</td>
<td>Reboiler pressure or temperature, and amine lean loading or heat duty</td>
</tr>
<tr>
<td>Washer</td>
<td>$10 + c$</td>
<td>$10 + c$</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
3.3 Model validation

CASTOR pilot plant data was used to validate the performance of the model presented in the previous section. The inputs of the model summarized in Table 3.3 were simulated in gPROMS in order to calculate the following quantities:

1. Reboiler duty (MJ/ton CO₂)
2. Solvent rich loading (mol CO₂/mol MEA)
3. Solvent lean loading (mol CO₂/mol MEA)
4. Absorber packed height (m)
5. Stripper packed height (m)
6. Absorber bulk liquid phase temperature profile

**Table 3.3:** CASTOR pilot plant input values in the simulation of carbon capture model\(^1\) (Abu-Zahra, 2009).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lean solvent flow rate (m(^3)/hr)</td>
<td>23</td>
</tr>
<tr>
<td>Lean solvent MEA composition (wt%)</td>
<td>30.4</td>
</tr>
<tr>
<td>Lean solvent temperature (°C)</td>
<td>58.8</td>
</tr>
<tr>
<td>Absorber inlet flue gas flow rate (Nm(^3)/hr)</td>
<td>4915</td>
</tr>
<tr>
<td>Absorber Inlet flue gas molar CO₂ composition (mol%)</td>
<td>11.86</td>
</tr>
<tr>
<td>Absorber inlet flue gas molar H(_2)O composition (mol%)</td>
<td>11.00(^2)</td>
</tr>
<tr>
<td>Absorber inlet flue gas temperature (°C)</td>
<td>47.3</td>
</tr>
<tr>
<td>Absorber pressure (kPa)</td>
<td>101.3</td>
</tr>
<tr>
<td>Stripper and Reboiler pressure (kPa)</td>
<td>181</td>
</tr>
<tr>
<td>Temperature rich solvent out of heat exchanger (°C)</td>
<td>100</td>
</tr>
<tr>
<td>Degree of capture (%)</td>
<td>90</td>
</tr>
<tr>
<td>IMTP 50 mm dry packing area (aₚ) (m(^2)/m(^3))</td>
<td>120</td>
</tr>
</tbody>
</table>

\(^1\) This comprises of closed loops of the absorber and stripper without DCC and compressor  
\(^2\) This was based on reported water content of coal-fired flue gas (Abu-Zahra et al., 2007b)
3.3.1 **Model Validation Results**

The performance of an unadjusted equilibrium stage model for the description of the absorption column was initially evaluated. As might be expected, the equilibrium stage model significantly underestimated the required size of the column (i.e., 12 m as opposed to 18 m). Thus, an efficiency factor (i.e., 0.25), which only affects the height of the column, was applied to the bottom 60% of the column.

The results are presented graphically in Figure 3.4 and numerically in Table 3.4. This table includes percentage relative error (PRE) of the model against experimental data obtained from Equation 3.2.1.

\[
\%PRE = \frac{|Model - EXP|}{EXP} \times 100 \tag{3.21}
\]

![Figure 3.4: Temperature profile of liquid inside the absorber column for the model against experimental data](image-url)
Table 3.4: Prediction of the model compared to CASTOR pilot plant data

<table>
<thead>
<tr>
<th></th>
<th>Model</th>
<th>Experiment(^1)</th>
<th>PRE(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reboiler duty (GJ/ton CO(_2))</td>
<td>4.428</td>
<td>3.897</td>
<td>13.63 %</td>
</tr>
<tr>
<td>Lean solvent loading (mol CO(_2)/mol MEA)</td>
<td>0.2806</td>
<td>0.28</td>
<td>0.21%</td>
</tr>
<tr>
<td>Rich solvent loading (mol CO(_2)/mol MEA)</td>
<td>0.492</td>
<td>0.46</td>
<td>6.96%</td>
</tr>
<tr>
<td>Stripper height prediction (m)</td>
<td>9.56(^3)</td>
<td>10</td>
<td>4.38%</td>
</tr>
<tr>
<td>Reboiler temperature (°C)</td>
<td>119.45</td>
<td>118.5</td>
<td>0.80%</td>
</tr>
<tr>
<td>Maximum solvent temperature (°C) in the absorber column</td>
<td>75</td>
<td>69.5</td>
<td>7.33%</td>
</tr>
</tbody>
</table>

\(^1\) Data source (Abu-Zahra, 2009)
\(^2\) Percent relative error %
\(^3\) Using 25 equilibrium stages

There is good agreement between model prediction and experiments in most of the variables outlined in Table 3.4. The predicted reboiler duty was higher than the experimental value; however, the predicted value is in a reasonable agreement with a typical reboiler duty of 3.9-4.2 (GJ/ ton CO\(_2\)) reported in simulation models and for a well designed commercial capture plant employing MEA as solvent (i.e., Fluor Econamine FG plants) (Abu-Zahra et al., 2007a; Abu-Zahra et al., 2007b; Chapel et al., 1999; Mac Dowell and Shah, 2013; Mariz, 1998; Singh et al., 2003).

The predicted absorber temperature profile for the model is shown in Figure 3.4. The predicted equilibrium stage model temperature profile was not expected to match the pilot plant temperature profile as outlined in the earlier studies (Abu-Zahra, 2009; Lawal et al., 2009; Luo et al., 2009; Taylor and Krishna, 1993). However, the equilibrium stage model was expected to have a good match for the column end temperature as shown in Figure 3.4 and noted by earlier studies. A better match of temperature profile that could be obtained by using a more sophisticated rate-based description of the capture process is acknowledged. However, this is out of the scope of this work as it focuses on the system trends, as opposed to the detailed behaviour at the individual unit level.
In summary, an equilibrium steady state model in which thermophysical properties were calculated using SAFT-VR was developed in gPROMS. The SAFT-VR thermodynamic model takes into account the chemical reaction of the system, which enhances the ability of the model to predict the mass transfer driven by the chemical potential gradient. The absorber column height was calculated using the two-film theory approach and the stripper column height was calculated using HETP approach. The validation of the model has presented the ability of equilibrium stage model to predict the overall system performance represented by the selected KPIs. A better accuracy could be obtained by adding complexity to the model such as developing a rate-based model in gPROMS, however, it demands more effort to develop and converge.

3.4 Parametric study and regional impact case study

The objective of this study was to initially assess the effects of key operating parameters (KOPs) on the performance of the CO₂ capture process and compression train model applied to a case study of an exhaust gas typical of a 400 MW combined cycle gas turbine (CCGT) power plant (Bailey and Feron, 2005) in hot countries where the availability of low temperature cooling water is severely limited. Then, the region-specific climate conditions effect on the performance of the system was studied.

The first objective was achieved by performing a number of simulations of the model while manipulating one degree of freedom, which represents the studied KOP at a time in the range listed in Table 3.5 while keeping the remainder DOFs outlined in 3.2.1.5 and represented by the input variables listed in Table 3.5 and Table 3.6 at their default values. The ranges listed in Table 3.5 were chosen using a combination of literature data and engineering judgment. The data listed in Table 3.6 includes the base plant input data, key design and operating variables that are set at their constant values in the entire study using data from the literature. The water make up into the capture plant listed in Table 3.6 was reduced through utilizing the condensate from the initial stages of the low-pressure compressors and through controlling
the scrubber-cooler to recover the water in the flue gas. This has the effect of reducing the water consumption of the CO₂ capture process – a concern in water strained areas.

**Table 3.5:** Key operating parameters range used in the simulations of the capture plant model.

<table>
<thead>
<tr>
<th>Variable name</th>
<th>Default value</th>
<th>Variable range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amine lean loading (mol CO₂/mol MEA)</td>
<td>0.25</td>
<td>0.2-0.36</td>
</tr>
<tr>
<td>Degree of capture</td>
<td>0.85</td>
<td>0.45-0.95</td>
</tr>
<tr>
<td>Stripper and reboiler pressure (kPa)</td>
<td>180</td>
<td>81-301</td>
</tr>
<tr>
<td>Tᵢₐₙ inlet to absorber (°C)</td>
<td>40</td>
<td>40-50</td>
</tr>
<tr>
<td>Tₑ after cooling (°C)</td>
<td>50</td>
<td>40.5-54</td>
</tr>
<tr>
<td>Parameter</td>
<td>Value</td>
<td></td>
</tr>
<tr>
<td>----------------------------------------------------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas flow rate (Nm$^3$/hr)</td>
<td>1800000$^1$</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas temperature (°C)</td>
<td>98</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas pressure (kPa)</td>
<td>101</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas molar H$_2$O composition (mol%)</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas molar CO$_2$ composition (mol%)</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>CCGT flue gas molar N$_2$ composition (mol%)</td>
<td>83</td>
<td></td>
</tr>
<tr>
<td>Pressure of the absorber (kPa)</td>
<td>101</td>
<td></td>
</tr>
<tr>
<td>Pressure drops in packing (kPa/m)</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Water makeup (kg/ton CO$_2$)</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Rich/lean heat exchanger ΔT (°C)</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Scrubber &amp; DCC cooler ΔT (°C)</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Absorber, scrubber, and DCC cooler diameter (m)</td>
<td>14.5</td>
<td></td>
</tr>
<tr>
<td>Stripper diameter (m)</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>Norton IMTP 50 mm dry packing area (a) (m$^2$/m$^3$)</td>
<td>120</td>
<td></td>
</tr>
<tr>
<td>CO$_2$ outlet pressure from compressor (kPa)</td>
<td>14000$^2$</td>
<td></td>
</tr>
<tr>
<td>CO$_2$ product content from condenser (mol%)</td>
<td>90.4$^3$</td>
<td></td>
</tr>
<tr>
<td>Compressor efficiency ($\eta_{ism}, \eta_{mec}$) (%)</td>
<td>(80,95)$^4$</td>
<td></td>
</tr>
<tr>
<td>Pumps efficiency (%)</td>
<td>75$^3$</td>
<td></td>
</tr>
</tbody>
</table>

$^1$(Bailey and Feron, 2005)
$^2$(Rao and Rubin, 2002)
$^3$(Iijima, 1998)
$^4$(Kvamsdal et al., 2007)
The effects of KOPs on the performance of the CO\textsubscript{2} capture plant and compression train were studied using the following KPIs:

1. Reboiler duty (MJ/ton CO\textsubscript{2})
2. Cooling duty (MJ/ton CO\textsubscript{2})
3. Volume of packing (m\textsuperscript{3}/ton CO\textsubscript{2} hr\textsuperscript{-1})
4. Ancillary power consumption (kWhr/ton CO\textsubscript{2})
5. Amine Slippage (kg/ton CO\textsubscript{2})
6. Solvent flow rate (m\textsuperscript{3}/ton CO\textsubscript{2})

These variables were used to determine the effect of key operating parameters on the capital cost, operating cost, and environmental impact of the CO\textsubscript{2} capture plant. The reboiler duty represents the main energy requirement for the CO\textsubscript{2} capture process. The ancillary power consumption highlights the energy required to run pumps, compressors and blowers in the system. The volume of the packing per ton of CO\textsubscript{2} per hour drives the capital cost requirement of both the absorber and stripper columns. The amine emission is indicative of the potential for deleterious environmental impact associated with the potential emission of amine degradation products such as nitrosamines.

The second objective was achieved by performing a number of simulations varying the cooling water temperature between 5-35°C in increments of 5°C in order to evaluate the effect of region-specific climate conditions on the cooling duty in addition to its effects on compression duties observed in section 3.2.1.4. The rest of the values listed in Table 3-5 and Table 3.6 were set at their default values. The amount of cooling water required (m\textsuperscript{3}/hr) is calculated using Equation (3.22); the maximum output temperature of water is assumed to be 40°C owing to environmental regulation of dumping hot water in the sea. The specific heat of water is assumed to be constant at 4.18 (kJ kg\textsuperscript{-1}K\textsuperscript{-1}) (Peters et al., 2004).

\[
    m_{cw}^* = 3.6 \frac{q}{c_p(T_{cw_{out}}-T_{cw_{in}})} \quad (3.22)
\]
3.5 Results and discussions

3.5.1 Parametric study

A number of simulations in gPROMS of the CO\textsubscript{2} capture process and compression train model applied to a case study of an exhaust gas typical of a 400 Mwe CCGT power plant in the UAE were performed. The default values listed in Table 3.5 and Table 3.6 were used as the input of the model while manipulating one of the key operating variables at an incremental step of 1% of the range specified in Table 3.6 while holding everything else constant. The model then specifies the required solvent circulation rate and height of the columns represented by the selected KPIs. The effects of each key operating parameter on all the selected KPIs are illustrated in figures in this section.

3.5.1.1 Effects of amine lean loading

As can be seen in Figure 3.5a, the reboiler duty is really high at low amine loading. This can be explained by noting the interconnectedness between components that contributes to the overall heat duty which consists of: (1) sensible heat required to raise the solvent to the required stripper inlet temperature, which is linked to the solvent circulation rate; (2) heat of absorption required to reverse the reaction, which depends on the amount of CO\textsubscript{2} captured and the type of the solvent used; (3) heat of vaporization, which represents the amount of steam required to maintain the driving force, which depends mainly on the partial pressure of CO\textsubscript{2} and water vapour in equilibrium with the liquid phase (i.e., chemical potential gradient) as highlighted by Oexmann (2010). At low amine lean loading, the driving force (i.e., the chemical potential gradient) at the bottom of the stripper column is low. Thus, more energy was required to generate more steam needed to maintain the driving force. This outweighed the benefits of lower sensible heat required with less solvent circulated into the system as noted in Figure 3.5f. Increasing the amine lean loading further by circulating more solvent into the system lowered the reboiler duty until reaching a global minimum at amine lean
loading of 0.31. This is due to increased solvent chemical potential gradient at the bottom of the stripper column, which reduced the amount of steam generated to maintain driving force. Increasing the amine lean loading beyond this point increased the reboiler duty again as this region was dominated by the sensible heat required to heat the increased solvent rate circulating into the system. A similar trend between amine loading and reboiler duty was observed in a study of MEA based CO$_2$ capture plant attached to a coal plant in which a minimum reboiler duty was observed at amine lean loading of 0.32 (Abu-Zahra et al., 2007b). The behaviour of the cooling duty against amine lean loading followed in line with the reboiler duty (see Figure 3.5b).

The required volume of packing representing the total height of both columns increases while increasing the amine lean loading as shown in Figure 3.5c. This resulted in a gradual increase in power consumption from pumps and blowers, as indicated by Figure 3.5d, because of higher solvent circulation rates and pressure drops having taller columns. Nevertheless, there is a noticeable reduction in amine slippage while increasing the amine lean loading (see Figure 3.5e); this can be explained from solvent entering the top of the absorber column at lower driving force and thus lowering flue gas temperatures exiting the absorber column, which in turn reduced the vaporization of the amine. To capture 85% of CO$_2$ while varying the lean loading, the liquid circulation rate was varied as shown in Figure 3.5f.
Figure 3.5: Effects of varying amine lean loading in the KPIs of the capture plant with compression.
3.5.1.2 Effects of degree of capture

This study shows that the specific reboiler duty did not change with higher DOC as shown in Figure 3.6a because solvent circulation rate per ton of CO$_2$ (see Figure 3.6f) and amine lean loading remained unchanged. This is contrary to the results of earlier studies (Abu-Zahra et al., 2007b; Rao and Rubin, 2006), which carried out under the assumption of fixed column height and thus increasing solvent flow rate was the remaining approach to increase DOC (Dugas, 2006; Lawal et al., 2009). This in turn increased the specific reboiler duty outlined in earlier studies. In this study, however, the volume of packing was not fixed and increased with higher DOC.

There was a slight reduction in cooling duty while increasing DOC as a result of distributing cooling duty consumed in cooling flue gas over increased amount of CO$_2$ captured (see Figure 3.6b). As can be seen in Figure 3.6c, there was a dramatic increase in the volume of packing required while capturing more than 85%. This also led to higher power consumption mainly from the blower because of the increase in pressure drops in taller columns while the liquid circulation rate remained unchanged (see Figure 3.6d). Furthermore, as can be seen in Figure 3.6e, there was a rapid loss of amine when capturing CO$_2$ at higher than 85% level; this was as a result of the flue gas exiting a taller absorber column at a high temperature, which in turn vaporized the amine. This can be prevented by applying many technologies that minimize slippage of amine and its degradation products to the atmosphere: the core technology is to use a water wash system installed at the top of the scrubber to cool the flue gas to a temperature that minimizes its vaporization. Other promising technologies such as acid water removal, filters and demisters in addition to utilizing UV-light minimize the slippage and reverse the degradation products (i.e., nitrosamine and nitramine) back to amine (Kolderup et al., 2011). These all can be applied once a well-defined amine emission standard is defined (e.g., 0.2ppmV). The solvent circulation rate per ton of CO$_2$ remained unchanged while changing the DOC as shown in Figure 3.6f due to increased volume of packing.
Figure 3.6: Effects of varying degree of capture on the KPIs of the capture plant with compression
3.5.1.3 Effects of stripper and reboiler pressure

The increase of stripper and reboiler pressure decreased both the reboiler duty and the cooling duty changing in line with the reboiler duty (see Figure 3.7a and Figure 3.7b). The increase in reboiler and stripper pressure was accompanied by consequent increase in operating temperature as shown in Figure 3.7a. This increased the solvent chemical potential gradient in the stripper column, which resulted in less steam generated to maintain the driving force. This outweighed the increase of solvent sensible heat linked with higher molar specific heat at higher pressure. Also, there was a slight decrease in the height of the stripper column (see Figure 3.7c) as a result of increased driving force while operating the stripper at high pressure. Further, there was a rapid decrease in power consumption (see Figure 3.7d) mainly from the compressor as a result of compressing CO\textsubscript{2} exiting at higher pressure from the condenser. The reboiler and stripper, however, cannot be operated at higher than 120°C-125°C (i.e., 180kPa-212kPa) owing to concerns associated with solvent degradation. Nevertheless, the development of degradation resistant solvents has a great potential on improving the overall performance of the capture plant.

Operating the stripper and the reboiler at vacuum pressure increased cooling duty by 34% and specific reboiler duty by 42% as a result of decreased solvent chemical potential gradient at low operating temperature. This demands more steam to be generated to maintain the driving force that outweighed the decrease in the solvent sensible heat linked with lower specific heat at low operating pressure. This result is in agreement with the earlier study of Oexmann and Kather (2010). The main benefit of operating at low pressure is that it allows using low temperature heating water that might be available from the waste heat. However, this increased power consumption by 17% mainly from the pump and the compressor (see Figure 3.7d) resulting from the increase in the height of the stripper column associated with driving force (see Figure 3.7c) and the decrease in the pressure exiting from the condenser.

The stripper and reboiler pressure did not affect slippage because there was no change in the inlet conditions to the absorber column. There was no change in the solvent circulation rate as
shown in the Figure 3.7f because the amount of CO₂ captured and the amine lean loading were constant while changing the reboiler and stripper pressures.
**Figure 3.7:** Effects of varying reboiler and stripper pressure on the KPIs of the capture plant with compression
3.5.1.4 Effects of lean solvent temperature inlet to absorber

As can be seen in Figure 3.8a and Figure 3.8b, there was a slight decrease in reboiler and cooling duty at low $T_{ls}$ owing to the lower circulation rate and hence sensible heat. This is due to the increase of driving force (i.e., chemical potential gradient) of CO$_2$ transfer to the liquid phase in the absorber at low temperature, which increased the rich loading at the exit of the absorber. In fact, the absorber inter-cooling is used to increase the rich loading exiting the bottom of the absorber to gain the abovementioned benefits (Amrollahi et al., 2012).

On the other hand, there was a gradual decrease in volume of packing while increasing the $T_{ls}$ because of diffusivity and reaction rate enhancements with higher temperature, which was captured by the overall mass transfer coefficient equation. This outweighed the decreased driving force of absorption at high temperature (see Figure 3.8c). This shorter column led to a lower pressure drop through the column; thus there was lower blower energy consumption as shown in Figure 3.8d. However, higher $T_{ls}$ increased the MEA vaporization as shown in Figure 3.8e. The results of decreasing solvent circulation rate shown in Figure 3.8f while reducing the $T_{ls}$ can be explained through the mass balance of the whole absorber column. When the $T_{ls}$ was reduced, it increased the rich loading for the liquid output of the absorber. This led to a larger net solvent loading ($\Delta \theta$) while keeping lean amine loading and the degree of capture ($G\Delta y$) at their constant values; thus decreasing the solvent circulation rate.
Figure 3.8: Effects of varying lean solvent temperatures in the KPIs of the capture plant with compression
3.5.1.5 Effects of flue gas temperature after cooling

There was slight decrease in reboiler duty at low $T_{fg}$ after cooling shown in Figure 3.9a as a result of increased driving force in the absorber, which increased the solvent rich loading and hence reduced the solvent circulation rate. Thus, lower sensible heat was required for the solvent. The cooling duty, however, was increased rapidly while operating at lower $T_{fg}$ as a result of higher direct contact cooler duty needed to cool the flue gas (see Figure 3.9b). As can be seen in Figure 3.9c, there was a similar gradual decrease in the volume of packing while increasing the $T_{fg}$ after cooling. This led to decreased blower power consumption needed to cover the pressure drops of the shorter column as shown in Figure 3.9d. Also, it increased the vaporization of the amine to the atmosphere as can be seen in Figure 3.9e. There was a gradual decrease in solvent circulation rate while operating at lower $T_{fg}$ as shown in Figure 3.9f; the reason for that increase was explained earlier in section 3.5.1.4.
Figure 3.9: Effects of various flue gas temperatures in the KPIs of the capture plant with compression
3.5.2 **REGIONAL IMPACT**

The regional aspects of cooling water effects on the amount of cooling water required was quantified by perfuming a number of simulations in gPROMS of the CO$_2$ capture process and compression train model applied to a case study of an exhaust gas typical of a 400 Mwe CCGT power plant. The default values listed in Table 3.5 and Table 3.6 were used as an input of the model while varying the cooling water temperature between 5-35°C in increments of 5°C to evaluate the region-specific climate conditions. The results of the simulations are presented in Figure 3.10. It shows that there was dramatic increase in the amount of cooling water required in hot countries where the cooling water temperature is higher than 25°C. This adds another challenge on applying the MEA-based post combustion capture plant in hot countries added to the ones observed in this study that can be summarized as follows: (1) Higher compression duty was observed in hot countries to maintain single phase flow as outlined in section 3.2.1.4; (2) More cooling water was needed in the washing-water system at the top of the absorber column in order to prevent the amine vaporization and formation of nitrosamine. Further, the availability of chilled water might limit the potential of utilizing ammonia-based post combustion capture plants in warm and hot countries. For example, recently, it has been shown that although energy penalty of the ammonia based capture plant is lower than MEA-based capture plant at chilled water temperature of 10°C, the ranking was opposite at cooling water temperature of 20°C (Linnenberg et al., 2012).
3.6 Concluding remarks

An equilibrium-stage model of a monoethanolamine-based CO₂ captures plant and CO₂ compression train was developed and implemented in gPROMS in which thermophysical properties were calculated using the SAFT-VR equation of state. The proposed model was validated using a data from the CASTOR project. The effects of key operating parameters on the performance of the CO₂ capture and compression process applied to exhaust gas typical of a 400 MW combined cycle gas turbine power plant in hot countries was assessed using selected key economic and environmental performance indicators. The results illustrate higher compression power and dramatic increase of cooling water requirements in coolers and washing water system used to minimize amine slippage in hot countries. This work elucidates the complex compromise between minimising capital and operating costs, and environmental impacts. Reboiler duty was observed to have a minimum value at a lean loading of 0.31, but at the cost of a larger absorber unit and increased power consumption in the flue gas blower. It was observed that the size of the absorption unit increased rapidly at capture rates greater than 85%. Operating the stripper and reboiler at high pressure reduces

![Graph showing the effects of cooling water temperature on the amount of cooling water required.](image)
the volume of packing, reboiler and cooling duty, and compression power but the process should be run at lower than degradation temperature. Reducing the temperature of the flue gas and/or lean solvent slightly reduced amine loss to the atmosphere and reboiler duty; however, this increased the size of the absorber unit, power consumption for the exhaust gas blower and cooling duty for reducing flue gas temperature, leading to an overall increased annualised cost. This highlights the importance of considering the whole process, as opposed to simply focusing on energy penalty associated with solvent regeneration. In the next chapter, we develop an optimization-oriented model of an MEA-based CO$_2$ capture plant and compression train that allow us to simultaneously find the cost optimal design and operating parameters.
4 A TECHNO-ECONOMIC ANALYSIS OF POST-COMBUSTION CO₂ CAPTURE AND COMPRESSION APPLIED TO A CCGT: PART II. IDENTIFYING THE COST-OPTIMAL OPERATING PARAMETERS

4.1 Introduction

In the literature, capture cost estimates vary widely because of the different technical assumptions regarding power plant size, load factor, fuel properties and net efficiency in addition to the diverse economic and financial assumptions such as, discount rate, plant life, and fuel cost (Mac Dowell and Shah, 2013; Metz et al., 2005; Rubin et al., 2007a; Rubin et al., 2007b). These cost estimates can be grouped into the those developed by governmental bodies (DECC, 2011; Finkenrath, 2011; GCCSI, 2011; Metz et al., 2005; NETL, 2010; ZEP, 2011), private companies and licensors of commercial solvents (Iijima, 1998; Mariz, 1998; Scottish Power, 2011), and those arising from detailed capture plant models (Abu-Zahra et al., 2007a; Mores et al., 2012a; Rao and Rubin, 2002, 2006; Singh et al., 2003). The former estimates are generated by organizations that do not make public the details of their assumptions and models. The latter option, which is based on coupling economic and physical models of the CO₂ capture plant, is the focus of this chapter. The efforts in this area can be classified as: (1) a step-wise approach where the simulation of the capture plant and the calculation of cost are performed separately and (2) a simultaneous approach in which the economic model is integrated within the physical model of the CO₂ capture plant. The following aspects are highlighted in the literature: (1) methodology of linking CO₂ source plant model to the cost model; (2) assumptions of control or state variables and design variables (e.g., diameter, height of the column); (3) main variables and size factors used to obtain the purchased cost of the CO₂ capture plant; (4) approach used to obtain the plant cost; (5) assumptions of the power plant size, life, and capacity factor; (6) inclusion of uncertainty and variability.

The earliest step-wise approach was carried out by the Carnegie Mellon University (CMU) group who developed a power plant simulation model (the integrated environmental control
model (IECM) for the US department of Energy) with an option to attach SO$_2$ and NO$_x$ emissions control technologies (Rubin et al., 1997). This model was subsequently extended with a carbon control technology (i.e., MEA, ammonia, membranes and oxyfuel-based decarbonisation). It was represented by a regression model containing the main variables that allow the calculation of the capital cost and operating cost such as MEA make-up, energy requirement, and environmental emissions generated from the MEA degradation and the bottom of reclamer (Rao, 2002). This regression model was based on a number of simulations for the CO$_2$ capture plant and a compression train with 4 compression stages developed on ProTreat and Aspen Plus respectively. The following main variables were obtained from the regression model which are functions of amine lean loading, CO$_2$ content, MEA concentration, flue gas temperature, and degree of CO$_2$ capture: (1) Liquid to gas flow rate; (2) Heat supplied per unit of liquid (KJ/kmol); (3) compression power required per kg of CO$_2$. The main equipment purchased cost was obtained by applying the sixth-tenth power relationship to the data obtained from Fluor as the reference size (Rao, 2002). The following size factors were used to scale the cost: volume and temperature of flue gas for blowers, absorbers and DCC; volume of lean solvent for stripper, lean amine cooler, storage tank and rich lean cooler; volume of solvent and amount of steam for the reboiler. The total capital cost were obtained using the Energy Power Research Institute (EPRI) costing methodology, which relates other cost components such as engineering as a fraction of the total equipment cost (EPRI, 1993).

Rao and Rubin (2002) initially used the IECM-CS model (i.e., the IECM model with carbon capture plant regression model) to find the effect of the assumptions made for the reference plant (i.e., coal fired power plant) and the interactions with the existing pollution control strategy in addition to the assumptions made about the performance parameters of the carbon capture plant. It was observed that the amine lean loading had an important effect on the total cost of CO$_2$ avoided. Rao and Rubin (2006) examined the effect of degree of capture between 70-90% on the energy penalty (i.e., electricity consumption and electricity loss of the power plant for steam derating) and the cost of CO$_2$ avoided. The study was based on
attaching a CO₂ capture plant to coal fired power plants with sizes of 600 Mwe and 1000 Mwe. The flue gas bypass option was also examined in the study to lower the cost of carbon capture plant. The benefits of using flue gas bypass option at higher than 60% DOC were anticipated as a result of treating less flue gas and solvent into the system. The main driver to use the flue gas bypass option in Rao and Rubin (2006) work is to minimize cost resulting from treating less flue gas and capturing the remaining flue gas at 95% DOC. This was driven by a combination of lower CAPEX associated with smaller equipment size and with similarly lower OPEX arising from reduced solvent flowrates and thus solvent regeneration costs. The assumption of fixed column height along with the absorber cost calculation method, which is based on the amount of flue gas treated, are the reasons for lower cost predicted in the earlier study. Further, it was found that the cost optimal degree of capture depends on the size of the plant, and it is less than the assumed value of 90% degree of capture. The main limitations of the study were the assumptions of a fixed 12 meter height column and an amine lean loading of 0.2 which might not be the optimum operating and design variables. Further, the assumption of having a maximum capacity for each train might affect the cost of CO₂ avoided.

In 2007, the IECM-CS model, which was originally integrated with a sub-critical coal fired power plant, was extended to include NGCC and IGCC power plants (Rubin et al., 2007a). The effects of varying fuel price and composition on the cost of electricity with and without CO₂ capture were investigated for three different power plants; sub-critical coal fired plant, IGCC and NGCC (Rubin et al., 2007a). Their results revealed that although the cost of electricity (COE) with and without capture for NGCC is lower at gas prices lower than $4/GJ; the order was different at a gas price of $6/ GJ at that time. The group also stressed the importance of accounting variability, which describes changes occurring over time such as learning by doing, innovation and technological development (Rubin et al., 2007b). Application of a higher premium capital charge factor for riskier technologies such as IGCC was suggested (Rubin et al., 2007a). Uncertainty in the capital cost and the effect of research and development in lowering important cost elements such as the reboiler duty were
examined by Singh et al. (2003). Further, the effect of varying interest rates on the cost of CO₂ avoided attached to a coal fired plant were also studied by Abu-Zahra et al. (2007a) and Klemes et al. (2007).

Abu-Zahra et al. (2007a) and Singh et al. (2003) used a step-wise approach in which the output of the simulation of CO₂ capture model developed in Aspen plus was used directly to obtain the CO₂ capture plant cost. Singh et al. (2003) assumed attaching a carbon capture plant to 400 Mwe coal plant while using a supplement gas turbine to supply the electricity and steam required to run the capture plant. They used the Icarus Process Evaluator within Aspen Plus to obtain the cost of the main equipment of the capture plant model and the compression system (i.e., absorption and regeneration columns, heat exchangers, tanks, pumps and compressor). The balance of the plant costs such as engineering, start-up costs and contractor fees were assumed to be the same as the ones obtained by Mariz (1998). The indirect cost and contingency were taken as percentage of the equipment cost. The effect of the control variables such as amine lean loading on the cost was not considered in this study. Abu-Zahra et al. (2007a), however, have examined the effect of amine lean loading, MEA weight, and stripper operating pressure and temperature on the cost per ton of CO₂ avoided. Their work was based on a detailed model developed in Aspen plus (Abu-Zahra et al., 2007b). The results of the model were used then to size the columns while the purchased costs of the rest of equipment were obtained using several references without enclosing details of the used sizing factors. The results of this study showed that the cost of CO₂ avoided was constant and minimum when operating at amine lean loading between 0.25-0.32 and 80-90% degree of capture. Operating the stripper at high pressure also minimized the cost of CO₂ avoided.

There are relatively few contributions in the literature, which evaluate the cost of an integrated CO₂ capture plant and compression train. Mores et al. (2012a) developed a detailed model of the CO₂ capture plant with compression and cost models in GAMS to simultaneously find the optimum design and operating conditions that minimize the total cost of CO₂ captured and compressed while meeting different CO₂ reduction targets. The
purchased equipment cost was obtained using the following size factors: superficial area and packing volume for packing; area for heat exchangers; volumetric capacity for water storage tanks; horsepower for compressors and pumps. These variables were used to scale the purchased cost using the sixth-tenth economies of scale rule while the reference unit sizes were selected randomly and their respective costs were calculated from correlations of Henao (2006) and Seider et al. (2009). The balance cost of the plant was based on the assumptions made in Abu-Zahra et al.’s (2007a) work. The results obtained from attaching a CO₂ capture plant to a theoretical plant with CO₂ content similar to NGCC plant predicted a relatively large reboiler duty of 5.7 GJ/tonne CO₂ in comparison to the 3.8-4.2 GJ/tonne CO₂ commonly found in the literature in the case of CCS on coal fired power plant. This is in line with previous observations that decarbonized gas-fired power plants are more costly in terms of GJ/tonne CO₂ recovered but they are relatively low cost in terms of $/MWhr of low-carbon electricity generated which is the ultimate aim (Rubin et al., 2007a).

The following limitations in current CO₂ capture cost estimations using detailed models are summarized: assumptions of scaling factor based on the sixth-tenth power relationship while obtaining the purchased equipment cost, which is not applicable to all units at the same rate (e.g., see Ulrich and Vasudevan (2009)); inconsistency in size factors and cost elements used to obtain the equipment cost and the balance cost of the plant respectively; separation of cost model from the capture plant model, which limits the response-capability of the model to different assumptions.

The objective of this chapter is to develop an optimization based mathematical model of the CO₂ capture plant and compression train in which a comprehensive costing approach is integrated and applied. This model is then used to simultaneously find the optimal process design and operating parameters (e.g. amine lean loading, reboiler and stripper pressure, absorber height and diameter) which minimize the total levelized cost of the CO₂ captured and compressed while meeting different degree of capture.

The remainder of the chapter is presented as follows: it starts by formulating the optimization problem of the CO₂ capture plant and compression train, followed by the comprehensive
economic model proposed for the process; then the optimum control and design variables attached to CO₂ capture and compression process with flue gas bypass option while considering different carbon prices are determined and analysed. It concludes with a summary of the main results of the chapter.

4.2 Methodology

4.2.1 Model Development

The engineering models of the CO₂ capture process and compression train illustrated in Figure 3.1 were developed in section 3.2.1. The packed sections of the absorber and desorber are described using an equilibrium-stage model. All thermophysical properties were calculated using the statistical associating fluid theory SAFT (Chapman et al., 1989; Chapman et al., 1990; Rubin et al., 2007a) for potentials of variable range: SAFT-VR (Galindo et al., 1998; Gil-Villegas et al., 1997) in which the chemical reaction between the amine and the CO₂ is explicitly described in thermodynamic model (Mac Dowell et al., 2010b). The engineering model presented in section 3.2.1 was extended with a detailed economic model in order to develop a tool capable of determining the cost optimal operating and control variables in addition to performing further analysis to study the effects of carbon price and the usage of flue gas bypass option on the process costs.

4.2.1.1 Cost model

The CO₂ capture and compression cost model was incorporated into the model developed in section 3.2.1. There are many approaches available to calculate the total cost of the plant, which is mainly based on obtaining the purchased equipment cost and then utilizing a factorisation approach to obtain the total cost of the plant. Purchased equipment cost was usually obtained using scaling approaches utilizing power relationships based on cost plots (Green and Perry, 2008; Peters et al., 2004; Ulrich and Vasudevan, 2004) in addition to using Douglas (1988) approach, which is based on Guthrie (1969) simplified cost correlations. Douglas (1988) and Peters et al. (2004) factorisation approaches were mainly used in the
literature to obtain the balance cost of the plant. The main challenge in applying these approaches is the difficulty in choosing fixed values for various factors contributing to the total cost of the plant. In this study, a standardised Chauvel et al. (1981) approach was used to calculate the total cost of the plant. This method is simple with fewer elements contributing to the total capital cost; thus eliminating errors accumulating with estimations of wide range of elements used in different methods (e.g., process pipelines, land, yard improvements, electrical). The purchased equipment cost was obtained from the updated cost correlations outlined in Couper (2010) work. Further, a decoupling between instrument cost and equipment cost based on Cran (1981) approach was applied in this study to obtain the direct equipment cost due to the fact that instrumentation cost depends mainly on the type of the equipment used.

There are variety of approaches used in the literature to report the cost of CO$_2$ capture and compression (Metz et al., 2005; Rubin, 2012). The cost of CO$_2$ avoided is mostly used in reporting the total cost of capture plant and compression train coupled with power plant. However, levelized cost of CO$_2$ capture and compression was used in this work to avoid the sensitivity of the assumptions made with regard to plant size, life and capacity and to apply it to different CO$_2$ sources. Further, this way of reporting is also flexible to study the effect of carbon price for each ton of CO$_2$ vented in addition to being expandable to account for the opportunity loss of utilizing steam and electricity instead of selling the electricity at market price. The total levelized cost of CO$_2$ capture and compression is based on calculating CAPEX and OPEX.

### 4.2.1.1 CO$_2$ capture and compression CAPEX

The total capital cost (TC) of the capture plant and compression train was calculated using Chauvel et al. (1981) approach as shown in Table 4.1. The first step was to calculate the purchased equipment cost, which depends on the grade of material, the operating conditions and the size factors representing key characteristics of the equipment (see Table 4.2). These size factors were obtained from simulations of the developed carbon capture plant and
compression train model. Further size factors such as weight of columns and heat exchanger areas were developed in the model.

The second step was to obtain the direct equipment cost representing the building and installation of primary equipment in addition to any secondary equipment in the site using equipment multiplying-factor listed in Table 4.2. Then, the cost of instrumentation was added separately using values and instrument multiplying factor listed in Table 4.2 because it does not vary proportionally with the size of the equipment. After which, indirect costs that cover transportation cost, site preparation for special equipment such as cranes, temporary buildings, and contingency to account for surprises during construction is added. Then, the offsite cost (i.e., storage and utilities) was calculated. The rest of the cost elements were obtained using the relationships that depend on the investment in units (see Table 4.1).
### Table 4.1: Elements to calculate the total capital cost (Chauvel et al., 1981)

<table>
<thead>
<tr>
<th>Code</th>
<th>Capital cost element</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Purchased equipment cost</td>
<td>$E_i \forall i = 1 \ldots n$</td>
</tr>
<tr>
<td>B</td>
<td>Instrument cost</td>
<td>$I_i \forall i = 1 \ldots n$</td>
</tr>
<tr>
<td>C</td>
<td>Direct equipment cost ($DEC$)</td>
<td>$\sum_i^n E_i F_E + \sum_i^n I_i F_I$</td>
</tr>
<tr>
<td>D</td>
<td>Indirect equipment cost</td>
<td>31% $DEC$</td>
</tr>
<tr>
<td>E</td>
<td>Inside Battery Limit Investment ($ISBL$)</td>
<td>$C + D$</td>
</tr>
<tr>
<td>F</td>
<td>Off sites ($OS$)</td>
<td>31% $DEC$</td>
</tr>
<tr>
<td>G</td>
<td>Process unit investment ($PUI$)</td>
<td>$ISBL + OS$</td>
</tr>
<tr>
<td>H</td>
<td>Engineering</td>
<td>12% $PUI$</td>
</tr>
<tr>
<td>I</td>
<td>Paid up royalties</td>
<td>7% $ISBL$</td>
</tr>
<tr>
<td>J</td>
<td>Process data book</td>
<td>265000 US$ in 2004(^1)</td>
</tr>
<tr>
<td>K</td>
<td>Facility capital cost ($FCC$)</td>
<td>$PUI + H + I + J$</td>
</tr>
<tr>
<td>L</td>
<td>Initial charge of feed stocks</td>
<td>Amine feedstock(^2) *Cost</td>
</tr>
<tr>
<td>M</td>
<td>Interest during construction</td>
<td>7% $FCC$</td>
</tr>
<tr>
<td>N</td>
<td>Start up cost</td>
<td>1 month of operating cost</td>
</tr>
<tr>
<td>O</td>
<td>Total capital ($TC$)</td>
<td>$FCC + L + M + N$</td>
</tr>
<tr>
<td>P</td>
<td>Working capital ($WC$)</td>
<td>1 month of operating cost</td>
</tr>
</tbody>
</table>

---

1. Average value scaled using Marshall and swift index
2. This is the liquid circulation rate in addition to amine hold up calculated from (Billet and Schultes, 1993)
Table 4.2: Elements to calculate the direct equipment cost (Couper, 2010; Cran, 1981).

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Size factor</th>
<th>Direct cost multiplying factor</th>
<th>Instrument cost $</th>
<th>Material of construction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blower</td>
<td>HP</td>
<td>1.4</td>
<td>2500$ per stage</td>
<td></td>
</tr>
<tr>
<td>Columns</td>
<td>Diameter, height and weight</td>
<td>2.1</td>
<td>44250$</td>
<td>SS</td>
</tr>
<tr>
<td>Columns packing</td>
<td>Volume</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Compressor</td>
<td>HP</td>
<td>1.3</td>
<td>2500$ per stage</td>
<td></td>
</tr>
<tr>
<td>Condenser</td>
<td>Area</td>
<td>2.2</td>
<td>10500$</td>
<td>CS/SS</td>
</tr>
<tr>
<td>Instrument</td>
<td></td>
<td>2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reboiler and coolers</td>
<td>Area</td>
<td>2.2</td>
<td>9750$</td>
<td>CS/SS</td>
</tr>
<tr>
<td>Rich/lean HE</td>
<td>Area</td>
<td>1.9</td>
<td>9750$</td>
<td>SS/SS</td>
</tr>
<tr>
<td>Pump</td>
<td>Head, HP and volumetric flow rate</td>
<td>2.0</td>
<td>2500$</td>
<td>SS</td>
</tr>
</tbody>
</table>

4.2.1.1.1 Weight of columns

The cost of the columns depends on the weight of the columns and the type of material. For our case, stainless steel was used for all the columns due to the high corrosion level: a rate of 0.286 mm per year in the absorber and 4.5-8.5 mm per year in the stripper were reported while using carbon steel (Kittel et al., 2009); this is higher than the accepted level of 0.1 mm (Kittel et al., 2009). The weight of the columns depends on the diameter, the height and the thickness. This in turn depends on the internal pressure, radius, material strength properties and wind speed. The thickness expressions obtained from Megyesey and Buthod (1986) and Richardson et al. (1999) in addition to diameter and height calculation obtained in Part I were incorporated in the cost model of the capture plant in gPROMS™.
4.2.1.1.2 Heat exchanger area

The required area for transferring the required heat duties (Q) in the coolers, the rich/lean heat exchanger, the condenser and the reboiler were obtained from Equation (4.1).

\[
\text{Area} = \frac{Q}{U \left( \frac{T_{\text{hot, in}} - T_{\text{cold, out}}}{\ln \left( \frac{T_{\text{hot, in}} - T_{\text{cold, out}}}{T_{\text{hot, out}} - T_{\text{cold, in}}} \right)} \right)} \tag{4.1}
\]

The overall heat transfer coefficient (U) depends on the type of medium and phases present in the heat exchanger and other dimensionless factors. A summary of the main overall heat transfer coefficients and types of heat exchanger used to calculate the capital cost in this study are outlined in Table 4.3.

**Table 4.3:** Overall heat transfer coefficients and type for the heat exchangers used within the capture plant and compression train (GPSA, 1987)

<table>
<thead>
<tr>
<th>Type of HE</th>
<th>U (W.m(^{-2}).K(^{-1}))</th>
<th>Type of HE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condenser and after-coolers</td>
<td>425</td>
<td>Shell and tube</td>
</tr>
<tr>
<td>Lean amine cooler</td>
<td>795</td>
<td>Shell and tube</td>
</tr>
<tr>
<td>Reboiler</td>
<td>850</td>
<td>Kettle</td>
</tr>
<tr>
<td>Rich lean HE</td>
<td>710</td>
<td>Shell and tube</td>
</tr>
<tr>
<td>Water cooler</td>
<td>1070</td>
<td>Shell and tube</td>
</tr>
</tbody>
</table>

4.2.1.2 CO\(_2\) capture and compression OPEX

Table 4.4 lists the main elements of the operating cost. The variable cost comprises utilities consumption and amine makeup cost. The fixed cost consists of maintenance, insurance, labour cost and overheads that cover the non-productive elements of the plant such as administration, workshops and office management (Chauvel et al., 1981).
Table 4.4: Elements to calculate fixed and variable operating and maintenance cost (Chauvel et al., 1981)

<table>
<thead>
<tr>
<th>Code</th>
<th>Capital cost element</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>OA</td>
<td>Electricity</td>
<td>$0.04/kWh</td>
</tr>
<tr>
<td>OB</td>
<td>Steam</td>
<td>$1.4/GJ</td>
</tr>
<tr>
<td>OC</td>
<td>Cooling water</td>
<td>$0.02/m³</td>
</tr>
<tr>
<td>OD</td>
<td>Utilities (U)</td>
<td>( U = OA + OB + OC )</td>
</tr>
<tr>
<td>OE</td>
<td>MEA make up</td>
<td>$1.2/kg</td>
</tr>
<tr>
<td>OF</td>
<td>Variable cost (VC)</td>
<td>( VC = U + OE )</td>
</tr>
<tr>
<td>OG</td>
<td>Labour</td>
<td>One operation engineer and four shift crews consisting of one foreman and two operators¹ ( (\frac{$398,000}{\text{year}}) )</td>
</tr>
<tr>
<td>OH</td>
<td>Maintenance</td>
<td>4%PUI</td>
</tr>
<tr>
<td>OI</td>
<td>Taxes and Insurance</td>
<td>2%PUI</td>
</tr>
<tr>
<td>OJ</td>
<td>Overhead</td>
<td>1%PUI</td>
</tr>
<tr>
<td>OK</td>
<td>Financing</td>
<td>9%WC</td>
</tr>
<tr>
<td>OL</td>
<td>Fixed operating &amp; maintenance (FOM)</td>
<td>( FOM = OG + OH + OI + OJ + OK )</td>
</tr>
</tbody>
</table>

¹ (Iijima, 1998)

4.2.1.1.3 Levelized capture and compression total cost

The total cost capture and compression cost (TCCC) is calculated using Equation (4.2).

\[
TCCC = \left( \frac{TC \text{CRF} + FOM}{CF \text{ m}^{\text{CO}_2}} \right) + VC + \left( \frac{CP \text{ m}^{\text{VOC}}}{\text{m}^{\text{CO}_2}} \right) \tag{4.2}
\]
The capital recovery factor (CRF) takes into account the depreciation of the plant and interest rates through its lifetime. A CRF of 15% was assumed for both the capture and compression train facilities (Rao and Rubin, 2002). $FOM$ is the fixed operation and maintenance cost including labor in $\text{year}^{-1}$, $CF$ is the capacity factor, $\dot{m}_{\text{CO}_2}^{\text{cap}}$ is the amount of CO$_2$ captured and compressed (tCO$_2$/year), $VC$ is the variable cost (e.g., utilities) ($/tCO_2$), CP is the carbon price ($/tCO_2$ emitted) and $\dot{m}_{\text{CO}_2}^{\text{vent}}$ is the amount of CO$_2$ vented (tCO$_2$/year) excluding any extra CO$_2$ vented from the capture plant and compression train.

### 4.2.2 Optimization Problem

The optimization problem is described as follows:

#### 4.2.2.1 Given

- The flue gas flow rate, temperature and composition
- The MEA concentration (i.e., 30 wt% MEA)
- DOC (25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%, 97%)
- Carbon price (CP)

#### 4.2.2.2 Decision variables

What are the optimum operating parameters (i.e., control or state variables) for the capture plant and compression train?

- Amine lean loading
- Flue gas temperature after cooling
- Lean solvent temperature inlet to absorber
- Reboiler and stripper pressure
- Temperature difference in DCC and scrubber cooler in addition to after-coolers.
- Temperature difference in rich and lean heat exchangers.
What are the optimum design variables?

- Area of heat exchangers (i.e., coolers, condensers, after-coolers and rich lean heat exchangers)
- Rate power (i.e., compressor, blower, and pumps)
- Volume and weight of packing columns (i.e., absorber, stripper, DCC, and scrubber)
- Flue gas utilization factor (i.e., considering bypassing portion of the flue gas)

### 4.2.2.3 Objective function

The objective function is to minimize the total levelized cost (i.e., CAPEX and OPEX) for the whole capture plant and compression train. This can be formulated in a general form as shown in Equation (4.3) being subject to equality and inequality constraints shown in Equations (4.4) and (4.5) respectively.

\[
\text{Min } F(x) \quad (4.3)
\]

Subject to:

\[
H(x) = 0 \quad (4.4)
\]

\[
G(x) \geq 0 \quad (4.5)
\]

$x$ is the vector that contains the above mentioned state or control variables and design variables in addition to operating variables such as utilities consumptions and amine make-up. Other economic variables that the vector contains are the economic factors such as finance and labour cost. $F(x)$ is the levelized total carbon capture and compression cost (TCCC) obtained in Equation (4.2). $H(x)$ is the set of equality constraints represented by the modelling equations in the earlier work such as mass and energy balance in addition to the economic equations presented here. $G(x)$ is the set of inequality constraints represented for the decision variables of the optimization problem as outlined in Equations (4.6)-(4.14).

\[
0.2 < \theta_{\text{lean}} < 0.38 \quad (4.6)
\]
\[ 40^\circ C < T_{\text{flue.gas}} < 50^\circ C \] (4.7)

\[ 40^\circ C < T_{\text{lean.solvent}} < 45^\circ C \] (4.8)

\[ 45^\circ C < T_{\text{out.after.cooler}} < 50^\circ C \] (4.9)

\[ 1 < \Delta T_{\text{DCC.cooler}} < 15 \] (4.10)

\[ 1 < \Delta T_{\text{Scrubber.cooler}} < 15 \] (4.11)

\[ 1 < \Delta T_{\text{Rich.lean.HE}} < 20 \] (4.12)

\[ D_{\text{column}}^{\text{Min}} < D_{\text{column}} < 15 \] (4.13)

\[ 0.2 < FFR < 1 \] (4.14)

The amine lean loading constraint (i.e., Equation (4.6)) covers the operating range considering technical performance using different KPIs (see previous chapter). The maximum operating temperature of the flue gas and the amine lean solvent loading were set to minimize the vaporization of the amine observed in the parametric study in the previous work (see previous chapter). The temperature differences for the heat exchangers are set within the feasible operating range. The minimum diameter of the column was obtained from the empirical correlation, which was based on capturing \%90 of the flue gas (Chapel et al., 1999).
4.3 Case study

The same indicative 400 MW CCGT flue gas data was used as a case study in which the main input parameters are listed in Table 4.5 (see section 4.3). The optimization model (i.e., cost model and CO$_2$ capture plant and compression train model) was developed in gPROMSTM, in order to find the cost optimal control or state variables in addition to design variables for different degrees of capture. The SRQPD solver based on the sequential quadratic programming (SQP) solution of the nonlinear programming (NLP) problem was used to find the optimum control or state variables. A number of optimization runs using different initial guesses for each degree of capture were done in gPROMSTM. These optimum control variables are then used as input for the simulation of the capture plant and compression train. In order to understand the trade-offs present in the system, technical performance of the system using KPIs outlined in section 3.4 will be used to analyse its behaviour at the optimum control variables.

This chapter will examine two case scenarios: The first case is based on attaching a CO$_2$ capture plant to the NGCC power plant with the assumption that there is no flue gas bypass option and no carbon price; the second case will explore the effects of carbon prices, which is reflective of current market prices (i.e., $0/ton$ CO$_2$ for no market price, $4/ton$CO$_2$ for certified emission reduction (CER) and $23/ton$ CO$_2$ for Australia levy), on the levelized cost of CO$_2$ captured and compressed while having flue gas bypass option.
**Table 4.5**: Case study of CCGT input values in the optimization of carbon capture plant and compression train.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCGT flue gas flow rate (Nm³/hr)</td>
<td>1800000¹</td>
</tr>
<tr>
<td>CCGT flue gas temperature (°C)</td>
<td>98</td>
</tr>
<tr>
<td>CCGT flue gas pressure (kPa)</td>
<td>101</td>
</tr>
<tr>
<td>CCGT flue gas molar H₂O composition (mol%)</td>
<td>12</td>
</tr>
<tr>
<td>CCGT flue gas molar CO₂ composition (mol%)</td>
<td>5</td>
</tr>
<tr>
<td>CCGT flue gas molar N₂ composition (mol%)</td>
<td>83</td>
</tr>
<tr>
<td>Pressure of the absorber (kPa)</td>
<td>101</td>
</tr>
<tr>
<td>Pressure drops in packing (kPa/m)</td>
<td>0.2</td>
</tr>
<tr>
<td>Water makeup (kg/ton CO₂)</td>
<td>0</td>
</tr>
<tr>
<td>Capacity factor (CF)</td>
<td>0.7</td>
</tr>
<tr>
<td>Cost year</td>
<td>2004</td>
</tr>
<tr>
<td>MEA make-up (kg/ton CO₂)</td>
<td>1.1 kg²</td>
</tr>
<tr>
<td>Norton IMTP 50 mm dry packing area (a) (m²/m³)</td>
<td>120</td>
</tr>
<tr>
<td>CO₂ outlet pressure from compressor (kPa)</td>
<td>14000³</td>
</tr>
<tr>
<td>CO₂ product content from condenser (mol%)</td>
<td>90.4⁴</td>
</tr>
<tr>
<td>Compressor efficiency (ηism, ηmec) (%)</td>
<td>(80, 95)⁵</td>
</tr>
<tr>
<td>Pumps efficiency (%)</td>
<td>75³</td>
</tr>
</tbody>
</table>

¹ (Bailey and Feron, 2005)
² (Chapel et al., 1999) predicted total of 1.6 kg/ton CO₂ of which 0.5 kg/ton CO₂ is vaporized at the optimum capture rate as predicted by the model. This increased model flexibility to account for vaporization
³ (Rao and Rubin, 2002)
⁴ (Iijima, 1998)
⁵ (Kvamsdal et al., 2007)
4.4 Results and discussions

4.4.1 BASE-CASE STUDY

4.4.1.1 Optimum operating parameters and KPIs for varying degree of capture

The optimization problem in gPROMS™ was solved to determine the optimum operating conditions that minimized the total levelized cost of the capture plant and compression train attached to CCGT power plant with no flue gas bypass option and no carbon price. The solution obtained from the model is the local optimum because it is a non-linear programming solver. In order to find the optimum variables that can be closer to the global optimum, different initialisation values of the control variables were used. It was observed that the reported control and design variables listed in Table 4.6 are the same with varying degree of capture. Thus, a constrained optimization was applied to find the optimum amine lean loading listed in Table 4.7. These optimum control variables are then used to simulate the whole capture plant and compression train at different degrees of capture to obtain the design variables listed in Table 4.7 and the Key Performance Indicators (KPIs) (i.e., reboiler and cooling duty, amine slippage, volume of packing, solvent flow rate and ancillary power consumption) listed in Table 4.8 (see section 3.4).
Table 4.6: Optimum constrained control and design variables for the CO\textsubscript{2} capture plant and compression train.

<table>
<thead>
<tr>
<th>Absorber, Scrubber and DCC diameter (m)</th>
<th>Stripper diameter (m)</th>
<th>( T_{\text{ls}} ) inlet to absorber column and ( T_{\text{s}} ) exiting after-cooler ( (^\circ \text{C}) )</th>
<th>Flue gas temperature after cooling ( (^\circ \text{C}) )</th>
<th>Reboiler and stripper pressure (Mpa)</th>
<th>( \Delta T ) DCC cooler</th>
<th>( \Delta T ) Rich lean HE</th>
<th>( \Delta T ) Scrubber cooler</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.5</td>
<td>8</td>
<td>45.0</td>
<td>50.0</td>
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Table 4.7: Optimum amine lean loading and design variables for the CO\textsubscript{2} capture plant and compression train.

<table>
<thead>
<tr>
<th>Degree of capture (%)</th>
<th>Absorber Height (m)</th>
<th>Amine lean loading</th>
<th>Blower power (kW)</th>
<th>Compressor after-cooler area (m\textsuperscript{2})</th>
<th>Compressor power (kW)</th>
<th>Condenser Area (m\textsuperscript{2})</th>
<th>DCC Height (m)</th>
<th>Lean amine cooler area (m\textsuperscript{2})</th>
<th>Reboiler Area</th>
<th>Rich lean HE area (m\textsuperscript{2})</th>
<th>Scrubber Height (m)</th>
<th>Stripper Height (m)</th>
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<td>25</td>
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<td>886</td>
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<td>4447</td>
<td>843</td>
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<td>803</td>
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<td>2535</td>
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<td>2903</td>
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<td>0.285</td>
<td>4590</td>
<td>1605</td>
<td>16010</td>
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<td>0.290</td>
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<td>2744</td>
<td>15280</td>
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<td>18.1</td>
</tr>
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</table>
Table 4.8 Key performance indicators for the optimum operation of the CO₂ capture plant and compression train.

<table>
<thead>
<tr>
<th>Degree of capture (%)</th>
<th>Amine Slippage (kg/ton CO₂)</th>
<th>Ancillary power consumption (kWhr/ton CO₂)</th>
<th>Cooling duty (MJ/ton CO₂)</th>
<th>Reboiler duty (MJ/ton CO₂)</th>
<th>Solvent flow rate (m³/ton CO₂)</th>
<th>Volume of packing (m³/ton CO₂ hr⁻¹)</th>
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</thead>
<tbody>
<tr>
<td>25</td>
<td>0.73</td>
<td>123.3</td>
<td>6651.6</td>
<td>4472.7</td>
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<td>31.0</td>
</tr>
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<td>0.64</td>
<td>122.7</td>
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<td>0.59</td>
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<td>6005.5</td>
<td>4473.4</td>
<td>24.0</td>
<td>27.9</td>
</tr>
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<td>0.55</td>
<td>122.3</td>
<td>5804.2</td>
<td>4473.6</td>
<td>24.0</td>
<td>27.1</td>
</tr>
<tr>
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<td>5648.0</td>
<td>4473.8</td>
<td>24.0</td>
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<td>4473.9</td>
<td>24.0</td>
<td>26.2</td>
</tr>
<tr>
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<td>5422.3</td>
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<td>24.0</td>
<td>26.1</td>
</tr>
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<td>0.49</td>
<td>124.3</td>
<td>5338.5</td>
<td>4474.1</td>
<td>24.0</td>
<td>26.2</td>
</tr>
<tr>
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<td>124.9</td>
<td>5268.3</td>
<td>4474.2</td>
<td>24.0</td>
<td>26.5</td>
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<tr>
<td>70</td>
<td>0.50</td>
<td>125.6</td>
<td>5209.1</td>
<td>4474.3</td>
<td>24.0</td>
<td>27.0</td>
</tr>
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<td>75</td>
<td>0.52</td>
<td>126.6</td>
<td>5158.8</td>
<td>4474.3</td>
<td>24.0</td>
<td>27.8</td>
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<tr>
<td>80</td>
<td>0.55</td>
<td>127.9</td>
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<td>4484.2</td>
<td>23.9</td>
<td>28.8</td>
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<td>5090.4</td>
<td>4484.2</td>
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<td>30.3</td>
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<td>5061.9</td>
<td>4484.1</td>
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<td>32.6</td>
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<td>5002.0</td>
<td>4443.2</td>
<td>24.3</td>
<td>36.6</td>
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<tr>
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<td>1.05</td>
<td>136.6</td>
<td>4965.2</td>
<td>4415.6</td>
<td>25.1</td>
<td>37.0</td>
</tr>
</tbody>
</table>

Table 4.6 highlights the fact that the diameter of the absorber and the stripper columns did not change with varying DOC because the same amount of flue gas was treated without considering flue gas bypass option. The optimum flue gas and lean solvent temperature are the highest ones obtained from the constraint equations. This is due to the increase of reaction rate constants and diffusivity, which decreased the absorber packing volume and hence cost. The optimum temperature differences for the heat exchangers are chosen to be the maximum one. This results in smaller heat exchange areas and hence CAPEX, which outweighs the incremented OPEX, acquired from larger amount of cooling water circulated into the system.
The optimum operating stripper and reboiler pressure shown in Table 4.6 is the highest one because of the gain in reducing the reboiler and cooling duty, the height of the stripper column and the compression power as outlined in section 3.5.1.3.

Table 4.7 illustrates that the optimum amine lean loading, which results from the trade-off between the CAPEX (e.g., the volume of packing required in the absorber column) and the OPEX (e.g., the amount of steam required in the reboiler), changes slightly with higher degree of capture. The results of the design variables vary linearly with DOC except for the absorber height and the blower power, which grow exponentially at higher than 60% DOC.

The optimum design variables presented in Table 4.7 were compared to the results presented by Mores et al. (2012a) in which they treated half of the flue gas used in this study. Thus, higher values for most of the design variables were expected. The projected design variables, which are less than those reported by the earlier study, are observed for the condenser, reboiler and rich lean HE areas. The assumption of 90% purity of CO₂ exiting the condenser in this study is reasonable, as more water will be condensed in the first stages of compression; this is also the reason for such a low condenser area predicted. The finding of an optimum lean loading that is higher than the one reported in the earlier work is the reason for lower reboiler duty and hence area. The optimum rich lean HE area was lower in this study because of the higher log mean temperature difference (i.e., the dominator in Equation (4.13)) predicted in this study.

Table 4.8 shows that the amine slippage, the ancillary power consumption, and the volume of packing have similar behaviour with different CO₂ reduction targets. Their values decrease slightly with higher degree of capture as a result of economies of scale. Then, the effect of economies of scale vanishes with higher DOC because of the difficulty associated with the process requiring a taller column with higher pressure drops. The table also illustrates that the cooling water duty decreases with higher DOC as a result of the economies of scale with higher amount of CO₂ being captured. There is slight change on the reboiler duty with varying DOC as it is highly linked with optimum amine lean loading, which was at an average value of 0.28. It is noteworthy to indicate that the reboiler duty obtained in this study
is lower than those reported in previous studies for a flue gas with low CO₂ content (Mores et al., 2012a).

### 4.4.1.2 Relationship between optimum cost and degree of capture

The optimum operating control variables outlined in Table 4.6 in addition to amine lean loading listed in Table 4.7 were used as the decision variables in the simulation of the capture plant and compression train in which the cost model was embedded. The results for the CAPEX, OPEX and TCCC are shown in Figure 4.1. It shows that the path for the capital cost and operating cost are similar at the optimum operating conditions. Initially, there is a gradual decrease in CAPEX, OPEX, and TCCC with higher degree of capture (i.e., 20%-55% DOC) as a result of economies of scale. Then, there is a shallow minimum between 55%-80% degree of capture arising from the simultaneous optimization of both design and operating parameters. After which, the cost of capture increases gradually with higher than 80% degree of capture as shown in Figure 4.1.

**Figure 4.1:** The profile of cost (i.e., OPEX, CAPEX and TCCC) against different DOC.
4.4.1.3 Distribution of cost between different equipment

This section highlights the distribution of the total cost between CAPEX and OPEX. The CAPEX distribution is presented here using ISBL while the OPEX are presented through variable cost and the utilities consumptions (i.e., steam, cooling water, electricity and amine make up).

Table 4.9 lists the contribution of each unit in the total CAPEX for different CO\textsubscript{2} removal targets. The most expensive units in this process are as follows: absorber; compressor train; stripper; rich lean heat exchanger. This order does not change with different DOC.

The DOC effects on different units can be summarized as follow. The absorber and blower contribution to the capital cost increases with higher degree of capture with no capture bypass as a result of having a taller column with higher pressure drops. The compressor train, stripper and DCC system contributions to CAPEX decrease with higher degree of capture as a result of economies of scale. The degree of capture has a slight effect on the CAPEX of the rest of the units.

Table 4.10 lists the contribution of the above units in addition to amine make-up to the variable cost of the CO\textsubscript{2} capture plant and compression train. The largest contributors to this cost are the reboiler; compressor; amine make-up. This order is not a function of the CO\textsubscript{2} degree of capture. In fact, aside from the blower and DCC system, the contributions of the other unit operations do not change with DOC. The blower contribution to variable cost increases with a higher degree of capture as a result of the extra power requirements to overcome the pressure drop in the system. The relative decrease in cost of the DCC system arises primarily from the increased cost associated with the significant increase in amine make-up costs arising from the increasing DOC.
Table 4.9: Distribution of the ISBL cost between the carbon capture plant and compression train.

<table>
<thead>
<tr>
<th>DOC (%)</th>
<th>Absorber (%)</th>
<th>Blower (%)</th>
<th>Compressor system (%)</th>
<th>Condenser (%)</th>
<th>DCC system (%)</th>
<th>Lean amine cooler (%)</th>
<th>Reboiler (%)</th>
<th>Rich &amp; lean pumps (%)</th>
<th>Rich lean HE (%)</th>
<th>Scrubber system (%)</th>
<th>Stripper system (%)</th>
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</thead>
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<td>8.2</td>
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<tr>
<td>85</td>
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<td>4.5</td>
<td>23.5</td>
<td>2.1</td>
<td>2.3</td>
<td>3.5</td>
<td>3.0</td>
<td>0.3</td>
<td>11.6</td>
<td>2.5</td>
<td>7.7</td>
</tr>
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<td>90</td>
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<td>22.6</td>
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<td>3.4</td>
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<td>11.2</td>
<td>2.4</td>
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<td>21.1</td>
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<td>3.2</td>
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<td>10.7</td>
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<tr>
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<td>4.8</td>
<td>20.9</td>
<td>1.7</td>
<td>2.0</td>
<td>3.4</td>
<td>2.6</td>
<td>0.3</td>
<td>10.8</td>
<td>2.0</td>
<td>6.5</td>
</tr>
</tbody>
</table>
Table 4.10: Distribution of the variable cost including amine make-up for different CO₂ reduction targets of the CO₂ capture plant and compression train.

<table>
<thead>
<tr>
<th>DOC (%)</th>
<th>Amine make-up (%)</th>
<th>Blower (%)</th>
<th>Compressor system (%)</th>
<th>Condenser (%)</th>
<th>DCC system (%)</th>
<th>Lean amine cooler (%)</th>
<th>Reboiler (%)</th>
<th>Rich &amp; lean pumps (%)</th>
<th>Scrubber system (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>15.7</td>
<td>4.5</td>
<td>24.7</td>
<td>3.5</td>
<td>7.0</td>
<td>5.4</td>
<td>35.9</td>
<td>0.4</td>
<td>2.8</td>
</tr>
<tr>
<td>30</td>
<td>15.3</td>
<td>4.6</td>
<td>25.2</td>
<td>3.6</td>
<td>6.0</td>
<td>5.5</td>
<td>36.6</td>
<td>0.4</td>
<td>2.9</td>
</tr>
<tr>
<td>35</td>
<td>15.0</td>
<td>4.6</td>
<td>25.5</td>
<td>3.7</td>
<td>5.2</td>
<td>5.6</td>
<td>37.1</td>
<td>0.5</td>
<td>2.9</td>
</tr>
<tr>
<td>40</td>
<td>14.8</td>
<td>4.6</td>
<td>25.7</td>
<td>3.7</td>
<td>4.6</td>
<td>5.7</td>
<td>37.4</td>
<td>0.5</td>
<td>3.0</td>
</tr>
<tr>
<td>45</td>
<td>14.6</td>
<td>4.7</td>
<td>25.9</td>
<td>3.7</td>
<td>4.2</td>
<td>5.7</td>
<td>37.6</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>50</td>
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<td>4.8</td>
<td>26.0</td>
<td>3.7</td>
<td>3.8</td>
<td>5.7</td>
<td>37.8</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>55</td>
<td>14.4</td>
<td>4.9</td>
<td>26.1</td>
<td>3.7</td>
<td>3.5</td>
<td>5.7</td>
<td>37.9</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>60</td>
<td>14.4</td>
<td>5.0</td>
<td>26.1</td>
<td>3.7</td>
<td>3.2</td>
<td>5.7</td>
<td>38.0</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>65</td>
<td>14.4</td>
<td>5.2</td>
<td>26.1</td>
<td>3.7</td>
<td>3.0</td>
<td>5.7</td>
<td>38.0</td>
<td>0.7</td>
<td>3.1</td>
</tr>
<tr>
<td>70</td>
<td>14.5</td>
<td>5.3</td>
<td>26.1</td>
<td>3.7</td>
<td>2.8</td>
<td>5.7</td>
<td>37.9</td>
<td>0.7</td>
<td>3.1</td>
</tr>
<tr>
<td>75</td>
<td>14.6</td>
<td>5.6</td>
<td>26.0</td>
<td>3.7</td>
<td>2.7</td>
<td>5.7</td>
<td>37.8</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>80</td>
<td>14.8</td>
<td>5.8</td>
<td>25.9</td>
<td>3.8</td>
<td>2.5</td>
<td>5.7</td>
<td>37.7</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>85</td>
<td>15.2</td>
<td>6.2</td>
<td>25.7</td>
<td>3.7</td>
<td>2.4</td>
<td>5.6</td>
<td>37.4</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>90</td>
<td>15.9</td>
<td>6.7</td>
<td>25.3</td>
<td>3.7</td>
<td>2.3</td>
<td>5.6</td>
<td>36.9</td>
<td>0.7</td>
<td>3.0</td>
</tr>
<tr>
<td>95</td>
<td>17.3</td>
<td>7.5</td>
<td>24.8</td>
<td>3.4</td>
<td>2.1</td>
<td>5.5</td>
<td>35.7</td>
<td>0.7</td>
<td>2.9</td>
</tr>
<tr>
<td>97</td>
<td>18.4</td>
<td>7.5</td>
<td>24.5</td>
<td>3.1</td>
<td>2.1</td>
<td>5.9</td>
<td>35.2</td>
<td>0.8</td>
<td>2.6</td>
</tr>
</tbody>
</table>
Table 4.11 lists the distribution of utilities cost against varying DOC. The order of their contributions in the total utility cost from higher to lower are as follows: steam; electricity; cooling water; MEA make-up. This order does not change with the DOC. Although, the steam contribution to the utility cost decreases at low and high degree of capture, it is steady between 45%-85% DOC. The cooling water consumption decreases with higher DOC as a result of economies of scale. Electricity consumption increases with higher DOC because of the higher solvent rate and higher mass of CO\textsubscript{2} that need to be compressed. MEA make-up increases at both high and low degree.

<table>
<thead>
<tr>
<th>DOC (%)</th>
<th>Cooling water (%)</th>
<th>Electricity (%)</th>
<th>MEA make-up (%)</th>
<th>Steam (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>20.1</td>
<td>28.3</td>
<td>15.7</td>
<td>35.9</td>
</tr>
<tr>
<td>30</td>
<td>19.5</td>
<td>28.7</td>
<td>15.3</td>
<td>36.6</td>
</tr>
<tr>
<td>35</td>
<td>19.0</td>
<td>29.0</td>
<td>15.0</td>
<td>37.1</td>
</tr>
<tr>
<td>40</td>
<td>18.6</td>
<td>29.2</td>
<td>14.8</td>
<td>37.4</td>
</tr>
<tr>
<td>45</td>
<td>18.2</td>
<td>29.6</td>
<td>14.6</td>
<td>37.6</td>
</tr>
<tr>
<td>50</td>
<td>17.9</td>
<td>29.8</td>
<td>14.5</td>
<td>37.8</td>
</tr>
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<td>55</td>
<td>17.7</td>
<td>30.0</td>
<td>14.4</td>
<td>37.9</td>
</tr>
<tr>
<td>60</td>
<td>17.5</td>
<td>30.1</td>
<td>14.4</td>
<td>38.0</td>
</tr>
<tr>
<td>65</td>
<td>17.3</td>
<td>30.3</td>
<td>14.4</td>
<td>38.0</td>
</tr>
<tr>
<td>70</td>
<td>17.1</td>
<td>30.4</td>
<td>14.5</td>
<td>37.9</td>
</tr>
<tr>
<td>75</td>
<td>16.9</td>
<td>30.6</td>
<td>14.6</td>
<td>37.8</td>
</tr>
<tr>
<td>80</td>
<td>16.7</td>
<td>30.7</td>
<td>14.8</td>
<td>37.7</td>
</tr>
<tr>
<td>85</td>
<td>16.5</td>
<td>30.9</td>
<td>15.2</td>
<td>37.4</td>
</tr>
<tr>
<td>90</td>
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<td>31.0</td>
<td>15.9</td>
<td>36.9</td>
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<tr>
<td>95</td>
<td>15.7</td>
<td>31.3</td>
<td>17.3</td>
<td>35.7</td>
</tr>
<tr>
<td>97</td>
<td>15.4</td>
<td>31.1</td>
<td>18.4</td>
<td>35.2</td>
</tr>
</tbody>
</table>
4.4.2 Effects of Flue Gas Bypass Option

The above described optimization problem with a flue gas bypass option and carbon price of $0, $4 and $23/ton CO$_2$ vented was solved. It was observed that similar control variables listed in Table 4.6 are the optimum for varying DOC and carbon price except for diameters of the columns. Thus, the previously described optimization problem was used to find the optimum amine lean loading, flue gas feed fraction ratio (FFR) and diameters of the columns listed in Table 4.12.

Table 4.12: Optimum design variables for CO$_2$ capture plant and compression train with flue gas bypass option

<table>
<thead>
<tr>
<th>CO$_2$ removal target (%)</th>
<th>25</th>
<th>30</th>
<th>35</th>
<th>40</th>
<th>45</th>
<th>50</th>
<th>55</th>
<th>60-97</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Fraction Ratio (FFR)</td>
<td>0.42</td>
<td>0.52</td>
<td>0.58</td>
<td>0.67</td>
<td>0.74</td>
<td>0.84</td>
<td>0.91</td>
<td>1.0</td>
</tr>
<tr>
<td>Absorber, DCC, and Scrubber diameter (m)</td>
<td>9.4</td>
<td>10.5</td>
<td>11.1</td>
<td>11.8</td>
<td>12.5</td>
<td>13.3</td>
<td>13.8</td>
<td>14.5</td>
</tr>
<tr>
<td>Stripper diameter (m)</td>
<td>5.3</td>
<td>5.8</td>
<td>6.2</td>
<td>6.6</td>
<td>7.0</td>
<td>7.4</td>
<td>7.7</td>
<td>8.0</td>
</tr>
<tr>
<td>Degree of capture (%)</td>
<td>59</td>
<td>58</td>
<td>60</td>
<td>61</td>
<td>61</td>
<td>59</td>
<td>61</td>
<td>60-97</td>
</tr>
<tr>
<td>Amine lean loading</td>
<td>0.283</td>
<td>0.283</td>
<td>0.283</td>
<td>0.283</td>
<td>0.283</td>
<td>0.283</td>
<td>0.283</td>
<td>0.282</td>
</tr>
</tbody>
</table>

The optimum FFR listed in Table 4.12 reveal that the flue gas bypass option is the cost optimal choice for lower than 60% overall DOC. The optimum degree of capture for the remaining flue gas listed in Table 4.12 is close to the optimum rate (i.e., 60% DOC) that has the lowest volume of packing and blower power consumption per ton of CO$_2$ captured.

In the literature, however, the flue gas bypass option was considered to be the optimum choice at higher than 60% overall DOC as a result of treating less flue gas and hence lower solvent circulation rate into the system (Rao and Rubin, 2006). This in turn reduced the reboiler duty, which decreased OPEX in addition to reducing CAPEX resulted from
anticipated smaller absorber column. However, our result shown in Figure 4.2 shows that the reboiler duty and liquid circulation rate per ton of CO₂ captured against degree of capture are constant and do not change with flue gas bypass option. This is in agreement with the earlier study of Sanpapertparnich et al. (2010). In fact, the solvent circulation rate per ton of CO₂ captured is observed to be linked to the optimum amine lean loading and the amount of CO₂ captured, which were similar at varying flue gas bypass ratio (see Figure 4.2).

![Figure 4.2: Effects of flue gas bypass option on optimal solvent flow rate and reboiler duty required for varying DOC.](image)

### 4.4.3 Effects of Carbon Price

The control and design variables listed in Table 4.12, which were similar at different carbon prices, are used to simulate the capture plant in order to obtain the levelized cost against DOC for different carbon prices shown in Figure 4.3.
Figure 4.3: Effects of flue gas bypass option and CP on the total cost of CO₂ capture and compression

Figure 4.3 shows the effects of flue gas bypass option and carbon prices (i.e., $0, $4 and $23 per ton of CO₂ vented) on the levelized cost of CO₂ captured and compressed from CCGT power plant. The results reflect the benefits of bypassing the flue gas while meeting lower than 60% CO₂ reduction targets because of a lower volume of packing required and hence lower CAPEX. The carbon price has a clear impact on the cost optimum DOC: at $0/ton CO₂, there is shallow minimum between 55%-80% DOC arising from the simultaneous optimization of both design and operating parameters; at $4/ton CO₂, there is shallow minimum between 70%-80% DOC; at $23/ton CO₂, there is shallow minimum between 85%-90% DOC. Thus, the cost optimum DOC will shift to more than 90% DOC at higher carbon prices which is in agreement with results obtained in the previous study (Mac Dowell and Shah, 2013).

It is also shown in Figure 4.1 that the lowest cost of CO₂ capture and compression is $59/ton CO₂ which is much higher than the current carbon price of $23/ton CO₂ vented assumed in this study. Thus, it will be cheaper to pay the costs associated with CO₂ emissions than investing in CCS. At the right carbon price (i.e. higher than $60/ton CO₂), which covers the cost of CO₂ capture and compression, there will be a motivation to capture the CO₂ at higher than 95% DOC.
This is potentially an important message to policy makers; if a suitably high carbon price does not materialize through a market mechanism, appropriate policies may need to be put in place to achieve decarburization targets. The Electricity Market Reform (EMR) tools currently being discussed in the UK provide one potential means to achieve this. Alternatively, stringent emissions performance standards (EPS) will be required to incentivize high rates of decarbonisation (i.e., >80%).

4.5 Concluding remarks

A detailed optimization-orientated model of an MEA-based CO₂ capture plant and compression train was developed and implemented in gPROMS™. The model is applied to an exhaust gas typical of a gas-fired combined cycle power plant. This integrated model was used to determine the cost optimal control and design variables including capture bypass ratio at different degree of capture (DOC). The effects of varying carbon prices on the levelized cost of CO₂ captured and compressed were also studied. The impact on cost vs DOC of plant designs that partially bypass the CO₂ capture process so as to achieve low to moderate reductions of CO₂, but at lower overall cost was investigated. The capture bypass option was observed to be the cost optimal choice for lower than 60% overall DOC. Carbon prices were observed to have a clear impact on the cost optimal DOC, with the cost-optimal DOC shifting from 70%-80% to 85%-90% at carbon prices of $4/ton CO₂ to $23/ton CO₂ respectively. The developed techno-economic model forms the first CCTS network component that can be coupled to different CO₂ sources in order to analyse their performance. In the next chapter, an optimization-oriented model of the CO₂ transportation system used to identify the key performance operating parameters and limiting uncertainties that need to be mitigated or optimized to ensure a safe cost-optimal design is developed.
5 OPTIMUM DESIGN OF CO₂ TRANSPORT SYSTEM UNDER UNCERTAIN TEMPERATURE AND FLOW COMPOSITION

5.1 Introduction

High-pressure supercritical carbon dioxide has commercially been transported in pipelines to oilfields for EOR activities in the last three decades. The main source of this CO₂ gas was natural underground deposits available at reasonable cost. In the future, more CO₂ will be transported due to large-scale implementation of carbon capture, transport and storage (CCTS) perceived as a short to medium-term measure to mitigate climate change in which CO₂ emissions contribute significantly. Thus, there is a need to configure a safe and cost-effective CO₂ transportation system that takes into account the interactions of the CO₂ flow with impurities, temperature, elevation change and compression.

The design of a CO₂ transport system involves a number of decisions that need to be made with regard to rating power and capacity of the compression train, location of booster or regulator stations, pipeline thickness, diameter, toughness, and route in addition to control variables such as operating velocity and pressure. The optimum design has to minimize cost, meet safety factors under transient and steady state operation, maintain flexibility under changes in composition, fluctuation in seasonal temperature and upset of CO₂ injection or capture.

The safe design of a CO₂ transport system is obtained through the following established design codes and regulations for similar fluid systems. For example, ASME B31.4 and ASME B31.8 codes that set the thickness and toughness of CO₂ pipelines are followed to minimize the effects of stresses (i.e., hoop stress and combined stress), surge pressure and ductile fracture in the pipe wall under transient and steady state operating condition (ASME B31.4, 2006; ASME B31.8, 2007). The safety factor used in the hoop stress equation is increased for pipelines crossing populated area and hence this increases the required thickness (ASME B31.8, 2007). The surge pressure (e.g., 0.4Mpa /m/s) resulting from a sudden blockage of the flow and loss of velocity has to be less than 10% of the pipeline
design pressure as embodied in the code (ASME B31.4, 2006; Kumar, 2010). The
propagating ductile fracture in the unrestrained tip of a fractured wall can tear the pipeline.
Thus, Battelle fracture arrest equations are used to find the required toughness or thickness of
the pipeline to prevent this damage (Cosham, 2007; Eiber, 1993; King, 1981). Alternatively,
mechanical crack-arrestor devices can be installed at different sections of the pipelines to
arrest ductile fracture and minimize the loss.

Further, it is important to consider the risks associated with CO₂ transportation and the
actions required to control and prevent leakage. CO₂ pipelines have been classified by the
Federal Regulations in the USA as highly volatile, low hazard, low risk facilities (Recht,
1986). The main risk associated with the gas is that, being denser than air, it can accumulate
in low areas and at concentrations higher than 10 % may cause asphyxiation. Accumulation
of the gas is difficult to detect due to its being colourless and odourless. It is therefore
important to add chemicals similar to the ones added to natural gas and coal gas to give the
gas a distinctive smell (Gale and Davison, 2004). In order to prevent leakage, high standard
sealing and packing are recommended. Increasing the number of block valves for pipelines
crossing densely populated areas are applied to shut off the gas flow in the event of a leak
being detected. Alternatively, an automatic control system similar to those used for H₂S
pipelines can be used to improve safety (Gale and Davison, 2004).

In the literature, the optimum design of CO₂ transport systems mainly involved finding the
optimum diameter of the pipeline while using hydraulic flow equations and economic-related
correlations. Many authors making dissimilar assumptions with regards to density, viscosity,
input pressure, topographical height difference and pressure drop per unit length and/or
operating velocity used the first approach purely (Bock et al., 2003; Hamelinck et al., 2001;
Heddle et al., 2003; IEA GHG, 2002, 2005; McCoy and Rubin, 2008; Vandeginste and
Piessens, 2008). However, there is limited work in utilizing developed regression based
formulae, which minimizes investment and operating cost of compression train and pipeline
(Zhang et al., 2006). This correlation has viscosity, density, and flow rate as main input
variables and it was driven while making many assumptions with regard to pipeline cost, input pressure and compressor efficiency.

It is clear that previous work focused on optimizing one design variable (i.e., pipeline diameter) while overlooking other interacting operating and design variables such as input pressure, compressor rating power, and operating velocity in addition to overlooking the fact that thermophysical properties (e.g., compressibility) behave non-linearly at pipeline operating temperatures and pressures (Farris, 1983). These will highly be affected by the presence of other impurities that result from having different CO₂ sources and capture technologies (e.g., hydrogen in pre-combustion technologies, oxygen in oxy-fuel technologies). This in turn was shown to influence pipeline capacity and nominal booster pump suction head needed to prevent cavitation in addition to pipeline thickness required to prevent ductile fracture (Cosham, 2007; Mohitpour et al., 2008). Further, the variation of pipeline operating temperature dictated by the soil seasonal temperature, as most of the pipelines are buried for safety reasons, is another design factor that was neglected.

The objective of this chapter is to develop a techno-economic model of the CO₂ transport system that integrates a multi-stage compression train model with the CO₂ flow in pipeline model. Equations of states (i.e., SAFT) and economic correlations are embodied in this model and thus helping in analysing and optimizing the system simultaneously. This model is used to perform a number of analyses including: finding the cost optimum variables for transferring CO₂ flow with certain capacity under uncertainty in composition and variability in seasonal temperature. Further, this model is used to find the optimum operating capacity of each nominal pipeline size (NPS) diameter, which can then be used for source-sink matching.

The remaining of this chapter is outlined as follows: first, a detailed model of the CO₂ flow in pipelines was developed and then validated in predicting the NPS diameter considering current practice. After this, an economic and optimization based model of the CO₂ transport system was developed. This model was then used to find the cost-optimal design and control variables for a case study representing 83% degree of capture from 600 MW natural gas fired
boiler plant. Finally, the optimal operating capacity for commercial NPS diameters considering flow transportation over a flat area to a storage site within a 100 km distance was found.

5.2 Methodology

5.2.1 Model development

The proposed model of CO₂ transport system shown in Figure 5.1 was developed in gPROMS™). Following the capture plant, CO₂ is compressed in a multi-stage compression train with an intercooler and hydration unit to the desired pipeline pressure (i.e., 10-14 Mpa). If a higher CO₂ pressure is required, a pump is more favourable to be used in the last stage of compression (Aspelund and Jordal, 2007; Skovholt, 1993). The dry CO₂ is then transferred using a carbon steel pipeline with specific diameter to the storage or utilization site.

![Figure 5.1: CO₂ transport system modelled in gPROMS™](image)

5.2.1.1 Compressor and pump model

The required multi-stage compression power was obtained assuming an isentropic compression path. First, the isentropic discharge enthalpy is calculated for the desired output
pressure using the SAFT-VR equation of state. Then, the actual enthalpy is corrected using
the isentropic efficiency (See Equation (5.1)).

\[ h_{\text{out}}(T_{\text{out}}, V_{\text{out}}, y_{\text{out}}) - h_{\text{in}}(T_{\text{in}}, V_{\text{in}}, y_{\text{in}}) = (h_{\text{out}} - h_{\text{in}})/\eta_{\text{isn}} \] (5.1)

After this, the power of the compressor was obtained while accounting for the mechanical
efficiency shown in Equation (5.2). The required amount of cooling water was obtained from
the after cooler equilibrium-stage model developed in section 3.2.1.2.

\[ W_c = G_{\text{in}}(h_{\text{out}}^g - h_{\text{in}}^g)/\eta_{\text{mec}} \] (5.2)

The dense phase pump power \((W_p)\) in watt was computed by:

\[ W_p = \frac{\dot{m}}{\eta_p} \left[ \frac{p_{\text{out}} - p_{\text{in}}}{p_{\text{in}}} \right] \] (5.3)

5.2.1.2 Pipeline flow model

The pipeline diameter design was based on the hydraulic and turbulent flow equation
(Mohitpour et al., 2003):

\[ D_{\text{pip}} = \left\{ \frac{-64Z^2\bar{\rho}R^2T_{\text{ave}}^2\bar{m}^2\text{Le}}{\pi^4 MZ_{\text{ave}}RT_{\text{ave}}(p_{\text{out}}^2 - p_{\text{in}}^2)} \right\}^{1/5} \] (5.4)

This depends on parameters such as elevation change, length, pressure drop, compressibility
and molecular weight in addition to mass flow rate.

This equation is solved for the average compressibility, temperature and compressibility:

\[ P_{\text{ave}} = 2/3 \left( P_{\text{out}} + P_{\text{in}} - \frac{p_{\text{out}}P_{\text{in}}}{P_{\text{out}} + P_{\text{in}}} \right) \] (5.5)
\[ Z_{ave} = \frac{P_{ave}}{R_f^{ave}} \]  

(5.6)

Where the fanning friction factor (Serghides, 1984) was approximated by:

\[ f = \left( f_A - \frac{(f_B - f_A)^2}{f_c - 2f_B + f_A} \right)^{-2} \]  

(5.7)

\[ f_A = -2 \log \left( \frac{\varepsilon/D_{pip}}{3.7} + \frac{12}{Re} \right), \]  

(5.8)

\[ f_B = -2 \log \left( \frac{\varepsilon/D_{pip}}{3.7} + \frac{2.51 f_A}{Re} \right), \]  

(5.9)

\[ f_c = -2 \log \left( \frac{\varepsilon/D_{pip}}{3.7} + \frac{2.51 f_B}{Re} \right). \]  

(5.10)

\( (\varepsilon/D_{pip}) \) is the relative roughness, \( \varepsilon \) is the internal surface roughness of pipe (i.e., 0.0457 \( \times 10^{-3} \) m for steel) and the Reynolds number was calculated by:

\[ Re = \frac{4m}{\mu_{ave} \pi D_{pip}} \]  

(5.11)

Where the viscosity was obtained from the empirical correlation for supercritical \( \text{CO}_2 \) (Heidaryan et al., 2011):

\[ \mu_{ave} = F(T_{ave}, P_{ave}) \]  

(5.12)

The mass and energy balances are outlined below:

Material balance

\[ G_{in} y_i^{in} = G_{out} y_i^{out}, \quad \forall i = 1 \cdots c, \]  

(5.13)
\[ y_i^{\text{in}} = y_i^{\text{out}} = y_i^{\text{ave}}, \quad \forall i = 1 \cdots c, \quad (5.14) \]

Energy transfer through enthalpy equations

\[ G_{\text{in}} h_{\text{in}}(T_{\text{in}}, V_{\text{in}}, y_i^{\text{in}}) = G_{\text{out}} h_{\text{out}}(T_{\text{out}}, V_{\text{out}}, y_i^{\text{out}}) + Q \quad \forall i = 1 \cdots c \quad (5.15) \]

The SAFT-VR equation of state was used to call the following thermophysical properties:

\[ h_{\text{in}} = F(T_{\text{in}}, V_{\text{in}}, y_i^{\text{in}}) \quad (5.16) \]

\[ h_{\text{out}} = F(T_{\text{out}}, V_{\text{out}}, y_i^{\text{out}}) \quad (5.17) \]

\[ P_{\text{in}} = F(T_{\text{in}}, V_{\text{in}}, y_i^{\text{in}}) \quad (5.18) \]

\[ P_{\text{ave}} = F(T_{\text{ave}}, V_{\text{ave}}, y_i^{\text{ave}}) \quad (5.19) \]

\[ P_{\text{out}} = F(T_{\text{out}}, V_{\text{out}}, y_i^{\text{out}}) \quad (5.20) \]

The superficial flow velocity in the pipeline is:

\[ u = \frac{4 m}{\pi D_{\text{pip}}^2 \rho_{\text{ave}}} \quad (5.21) \]

The density can be obtained from knowing the specific molar volume and molecular weight:

\[ \rho_{\text{ave}} = M/V_{\text{ave}} \quad (5.22) \]

The output temperature of the pipeline is equal to the average temperature:
\[ T_{out} = T_{ave} \] (5.23)

The diameter obtained from the earliest steps is equal to pipelines smaller than or equal to NPS 12. The thickness of the outer diameter for pipelines larger than 0.324\text{m} (12.76\text{ inch}) can be calculated from the equations below:

\[
t = \frac{p_{\text{max}} b_{\text{pip}}}{2[SMYS \rho E - p_{\text{max}}]} \] (5.24)

\[ OD_{\text{pip}} = 2t + D_{\text{pip}} \] (5.25)

The degree of freedom analysis performed is shown in Table 5.1. It lists the number of equations, variables, DOF and assigned DOF of the transport system.

**Table 5.1**: DOF analysis for the transport system

<table>
<thead>
<tr>
<th>Number of equations</th>
<th>Number of variables</th>
<th>DOF</th>
<th>Assigned DOF</th>
</tr>
</thead>
<tbody>
<tr>
<td>19 + 2c</td>
<td>26 + 2c</td>
<td>7</td>
<td>( p_{\text{out}}, T_{\text{ave}}, h_{\text{in}}, h_{\text{out}}, \text{Le}, )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( u ) and ( m ) or ( D_{\text{pip}} )</td>
</tr>
</tbody>
</table>

**5.2.1.2.1 Pipeline flow model validation**

The data of existing CO\textsubscript{2} pipelines in operation in the USA was used to validate the developed flow model. The input data were pipeline capacity, length and elevation difference. The remaining variables were assumed as follows: operating velocity of 2 m/s considered to be the optimum operating velocity in the literature (IEA GHG, 2005); discharge
pressure of 8.69 Mpa leaving a buffer above critical pressure (i.e., 7.38 Mpa) (Farris, 1983); and operating temperature of 27°C representing the soil temperature in Texas as most of the reported CO_2 pipelines were built in that region. These variables were used in the simulation of the flow model in gPROMS™ in order to predict the NPS diameters of the pipelines listed in Table 5.2. When the diameter exceeded the lower NPS diameter, it was corrected to the next NPS diameter. There was a good agreement in the entire NPS diameters ranges predicted by the model.

**Table 5.2:** Existing CO_2 pipelines capacity, length, elevation difference (Vandeginste and Piessens, 2008) vs. diameter predicted by the developed flow model in gPROMS

<table>
<thead>
<tr>
<th>Pipeline</th>
<th>Location</th>
<th>CO_2 capacity (Mt/year)</th>
<th>Length (km)</th>
<th>Elevation difference (m)</th>
<th>Pipe diameter m (in)</th>
<th>Predicted Pipe diameter m (in)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bravo</td>
<td>Bravo Dome to Denver City</td>
<td>7.3</td>
<td>350</td>
<td>955</td>
<td>0.51 (20”)</td>
<td>0.51 (20”)</td>
</tr>
<tr>
<td>Cortez</td>
<td>Cortez to Denver City</td>
<td>19.3</td>
<td>808</td>
<td>800</td>
<td>0.76 (30”)</td>
<td>0.76 (30”)</td>
</tr>
<tr>
<td>Sheep Mountain part-1</td>
<td>Sheep Mountain to Rosebud</td>
<td>6.4</td>
<td>296</td>
<td>893</td>
<td>0.51 (20”)</td>
<td>0.51 (20”)</td>
</tr>
<tr>
<td>Sheep Mountain part-2</td>
<td>Rosebud to Seminole</td>
<td>9.3</td>
<td>360</td>
<td>464</td>
<td>0.61 (24”)</td>
<td>0.61 (24”)</td>
</tr>
<tr>
<td>Transpetco</td>
<td>Bravo Dome to Guymon</td>
<td>3.4</td>
<td>193</td>
<td>1094</td>
<td>0.51 (20”)</td>
<td>0.51 (20”)</td>
</tr>
<tr>
<td>Weyburn</td>
<td>Beulah to Weyburn</td>
<td>5</td>
<td>330</td>
<td>46</td>
<td>0.36 (14”)</td>
<td>0.36 (14”)</td>
</tr>
</tbody>
</table>
5.2.1.3 CO₂ transport cost

The total capital cost of the compressor, after coolers and pumps was obtained by first calculating the purchased equipment cost that depends on the material of construction, operating condition and size factor (e.g. rate power, area). Then, the balance of plant costs including equipment erection, site preparation, instruments and engineering were added as outlined in Table 4.1 and Table 4.2. The operating cost of the equipment was calculated from the electricity and cooling water consumption outlined in Table 4.4.

Total pipeline capital cost was estimated using a developed regression model shown in Equation (5.26) and Equation (5.27) (McCoy and Rubin, 2008), which depends on the diameter and the length of the pipeline. The capital cost is broken into four construction cost components: Material (e.g. amount of steel, coating and cathode protection); Labour (i.e., construction labour); Right of Way (ROW) (i.e., land usage compensation and permits); Miscellaneous (e.g., surveying, engineering, overhead, supervision, contingencies and filing fees). Table 5.3 lists all the parameters needed to calculate the cost of pipelines constructed in the south-eastern United States (McCoy and Rubin, 2008).

\[ PCC_f = a_0^f (0.001 L e_{pip})^{a_1^f} (39.37 D_{pip})^{a_2^f} \]  \hspace{1cm} (5.26)

\[ TPCC = \sum PCC_f \]  \hspace{1cm} (5.27)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Materials</th>
<th>Labour</th>
<th>ROW</th>
<th>Miscellaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a_0)</td>
<td>1534.6</td>
<td>18663.8</td>
<td>8912.5</td>
<td>33265.96</td>
</tr>
<tr>
<td>(a_1)</td>
<td>0.901</td>
<td>0.820</td>
<td>1.049</td>
<td>0.783</td>
</tr>
<tr>
<td>(a_2)</td>
<td>1.590</td>
<td>0.940</td>
<td>0.403</td>
<td>0.791</td>
</tr>
</tbody>
</table>

The total compression and transportation cost (TCTC) to a storage site or to a CO₂ network is calculated using below Equation:

\[ \text{TCTC} = \sum \text{PCC}_f \]
The capital recovery factor (CRF) takes into account the depreciation of the equipment and interest rates through its lifetime. A CRF of 15% was assumed for both the compression train facilities and the CO₂ transportation. *FOM* is the fixed operation and maintenance cost including labour in $ year⁻¹ (i.e., 2% of TPCC (IEA GHG, 2009b)), *CF* is the capacity factor of the whole transportation system facility, *tCO₂* is the tons of CO₂ compressed and transported, and *VC* is the variable cost (i.e., utilities) ($/tCO₂).

### 5.2.1.4 Optimization of CO₂ transport system

The optimization model of the CO₂ transport system can be described as follows:

#### 5.2.1.4.1 Given

- CO₂ flow rate
- Pipeline operating temperature (i.e., the soil temperature as most pipelines will be buried for safety reasons)
- Flow feed composition (e.g., CO₂ content %)
- Pipeline delivery pressure (i.e., outlet pressure)
- Pipeline length
- Elevation change
5.2.1.4.2 Decision variables

What are the optimum control variables?
- Pipeline operating velocity
- Compressor output pressure
- Average operating compressibility
- Average operating pressure drop

What are the optimum design variables?
- NPS diameter
- Compressor rate power

5.2.1.4.3 Objective function

The objective function is to minimize the TCTC as shown in Equation (5.28). This is subject to equality constraints outlined in Equations (5.1-5.27) in addition to compression train equations outlined in section 3.2.1.4 and inequality constraints presented below:

\[ 0.1 < u < 4 \]  \quad (5.29)

\[ 0.273 < D_{pip} < 1.016 \]  \quad (5.30)

\[ 8.8 \text{ Mpa} < P_{out}^{com} < 14 \text{ Mpa} \]  \quad (5.31)

The operating velocity range is obtained from the literature while the pipeline diameter represents the nominal pipeline sizes available within the market. The minimum operating pressure is set to ensure single flow operation (i.e., dense phase) within the CO$_2$ transport system (Farris, 1983).
5.2.2 OPTIMUM CO₂ TRANSPORT SYSTEM UNDER UNCERTAINTY IN TEMPERATURE AND COMPOSITION

An indicative case study of transporting 84% of the captured CO₂ from 600 a MW natural gas fired boiler power plant (Mimura et al., 1995) located within the region of UAE was used. This was selected to assess the effects of seasonal variability in soil temperature (i.e., 13°C - 38°C) between summer and winter, as most of the pipelines will be buried for safety reasons. The effects of transporting flows with different CO₂ purity (i.e., 92%-99.99%) were also examined in this case study. Table 5.4 lists the main input variables and assumptions used in the developed techno economic model in gPROMS.

Table 5.4: Case study input values in the simulation of the CO₂ transport system model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow rate (Mt/year)</td>
<td>2</td>
</tr>
<tr>
<td>Capacity factor (CF)</td>
<td>1</td>
</tr>
<tr>
<td>Length (km)</td>
<td>100</td>
</tr>
<tr>
<td>Cost year</td>
<td>2004</td>
</tr>
<tr>
<td>Compressor efficiency (η_{Ish}, η_{I mec}) (%)</td>
<td>(80.95)</td>
</tr>
<tr>
<td>Pumps efficiency (%)</td>
<td>75</td>
</tr>
<tr>
<td>Operating temperature</td>
<td>13°C -38°C</td>
</tr>
<tr>
<td>Flow feed quality</td>
<td>92%-99.99% CO₂</td>
</tr>
<tr>
<td>Pipeline delivery pressure</td>
<td>8.69 MPa</td>
</tr>
<tr>
<td>Elevation difference</td>
<td>0 m</td>
</tr>
<tr>
<td>Electricity</td>
<td>$0.04/Kwh</td>
</tr>
<tr>
<td>Cooling water</td>
<td>$0.02/m³</td>
</tr>
<tr>
<td>Specified minimum yield strength (SMYS)</td>
<td>483 MPa</td>
</tr>
<tr>
<td>Basic design factors (F)</td>
<td>0.72⁵</td>
</tr>
<tr>
<td>Weld joint factor (E)</td>
<td>1</td>
</tr>
</tbody>
</table>

¹ (Kvaisdalen et al., 2007)
² (Iijima, 1998)
³ (Farris, 1983; Mohitpour et al., 2003)
⁴ (Farris, 1983; Mohitpour et al., 2003)
⁵ (ASME B31.8, 2007)
A scenario-based approach that represents discrete variables of operating temperature and flow composition as listed in Table 5.5 was used. This leaves the whole CO₂ transport system with one degree of freedom that can be manipulated. Thus, the optimum control and design variables (e.g. compressor output pressure, pipe diameter and operating velocity) of the whole CO₂ transport system were found graphically for each scenario by performing a number of simulations while manipulating the operating velocity. Further, the optimum design and control strategy under uncertainty can be interpolated using these results.

<table>
<thead>
<tr>
<th>Cases</th>
<th>Temperature</th>
<th>CO₂ composition (mol %)</th>
<th>N₂ composition (mol %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>26°C</td>
<td>99.99</td>
<td>0.001</td>
</tr>
<tr>
<td>High temp</td>
<td>38°C</td>
<td>99.99</td>
<td>0.001</td>
</tr>
<tr>
<td>Low temp</td>
<td>13°C</td>
<td>99.99</td>
<td>0.001</td>
</tr>
<tr>
<td>92% CO₂</td>
<td>26°C</td>
<td>92</td>
<td>8</td>
</tr>
<tr>
<td>95% CO₂</td>
<td>26°C</td>
<td>95</td>
<td>5</td>
</tr>
</tbody>
</table>

5.2.3 **Optimum Operating Pipeline Capacity for Each Nominal Pipeline Size**

In order to find the optimum operating pipeline capacity for each NPS pipeline diameter, a number of simulations of the techno-economic model using data listed in Table 5.4 at the nominal conditions listed in Table 5.5 while having flow rate as design variable instead of pipe diameter were performed. The generated data of the simulations while manipulating velocity was graphically used to find the cost optimum operating capacity in addition to control and design variables such as compressor output pressure and operating velocity. These results can then be used in the analysis of the whole CO₂ network design.
5.3 Results and discussion

5.3.1 COST OPTIMUM CO₂ TRANSPORT SYSTEM UNDER UNCERTAINTY IN TEMPERATURE AND COMPOSITION

The total cost of compressing 2 million tons per annum of CO₂ and transporting it to a storage site located within 100 Km against operating velocity is shown in Figure 5.2. This was obtained while simulating the developed techno-economic model in gPROMS™ for all the cases considered in the study. The cost optimum control and design variables considering both continuous and NPS diameters are shown in Figure 5.2 and Table 5.6.

![Cost of compressing and transporting 2 Mt/yr CO₂ against operating velocity using different scenarios.](image)

**Figure 5.2:** Cost of compressing and transporting 2 Mt/yr CO₂ against operating velocity using different scenarios.
Table 5.6: Cost optimum operating design and control variables for the case study

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Velocity (m s(^{-1}))</th>
<th>Cost ($ t^{-1} CO_2$)</th>
<th>Input Pressure (MPa)</th>
<th>Diameter (m)</th>
<th>Compressibility (Z)</th>
<th>Pressure drop (Pa m(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>92% CO2</td>
<td>1.39</td>
<td>10.63</td>
<td>10.96</td>
<td>0.2917</td>
<td>0.2413</td>
<td>23.4</td>
</tr>
<tr>
<td>95% CO2</td>
<td>1.30</td>
<td>10.29</td>
<td>10.91</td>
<td>0.2873</td>
<td>0.2226</td>
<td>23.0</td>
</tr>
<tr>
<td>Low Temp</td>
<td>1.14</td>
<td>9.85</td>
<td>10.88</td>
<td>0.2793</td>
<td>0.1989</td>
<td>22.6</td>
</tr>
<tr>
<td>High Temp</td>
<td>1.34</td>
<td>9.91</td>
<td>10.98</td>
<td>0.2867</td>
<td>0.2280</td>
<td>23.6</td>
</tr>
<tr>
<td>Nominal</td>
<td>1.21</td>
<td>9.87</td>
<td>10.85</td>
<td>0.2834</td>
<td>0.2073</td>
<td>22.3</td>
</tr>
<tr>
<td>Nominal N</td>
<td>1.30</td>
<td>9.88</td>
<td>11.32</td>
<td>0.2730</td>
<td>0.2121</td>
<td>27.0</td>
</tr>
<tr>
<td>92% CO2 N</td>
<td>1.56</td>
<td>10.66</td>
<td>11.88</td>
<td>0.2730</td>
<td>0.2489</td>
<td>32.6</td>
</tr>
<tr>
<td>95% CO2 N</td>
<td>1.43</td>
<td>10.30</td>
<td>11.59</td>
<td>0.2730</td>
<td>0.2293</td>
<td>29.7</td>
</tr>
<tr>
<td>Low Temp N</td>
<td>1.19</td>
<td>9.85</td>
<td>11.15</td>
<td>0.2730</td>
<td>0.2017</td>
<td>25.3</td>
</tr>
<tr>
<td>High Temp N</td>
<td>1.47</td>
<td>9.93</td>
<td>11.64</td>
<td>0.2730</td>
<td>0.2340</td>
<td>30.2</td>
</tr>
</tbody>
</table>

As can be seen in Figure 5.2 for all the cases considered in the study, there was an exponential decrease in total cost of transportation while increasing the operating velocity until it reached a global minimum as a result of decreasing pipeline diameters and hence capital cost. Increasing the operating velocity beyond this point increased the total cost of transport because of the increased pressure drop, compressibility and compressor rating power and pressure, which in turn increased the operating cost such that it outweighs the benefits of minimizing CAPEX. There was a change in direction when operating at higher velocity which reflects utilizing a cheaper pump at high pressure (i.e., >14 MPa) instead of compression stages. This results in a decrease in pressurizing capital and operating cost that minimized the total cost gradually until it reached another local minimum. There was again an increase in the total cost beyond this point as the benefit of utilizing a booster pump is lost and the effects of higher OPEX dominate the total cost of transportation.

The CO\(_2\) content of the flow has a large impact on the total cost of transportation as shown in Figure 5.2. The lower the CO\(_2\) content in the flow, the higher the transportation cost incurred. This is due to the increase of flow compressibility with enlarged presence of non-condensable gas (i.e., nitrogen), which reduces the capacity of transportation. Thus, a higher operating pressure is required to maintain transporting the same capacity of flow in the same pipeline.
size as shown in Table 5.6. This result indicates that transportation companies have to levy extra charges to discourage transporting flow from low CO\textsubscript{2} content sources. For example, an extra charge of 0.5-0.8 $ per ton of flow should be implemented for compressing and transporting flow having a 92\% CO\textsubscript{2} purity instead of 99.99\% in order to cover the extra operating expenses that can be calculated from Table 5.6.

Another important factor that affects the total cost of transportation is the variability in seasonal temperature as shown in Figure 5.2. The total cost of transporting the CO\textsubscript{2} is higher in the summer as a result of higher compressibility, which in turn reduces the operating capacity. Thus, a higher operating pressure is required to cover these loses. However, the total cost of transportation is lower in the winter as a result of decreased compressibility, which reduces the pressure drop. Thus, there is an opportunity to reduce the total cost of transportation by lowering the operating velocity in cooler temperatures.

The results outlined in Table 5.6 reveal that the cost optimum NPS pipeline diameter under uncertainty in composition and variability in ground temperature is NPS 10 (0.273 m). The remaining optimum control and design variables (e.g., compressor power, operating velocity) have to be designed for the worst cases being the maximum temperature in the summer and the lower CO\textsubscript{2} content in the flow (see Table 5.6). This allows the optimum operating velocity and pressure to be adjusted (see Table 5.6) accordingly in order to maintain the flow capacity in the pipelines.

5.3.2 COST OPTIMAL PIPELINE OPERATING CAPACITY

The total cost of transportation against operating capacity that results from simulating the techno-economic model developed in gPROMS\textsuperscript{TM} using various operating velocities (i.e., 0.25-3.5 m/s) for each NPS diameter is shown in Figure 5.3. Similar profiles were obtained in which a reduction in total cost of transportation was initially seen as a result of economies of scale. Then, the OPEX outweighed the benefits of CAPEX. After this, the usage of booster pumps reduced the total cost initially before having another rise in OPEX.
Figure 5.3: Cost of transportation against operating capacity for each NPS diameter using various operating velocity

The cost optimum operating capacity for each NPS diameter was obtained graphically and reported along with the optimum operating velocity, operating pressure, pressure drop and cost in Table 5.7. As shown in Figure 5.3, the cost optimum operating capacity for NPS 14 and NPS 16 was similar. Thus, the NPS 14 was not reported in Table 5.7 due to the fact that the NPS 16 has a lower pressure drop with similar total cost of transportation.
Table 5.7: Optimum operating pipeline variables including capacity and cost for each nominal pipeline size.

<table>
<thead>
<tr>
<th>Pipeline diameter</th>
<th>Capacity (Mt CO₂/year)</th>
<th>Velocity (m/s)</th>
<th>Input pressure (MPa)</th>
<th>Compressibility (Z)</th>
<th>Pressure drop (Pa/m)</th>
<th>Cost ($/ton CO₂/100km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>168 mm (6 in)</td>
<td>0.4-1.19</td>
<td>0.3-2</td>
<td>8.8-21</td>
<td>0.19-0.32</td>
<td>1.9-124</td>
<td>28.0-11.1</td>
</tr>
<tr>
<td>219 mm (8 in)</td>
<td>1.2-1.5</td>
<td>1.2-1.5</td>
<td>10-13.5</td>
<td>0.20-0.24</td>
<td>13-49</td>
<td>11.11-10.6</td>
</tr>
<tr>
<td>273 mm (10 in)</td>
<td>1.51-2.2</td>
<td>1-1.4</td>
<td>10.2-11.9</td>
<td>0.20-0.22</td>
<td>15.6-32.8</td>
<td>10.5-9.7</td>
</tr>
<tr>
<td>324 mm (12 in)</td>
<td>2.21-3.0</td>
<td>1-1.4</td>
<td>10.0-11.1</td>
<td>0.20-0.21</td>
<td>13.7-24.9</td>
<td>9.71-9.1</td>
</tr>
<tr>
<td>406 mm (16 in)</td>
<td>3.01-4.67</td>
<td>1.0-1.6</td>
<td>9.8-11.3</td>
<td>0.20-0.21</td>
<td>12.9-27.2</td>
<td>9.11-8.5</td>
</tr>
<tr>
<td>507 mm (20 in)</td>
<td>4.68-7.02</td>
<td>1.0-1.5</td>
<td>9.5-10.5</td>
<td>0.19-0.20</td>
<td>8.7-19.2</td>
<td>8.4-7.9</td>
</tr>
<tr>
<td>610 mm (24 in)</td>
<td>7.03-11.04</td>
<td>1.1-1.7</td>
<td>9.4-10.5</td>
<td>0.19-0.20</td>
<td>7.6-18.4</td>
<td>7.9-7.4</td>
</tr>
<tr>
<td>762 mm (30 in)</td>
<td>11.05-17.01</td>
<td>1.1-1.7</td>
<td>9.2-10.0</td>
<td>0.19-0.20</td>
<td>6-13.8</td>
<td>7.4-7.0</td>
</tr>
</tbody>
</table>
The results in Table 5.7 highlight that it is more cost effective to design a CO$_2$ transport system operating at low pressure and velocity when considering flow transportation in a flat area within a 100 km distance. This result is different from that of Farris (1983) in which a higher operating capacity was obtained as a result of using higher operating velocity (i.e., 2-4 m/s) considered to be the optimum choice in the earlier study. Further, Kumar and King (2012) predicted a higher operating pipeline capacity as a result of having a thicker pipeline diameter that allows operation at high pressure (i.e., 21 MPa). In this earlier study, a thicker pipeline was considered to be a cheaper choice than increasing the toughness of the pipeline in order to prevent ductile fracture. However, a thicker pipeline does not necessitate that a higher operating pressure should be implemented. This is due to the escalation in compressor rating power and pressure drops, which increases OPEX and outweighs the benefits of reducing CAPEX (e.g., reducing pipeline diameter) as outlined above.

5.4 Concluding remarks

More CO$_2$ containing different impurities will be transported due to large-scale implementation of carbon capture, transport and storage. Thus, a detailed optimization-based model of the whole CO$_2$ transport system including compression train, booster pump and pipeline was developed and implemented in gPROMS$^\text{TM}$ and then was successfully used to simultaneously find the cost optimal design considering a case study under variability in seasonal temperature and uncertainty in composition. The decision variables obtained included pipeline diameter in addition to design and control variables (i.e., compressor output pressure and rating power, pipeline operating velocity, compressibility and pressure drop) that were overlooked or assumed to be at constant values in the literature. The results reveal that the optimum design has to be made for the worst-case scenarios (i.e., high temperature and low CO$_2$ content) while optimizing control variables (e.g., operating velocity) to minimize cost. It was also observed that transportation companies should levy a charge to discourage transporting flow from low CO$_2$ content sources in order to cover the charges
associated with higher compression power required to maintain flow capacity. The results of finding the optimal operating capacity for commercial pipeline sizes reveal optimal designs with lower operating velocity (i.e., 1-2 m/s) and pressure compared to the ones reported in the literature.

All the main sub-process models forming CCTS network components were developed. In the next chapter, a systematic multiscale CCTS network model that integrates all these sub-process models was developed and used to design the cost-optimum network linking CO₂ sources (e.g., power stations) with potential sinks (e.g., depleted oil reservoirs).
A layout of the multi-scale detailed carbon capture, transport and storage system is shown in Figure 6.1. There are four macro components within CCTS system: CO$_2$ sources at fixed locations, CO$_2$ capture plants that need to be built, CO$_2$ transportation links that need to be picked among different potential nodes and CO$_2$ storage sites at fixed locations. The CO$_2$ source plants (e.g., power plant, process plant) emit certain amounts of CO$_2$ with varying compositions. The level of CO$_2$ emission changes in response to demand changes for services, products and utilities throughout the year. The CO$_2$ is assumed to be transported to a storage site via a pipeline network. Different sections of the network are composed of pipelines with different diameters with a minimum and a maximum capacity. The CO$_2$ can be stored in a permanent storage site such as depleted oil reservoir or it can be used for EOR projects. Each storage site has a certain capacity and injectivity that allow it to accommodate certain amount of CO$_2$ per year.

The multiscale approach comprises a series of interacting models that are able to capture behaviours at specific length and time scales. The following scale models are incorporated (see Figure 6.2):

(1) **Molecular scale**: a detailed thermodynamic model using SAFT-VR (i.e., molecular model based on Helmholtz free energy) approach is used (Chapman et al., 1989; Chapman et al., 1990; Galindo et al., 1998; Gil-Villegas et al., 1997) to evaluate thermophysical properties and reaction equilibria of the MEA-based solvent and flue gas (Mac Dowell et al., 2010b; Mac Dowell et al., 2011b; Rodriguez et al., 2012);

(2) **Film scale**: a two film theory is utilized to find the height required for the diffusion of CO$_2$ through a packed column;
(3) **Unit scale:** an equilibrium-based model comprising of mass and energy transfer equations for the whole amine-based CO₂ capture plant are used to analyse its performance;

(4) **Regional scale:** a high-level supply chain network model is utilized to map the cost optimum deployment of the CCTS network at the national or global level.
Figure 6.1: Multiscale CCTS modelling components
In order to inform the decisions at the macro level (e.g., select a source or not, degree of capture, network topology), a number of optimization runs are performed for attaching a CO$_2$ capture plant to each potential CO$_2$ source while using detailed fine scale sub-process models (e.g., units of the capture plant, cost model). Each of these units is affected by the local and regional parameters. For example, the availability and temperature of cooling water which in turn affect details of the design such as compression path. Further, the corrosion rate when considering the type of material and solvent used is another important factor that is quantified when incorporated in details of the capture plant. Other global parameters are reflective of the economic conditions such as fuel, water and electricity price.
The results obtained by the fine scale models are then passed to the macro scale models through the development of meta-models, which summarise their behaviour in terms of a small number of key variables. For example, these are derived from the database including energetic and economic performance of attaching amine-based post-combustion CO₂ capture plants and compression trains to different CO₂ sources is used in high-level network design. The remainder of this chapter is laid out as follows: it starts by developing a multiscale model of the CO₂ network system. Then, it demonstrates the use of the model in finding the cost-optimal CO₂ network considering four major CO₂ sources and three potential oil recoveries fields amenable to CO₂ flooding in the UAE. After this, it examines the effect of having various CO₂ reduction mandates in the overall cost of the network. Finally, it presents some concluding remarks.

6.1 Model development

The following steps were taken to develop the integrated multi-scale optimization based model of CO₂ capture, transport and storage networks:

(1) Build an inventory of CO₂ sources that include composition, flowrate and temperature of the flue gas in addition to CO₂ source location

(2) Build an inventory of CO₂ storage and potential EOR sites including location, capacity and injectivity.

(3) Develop economic-performance relationships for attaching MEA based CO₂ capture plants and compression trains to each potential CO₂ source. This is obtained by performing a number of optimizations using the detailed techno-economic model developed in gPROMS (see chapter 3 and 4). A database of the optimum operating,
control and design variables in addition to the cost of capture and compression against degree of capture will be developed for these sources.

(4) Obtain the optimum operating capacity and velocity for each pipeline diameter while considering the techno-economic interactions between the CO$_2$ compression train and transportation system (see previous chapter).

(5) Run the network model while using information obtained from steps (1)-(4) as inputs to find the optimal design of CCTS network:

**Given**
- Number, location, flue gas characteristics of potential CO$_2$ sources
- Database of economic performance (i.e., capital and operating cost) of CO$_2$ capture (for different degrees of capture, in the form of data points or meta-models) from all potential sources using the developed amine based post-combustion capture plant in gPROMS™ (Process Systems Enterprise)
- CO$_2$ reduction target or potential market for EOR
- Number, location and capacity of each storage site
- Financial and technical data such as discount rate, capacity factor, life time of the plant

**Decision variables**
- Which CO$_2$ sources to select?
- Which degree of capture and operating conditions the capture plant is designed for?
- Where to establish pipelines and at which size?
- How to connect these pipelines in a network?
- Which CO$_2$ storage sites to exploit?
**Objective Function**

- The objective function is the minimization of the total levelized cost (i.e., capital and operating cost) of the whole system (i.e., CO$_2$ capture, compression, transport and storage).

### 6.1.1 Mathematical Formulation of the CO$_2$ Network Model

The multiscale model was formulated as a MILP problem in which the complex system was described by a set of equality equations that describe the behaviour of the system, a set of inequality constraints that constrain the solutions in a feasible region and an objective function that the model minimizes in order to identify the optimum set of decisions that represent the deployment of the CCTS system. The mathematical formulation consists of nomenclature components namely indices, parameters, continuous variables, and binary variables, constraints and an objective function.

#### 6.1.1.1 Nomenclature

**6.1.1.1.1 Indices**

- $i$: grid squares
- $j$: grid squares such that $i \neq j$
- $k$: Degree of capture from each potential source (e.g., 25%-99%)
- $l$: Transportation modes using pipes with different diameter (i.e., 6 inch, 8 inch, 10 inch, 12 inch, 16 inch, 20 inch, 24 inch, 30 inches)
6.1.1.1.2 Parameters

- $a_{j}^{\text{max}}$: Maximum amount of CO$_2$ emitted in grid square $j$, t d$^{-1}$
- $a_{k,j}$: Amount of CO$_2$ captured in each grid square $j$ at degree of capture $k$
  
  \[ a_{k,j} = z_{k} a_{j}^{\text{max}} \]

- $a_{j}^{\text{max}}_{\text{total}}$: Total amount of CO$_2$ emitted from the CO$_2$ sources
  
  \[ a_{j}^{\text{max}}_{\text{total}} = \Sigma_j a_{j}^{\text{max}} \]

- $b_{j}^{\text{max}}$: Maximum amount of CO$_2$ that can be sequestered for EOR in grid square $j$, t d$^{-1}$ or maximum injection capacity

- $\text{Capex}_l$: Pipeline capital cost charge factor for each transpiration mode $l$, $\text{\$/km}^{-1}$
- $\text{Capex}_l^{\text{cor}}$: Pipeline capital cost charge factor for each transpiration mode $l$ corrected for uncertainty factor, $\text{\$/km}^{-1}$
  
  \[ \text{Capex}_l^{\text{cor}} = \text{UMF} \text{Capex}_l \]

- $CF$: Capacity factor

- $CRF$: Capital recovery factor, (i.e., 15%)

- $d_{ij}$: Distance between grid $i$ and grid $j$, km
  
  \[ d_{ij} = \sqrt{(d_{yj} - dy_{i})^2 + (dx_{j} - dx_{i})^2} \]

- $dx_{j}$: Horizontal distance relative to origin for each grid square $j$, km

- $dy_{j}$: Vertical distance relative to origin for each grid square $j$, km

- $\text{Opex}$: Pipeline operating cost charge factor for each transpiration mode $l$ (i.e., 2% of $\text{Capex}_l$), $\text{\$/km}^{-1}$

- $Q_{l}^{\text{max}}$: Maximum optimum flow rate via transportation mode $l$, t d$^{-1}$

- $Q_{l}^{\text{min}}$: Minimum optimum flow rate via transportation mode $l$, t d$^{-1}$

- $RT$: CO$_2$ reduction target that need to be met, %

- $TCC_{k,j}$: Total levelized cost of CO$_2$ captured and compressed to 140 bar in grid square $j$ at degree of capture $k$, $\text{\$/t}^{-1}$

- $\text{UMF}$: Uncertainty multiplying factor used to take into account the uncertainty in the pipeline cost (e.g., 1.25, 1.5)

- $z_{k}$: Number represent degree of capture for each $k$ (e.g., 0.25, 0.26, …, 0.99)
### 6.1.1.1.3 Continuous variables

- \( b_j \): Amount of CO\(_2\) sequestered in grid square \( j \) for EOR, \( t \ d^{-1} \)
- \( c_{kj} \): Optimum amount of CO\(_2\) captured in grid square \( j \) at degree of capture \( k \), \( t \ d^{-1} \)
- \( CC_l \): Capital cost for each transportation mode \( l \), $
- \( FCC_j \): Total levelized cost of establishing capture plant and compression train in grid square \( j \), $ \ d^{-1} 
- \( OC_l \): Operating cost for each transportation mode \( l \), $
- \( Q_{iij} \): CO\(_2\) flow rate between grid square \( i \) and grid square \( j \) by transportation mode \( l \), \( t \ d^{-1} \)
- \( TC \): Total cost of the whole CCTS network, $ \ d^{-1} 
- \( TD_l \): Total distance of each transportation mode \( l \), km
- \( TFCC \): Total levelized cost of establishing all capture plants and compression trains in the network, $ \ d^{-1} 
- \( TPCC \): Total pipeline capital cost, $
- \( TPOC \): Total pipeline operating cost, $ \ d^{-1} 

### 6.1.1.4 Binary variables

- \( X_{iij} \): 1 if transportation between grid square \( i \) and square \( j \) by mode \( l \) exists, 0 otherwise
- \( Y_{kj} \): 1 if CO\(_2\) capture plant will exist in grid square \( j \) at degree of capture \( k \), 0 otherwise
6.1.1.2 Constraints

6.1.1.2.1 Logical constraints

The total amount of CO$_2$ sequestered in each sink $j$ for EOR should not exceed the maximum injectivity per day as shown in Constraint (6.1).

$$b_j \leq b_j^{\text{max}} \forall j$$ (6.1)

Constraints (6.2) and (6.3) indicate that only one capture plant with specific degree of capture can be built at each prospective CO$_2$ source.

$$c_{kj} = a_{kj} Y_{kj}$$ (6.2)

$$\sum_k Y_{kj} \leq 1$$ (6.3)

The CO$_2$ reduction target that needs to be satisfied puts a constraint on the total imported flow from other grid squares by Constraint (6.4), which must not exceed the total reduction target. This limits the feasible region and hence minimizes the computation time.

$$\sum_l Q_{l,j} \leq RT a_{j,\text{total}}^{\text{max}} \forall j$$ (6.4)
6.1.1.2.2 Material balance constraints

Assuming steady state operation of the system, Constraint (6.5), which represents the mass balance, indicates that CO\textsubscript{2} captured or transported within each grid square must be transported out of the grid square or injected for EOR in the grid square.

\[ b_j = \sum_{l,i} Q_{li,j} - \sum_{l,i} Q_{lji} + \sum_k C_{kj} \quad \forall \ j \]  \hspace{1cm} (6.5)

Constraint (6.6) sets the operating capacity for each transportation mode (i.e., pipeline with different diameter) while assuring flow is only allowable once pipeline is established.

\[ Q_{l}^{\text{max}} X_{ij} \leq Q_{ij} \leq Q_{l}^{\text{min}} X_{ij} \quad \forall \ l, i, j; \ i \neq j \]  \hspace{1cm} (6.6)

Constraint (6.7) ensures that the flow between two grid squares can only exist in one direction.

\[ X_{ii} + X_{ij} \leq 1 \quad \forall \ i, j; \ i \neq j \]  \hspace{1cm} (6.7)

6.1.1.2.3 Reduction target objective constraint

The objective is to meet a reduction target of capturing certain amount of CO\textsubscript{2} emitted per year from all CO\textsubscript{2} sources as indicated in Constraint (6.8).

\[ RT \ a_{j,\text{total}}^{\text{max}} \leq \sum_{k,j} c_{kj} \]  \hspace{1cm} (6.8)
6.1.1.2.4 Non-negative constraints

All decision variables must not be negative as shown in the following equations.

\[ c_{k,j} \geq 0 \ \forall \ j \]  
\[ (6.9) \]

\[ Q_{l ij} \geq 0 \ \forall \ l, i, j: i \neq j \]  
\[ (6.10) \]

\[ b_j \geq 0 \ \forall \ j \]  
\[ (6.11) \]

6.1.1.3 Objective function

In order to find the cost-optimum CO\(_2\) infrastructure, the objective function here is to minimize the total levelized cost (i.e., capital and operating cost) incurred with establishing and operating CO\(_2\) capture plants and pipelines, and subject to the constraints outlined earlier. The total cost assumed in this study is the gate delivery cost to the potential EOR site. Any additional cost associated with pressurizing the gas further or modifying the existing storage sites infrastructure is not included in this study.

6.1.1.3.1 Capture plant and compression train levelized cost

The total daily levelized cost of establishing capture plant and compression train in grid square \( j \) is shown in Equation (6.12). The total facilities cost associated with building all the capture plants and compression trains for the CCTS network is shown in Equation (6.13).

\[ FCC_j = \sum_j TCC_{k_j} c_{k_j} \ \forall \ j \]  
\[ (6.12) \]

\[ TFCC = \sum_j FCC_j \]  
\[ (6.13) \]
6.1.1.3.2 Pipelines capital cost

The capital cost of establishing pipelines given the uncertainty in reported cost data is obtained by first calculating the total distance being built of each mode as shown in Equation (6.14); then, the capital cost of establishing specific pipelines are obtained as in Equation (6.15); finally, the total capital cost incurred for building all the pipelines in the network is calculated in Equation (6.16).

\[ TD_t = \sum_{i,j} d_{ij} X_{ijt} \]  \hspace{1cm} (6.14)

\[ CC_i = Capex_i^{cor} TD_t \hspace{0.5cm} \forall \hspace{0.5cm} l \]  \hspace{1cm} (6.15)

\[ TPCC = \sum_d CC_i \]  \hspace{1cm} (6.16)

6.1.1.3.3 Pipelines operating Cost

Pipeline operating costs depend mainly on the length of the pipeline, as shown in Equation (6.17), regardless of the pipe diameter. The daily total operating cost is outlined in Equation (6.18).

\[ OC_i = Opex_i TD \hspace{0.5cm} \forall \hspace{0.5cm} l \]  \hspace{1cm} (6.17)

\[ TPOC = \sum_l OC_i \]  \hspace{1cm} (6.18)
6.1.1.3.4 Overall objective function

The objective function is to minimize the total daily cost incurred in establishing and operating the CCTS infrastructure as shown in Equation (6.19). Any generic high-performance MILP solver can be used to find the optimum decision variables that optimise the objective function in addition to satisfying the equality and inequality constraints obtained from equations (6.1)-(6.19).

\[ \min TC = \frac{CRF \times (TPCC)}{365 \times CF} + TFCC + TPOC \]  

(6.19)

6.2 Case study

The feasibility of multiscale approach was demonstrated within the region of the United Arab Emirates (UAE). As this region has the sixth highest carbon emissions per capita in the world, it has an ambitious primary target to reduce Abu Dhabi’s carbon footprint by a third through implementing large scale CCTS networks for enhanced oil recovery (EOR) (Nader, 2009). The key drivers are the proximity of large CO\(_2\) sources and reservoirs and the benefit of releasing natural gas currently being used for EOR.

The phase 1 CO\(_2\) reduction mandate announced in Abu Dhabi was to capture 5 million tons of CO\(_2\) from three different sources namely boiler flue gas from Tawelal power company (TAWEELA), combined cycle gas turbine (CCGT) flue gas from Emirates Aluminium plant (EMAL) and a pure stream of CO\(_2\) from Emirates Steel Industry (ESI), shown in Table 6.1 and Figure 6.3 (Nader, 2009).

The objective here is to find the cost-optimum deployment of the CCTS network while capturing different amounts of CO\(_2\) emitted from all the three CO\(_2\) sources (i.e., 25%, 50%, 75%, 95%) and satisfying a portion of CO\(_2\) potential demand for EOR projects. This was calculated for three major oil fields (i.e., Asab, Bab, Bu Hasa) assuming a 17% incremental in oil production while employing CO\(_2\) in miscible floods considering that 1 ton of CO\(_2\) is capable of producing 4 barrels of oils per day on average (Beecy and Kuuskraa, 2005).
Table 6.1: Case scenario represents phase 1 of announced UAE reduction target of 5 million tons of CO$_2$ per year.

<table>
<thead>
<tr>
<th>Source/ sink type</th>
<th>Name and location</th>
<th>Flow rate, temperature, pressure and composition / capacity</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel production plant</td>
<td>Emirates Steel Industry (S1)</td>
<td>46,920 (Nm$^3$/ hour) 98(°C) 1.01 (bar) 90.4 (mol.%$_2$) CO$_2$ 9.6% (mol.%$_2$) H$_2$O</td>
<td>No capture required, just compression and dehydration unit</td>
</tr>
<tr>
<td>Boiler based power plant</td>
<td>Taweela power company (S2)</td>
<td>1,741,000 (Nm$^3$/ hour) 150 (°C) 1.01 (bar) 8.55 (mol.%$_2$) CO$_2$ 17 (mol.%$_2$) H$_2$O 74.45 (mol.%$_2$) N$_2$</td>
<td>An indicative 600 MW boiler based power plant data from Iijima (1998) was used</td>
</tr>
<tr>
<td>NGCC power plant</td>
<td>Emirates Aluminum (S3); (S4)</td>
<td>1,800,000 (Nm$^3$/ hour) 98 (°C) 1.01 (bar) 5.06 (mol.%$_2$) CO$_2$ 12 (mol.%$_2$) H$_2$O 82.94 (mol.%$_2$) N$_2$</td>
<td>An indicative 400 MW CCGT plant data from Bailey and Feron (2005) was used</td>
</tr>
<tr>
<td>Oil field</td>
<td>Bu Hasa (O$_1$)</td>
<td>9.13 (Mt CO$_2$/year)</td>
<td></td>
</tr>
<tr>
<td>Oil Field</td>
<td>Bab (O$_2$)</td>
<td>3.91 (Mt CO$_2$/year)</td>
<td></td>
</tr>
<tr>
<td>Oil Field</td>
<td>Asab (O$_3$)</td>
<td>3.88 (Mt CO$_2$/year)</td>
<td></td>
</tr>
</tbody>
</table>
Figure 6.3: Location of CO$_2$ sources ($S_1$, $S_2$, $S_3$) and sinks ($O_1$, $O_2$, $O_3$) of case study

### 6.3 Results and discussions

The cost optimal operational and design variables including capture bypass ratio at varying degree of capture (DOC) (i.e., 25%-99%) were obtained by performing a number of optimizations of the 30wt% MEA-based CO$_2$ capture plant and compression train techno-economic model (see chapters 3 and 4) attached to all the sources in the case study. These optimal operational variables listed in Table 6.2 along with the data listed in Table 6.3 were used to simulate the capture plant compression train in order to obtain the levelized cost relationships against degree of capture which in turn is used as a meta-model input in the network model.
Table 6.2: The cost-optimum control variables obtained for the capture plant and compression train attached to CCGT and boiler based power plant.

<table>
<thead>
<tr>
<th>Amine lean loading</th>
<th>$T_{fg}$ after cooling (°C)</th>
<th>$T_{ls}$ inlet to absorber (°C)</th>
<th>Reboiler and stripper pressure (Mpa)</th>
<th>$\Delta T$ Rich lean HE (°C)</th>
<th>$\Delta T$ Scrubber cooler (°C)</th>
<th>$\Delta T$ Scrubber cooler (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.28-0.29</td>
<td>50.0</td>
<td>45.0</td>
<td>0.202</td>
<td>20.0</td>
<td>15.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>

Table 6.3: Parameters and nominal variables used in the optimization and simulation of carbon capture plant and compression train.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure of the absorber (kPa)</td>
<td>101</td>
</tr>
<tr>
<td>Pressure drops in packing (kPa/m)</td>
<td>0.2</td>
</tr>
<tr>
<td>Water makeup (kg/ton CO$_2$)</td>
<td>0</td>
</tr>
<tr>
<td>Capacity factor (CF)</td>
<td>0.7</td>
</tr>
<tr>
<td>Cost year</td>
<td>2004</td>
</tr>
<tr>
<td>MEA make-up (kg/ton CO$_2$)</td>
<td>1.1 kg$^1$</td>
</tr>
<tr>
<td>Norton IMTP 50 mm dry packing area (a) (m$^2$/m$^3$)</td>
<td>120</td>
</tr>
<tr>
<td>CO$_2$ outlet pressure from compressor (kPa)</td>
<td>14000$^2$</td>
</tr>
<tr>
<td>CO$_2$ product content from condenser (mol%)</td>
<td>90.4$^3$</td>
</tr>
<tr>
<td>Compressor efficiency ($\eta_{lsn}, \eta_{mec}$) (%)</td>
<td>(80, 95)$^4$</td>
</tr>
<tr>
<td>Pumps efficiency (%)</td>
<td>75$^2$</td>
</tr>
</tbody>
</table>

$^1$ Chapel et al., 1999 predicted total of 1.6 kg/ton CO$_2$ of which 0.5 kg/ton CO$_2$ is vaporized at the optimum capture rate as predicted by the model. This increased model flexibility to account for vaporization

$^2$ Rao and Rubin, 2002

$^3$ Iijima, 1998

$^4$ Kvamsdal et al., 2007

The cost-optimal operating capacity and velocity for each nominal pipeline size (NPS) listed in Table 6.4 was obtained by performing a number of simulations of the techno-economic
model developed in the previous chapter while assuming a minimum delivery pressure of 8.7 MPa, a maximum operating pressure of 14 MPa, a distance of 100 km and a pipeline cost data based on a regression model obtained for the south-eastern region of the USA (McCoy and Rubin, 2008). In order to account for the uncertainty in this reported data, compared to published work in the literature in which double the cost was reported (van der Zwaan et al., 2011), an uncertainty multiplying factor that represents the following increments in pipeline capital cost (i.e., +25%, +50%, +75%, +100%) was included. An operating cost of ($3100/km/year) was used in the study (Herzog 2003).

<table>
<thead>
<tr>
<th>Pipeline diameter</th>
<th>Capacity (Mt CO₂/year)</th>
<th>Velocity (m/s)</th>
<th>Input pressure (MPa)</th>
<th>Compressibility (Z)</th>
<th>Pressure drop (Pa/m)</th>
<th>Cost (k$/km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>168 mm (6 in)</td>
<td>0.4-0.79</td>
<td>0.3-1.4</td>
<td>8.8-14</td>
<td>0.19-0.24</td>
<td>1.9-54</td>
<td>146</td>
</tr>
<tr>
<td>219 mm (8 in)</td>
<td>0.8-1.5</td>
<td>0.8-1.5</td>
<td>10-13.5</td>
<td>0.20-0.24</td>
<td>13-49</td>
<td>186</td>
</tr>
<tr>
<td>273 mm (10 in)</td>
<td>1.51-2.2</td>
<td>1-1.4</td>
<td>10.2-11.9</td>
<td>0.20-0.22</td>
<td>15.6-32.8</td>
<td>228</td>
</tr>
<tr>
<td>324 mm (12 in)</td>
<td>2.21-3.0</td>
<td>1-1.4</td>
<td>10.0-11.1</td>
<td>0.20-0.21</td>
<td>13.7-24.9</td>
<td>268</td>
</tr>
<tr>
<td>406 mm (16 in)</td>
<td>3.01-4.67</td>
<td>1.0-1.6</td>
<td>9.8-11.3</td>
<td>0.20-0.21</td>
<td>12.9-27.2</td>
<td>311</td>
</tr>
<tr>
<td>507 mm (20 in)</td>
<td>4.68-7.02</td>
<td>1.0-1.5</td>
<td>9.5-10.5</td>
<td>0.19-0.20</td>
<td>8.7-19.2</td>
<td>388</td>
</tr>
<tr>
<td>610 mm (24 in)</td>
<td>7.03-11.04</td>
<td>1.1-1.7</td>
<td>9.4-10.5</td>
<td>0.19-0.20</td>
<td>7.6-18.4</td>
<td>469</td>
</tr>
<tr>
<td>762 mm (30 in)</td>
<td>11.05-17.01</td>
<td>1.1-1.7</td>
<td>9.2-10.0</td>
<td>0.19-0.20</td>
<td>6-13.8</td>
<td>592</td>
</tr>
</tbody>
</table>

These results were then fed into the supply chain CCTS network model in which the decision variables are picked from sets of potential variables that should meet the above-mentioned constraints and the objective function. This was formulated as a mixed integer linear programming (MILP) problem and solved in the GAMS environment using the CPLEX solver. The results of running our multiscale model using 4 national reduction targets (i.e., 25%, 50%, 75%, 95%) that minimized the total levelized cost of the system were obtained including: the prospective network topologies shown in figures 6.4-6.7; the rate of capture and potential exploitation for EOR from selected sources and sinks shown in Table 6.5. It
was observed that the uncertainty in the pipeline construction cost did not change the optimal results obtained for the entire chosen CO$_2$ reduction targets.

**Figure 6.4:** Prospective network while meeting 25% CO$_2$ reduction target: 168 mm (6 in) pipeline transferring 2148 (tCO$_2$/day) between $S_1$ and $O_2$; 168 mm (6 in) pipeline transferring 2316 (tCO$_2$/day) between $S_2$ and $O_3$. 
Figure 6.5: Prospective network while meeting 50% CO₂ reduction target: 168 mm (6 in) pipeline transferring 1116 (tCO₂/day) between S₁ and S₂; 324 mm (12 in) pipeline transferring 6730 (tCO₂/day) between S₂ and S₁; 324 mm (12 in) pipeline transferring 6758 (tCO₂/day) between S₁ and O₂; 168 mm (6 in) pipeline transferring 2164 (tCO₂/day) between S₁ and O₃.
Figure 6.6: Prospective network while meeting 75% CO$_2$ reduction target: 219 mm (8 in) pipeline transferring 2619 (tCO$_2$/day) between S$_4$ and S$_3$; 273 mm (10 in) pipeline transferring 5282 (tCO$_2$/day) between S$_3$ and S$_2$; 406 mm (16 in) pipeline transferring 11176 (tCO$_2$/day) between S$_2$ and S$_1$; 406 mm (16 in) pipeline transferring 11204 (tCO$_2$/day) between S$_1$ and O$_2$; 168 mm (6 in) pipeline transferring 2164 (tCO$_2$/day) between S$_1$ and O$_3$. 
Figure 6.7: Prospective network while meeting 95% CO₂ reduction target: 219 mm (8 in) pipeline transferring 3950 (tCO₂/day) between S₄ and S₃; 12 inch pipeline transferring 3950 (tCO₂/day) between S₃ and S₂; 507 mm (20 in) pipeline transferring 7900 (tCO₂/day) between S₂ and S₁; 507 mm (20 in) pipeline transferring 14778 (tCO₂/day) between S₁ and O₂; 168 mm (6 in) pipeline transferring 2164 (tCO₂/day) between S₁ and O₃.

Table 6.5: The cost-optimum capture rate for each selected source and injectivity in each potential reservoir

<table>
<thead>
<tr>
<th>CO₂ reduction target</th>
<th>S₁ (DOC %)</th>
<th>S₂ (DOC %)</th>
<th>S₃ (DOC %)</th>
<th>S₄ (DOC %)</th>
<th>O₁ (Mt CO₂/year)</th>
<th>O₂ (Mt CO₂/year)</th>
<th>O₃ (Mt CO₂/year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25%</td>
<td>98</td>
<td>33¹</td>
<td>0</td>
<td>0</td>
<td>0.78</td>
<td>0.85</td>
<td></td>
</tr>
<tr>
<td>50%</td>
<td>100</td>
<td>80</td>
<td>26²</td>
<td>0</td>
<td>2.2</td>
<td>1.06</td>
<td></td>
</tr>
<tr>
<td>75%</td>
<td>100</td>
<td>84</td>
<td>62</td>
<td>61</td>
<td>4.08</td>
<td>0.80</td>
<td></td>
</tr>
<tr>
<td>95%</td>
<td>99</td>
<td>98</td>
<td>92</td>
<td>92</td>
<td>5.39</td>
<td>0.79</td>
<td></td>
</tr>
</tbody>
</table>

¹ This was obtained by bypassing 53% of the flue gas while capturing the remaining flue gas at 70% DOC
² This was obtained by bypassing 58% of the flue gas while capturing the remaining flue gas at 60% DOC
**Table 6.6:** Optimum design variables of capture plant and compression train attached to selected CO₂ sources

<table>
<thead>
<tr>
<th>Reduction target (%)</th>
<th>Sources</th>
<th>Absorber &amp; DCC diameter (m)</th>
<th>Absorber height (m)</th>
<th>Blower power (kW)</th>
<th>Compressor after-cooler area (m²)</th>
<th>Compressor power (kW)</th>
<th>Condenser area (m²)</th>
<th>DCC height (m)</th>
<th>Lean amine cooler area (m²)</th>
<th>Reboiler area (m²)</th>
<th>Rich lean HE area (m²)</th>
<th>Stripper Diameter (m)</th>
<th>Stripper Height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>S₁</td>
<td>10.6</td>
<td>16.3</td>
<td>1155</td>
<td>962</td>
<td>9594</td>
<td>1625</td>
<td>10.3</td>
<td>2871</td>
<td>1470</td>
<td>8168</td>
<td>7.1</td>
<td>16.4</td>
</tr>
<tr>
<td>50</td>
<td>S₁</td>
<td>15.4</td>
<td>20.6</td>
<td>3096</td>
<td>2331</td>
<td>23246</td>
<td>3797</td>
<td>10.3</td>
<td>7030</td>
<td>3535</td>
<td>19955</td>
<td>10.3</td>
<td>17.1</td>
</tr>
<tr>
<td></td>
<td>S₂</td>
<td>9.5</td>
<td>16.4</td>
<td>950</td>
<td>4934</td>
<td>4572</td>
<td>9348</td>
<td>7.9</td>
<td>1459</td>
<td>748</td>
<td>4097</td>
<td>5.3</td>
<td>15.9</td>
</tr>
<tr>
<td>75</td>
<td>S₁</td>
<td>15.4</td>
<td>22.9</td>
<td>3428</td>
<td>2447</td>
<td>24406</td>
<td>3987</td>
<td>10.3</td>
<td>7385</td>
<td>3711</td>
<td>20946</td>
<td>10.3</td>
<td>17.3</td>
</tr>
<tr>
<td></td>
<td>S₂</td>
<td>14.5</td>
<td>17.1</td>
<td>2309</td>
<td>1103</td>
<td>11002</td>
<td>2090</td>
<td>7.9</td>
<td>3511</td>
<td>1800</td>
<td>9860</td>
<td>8.1</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>S₃</td>
<td>14.5</td>
<td>16.8</td>
<td>2272</td>
<td>1090</td>
<td>10871</td>
<td>2065</td>
<td>7.9</td>
<td>3469</td>
<td>1778</td>
<td>9742</td>
<td>8.1</td>
<td>16</td>
</tr>
<tr>
<td>95</td>
<td>S₁</td>
<td>15.4</td>
<td>35.6</td>
<td>5302</td>
<td>2857</td>
<td>28497</td>
<td>4803</td>
<td>10.4</td>
<td>9702</td>
<td>4448</td>
<td>23428</td>
<td>10.3</td>
<td>18.3</td>
</tr>
<tr>
<td></td>
<td>S₂</td>
<td>14.5</td>
<td>35.5</td>
<td>4883</td>
<td>1638</td>
<td>16333</td>
<td>3103</td>
<td>8.1</td>
<td>5212</td>
<td>2672</td>
<td>14636</td>
<td>8.1</td>
<td>17.9</td>
</tr>
<tr>
<td></td>
<td>S₃</td>
<td>14.5</td>
<td>36.5</td>
<td>4883</td>
<td>1638</td>
<td>16333</td>
<td>3103</td>
<td>8.1</td>
<td>5212</td>
<td>2672</td>
<td>14636</td>
<td>8.1</td>
<td>17.9</td>
</tr>
<tr>
<td></td>
<td>S₄</td>
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<td>4883</td>
<td>1638</td>
<td>16333</td>
<td>3103</td>
<td>8.1</td>
<td>5212</td>
<td>2672</td>
<td>14636</td>
<td>8.1</td>
<td>17.9</td>
</tr>
</tbody>
</table>
The results reveal the effects of having different CO$_2$ reduction targets on the cost-optimal CO$_2$ network topology. At a 25% CO$_2$ reduction target, a single-source single-sink network was deployed in which the steel production plant was exploited completely in addition to the boiler based power plant (i.e., the second highest CO$_2$ content source) being exploited proportionally and then transported to the closest sinks. At a 50% CO$_2$ reduction target, a hub at Taweelah region was developed to transport the CO$_2$ through a 324 mm (12 in) trunk line to the steel production plant in which a combination of 324 mm (12 in) trunk line and new 168 mm (6 in) pipeline were built to transport the CO$_2$ to the closest two oil reservoirs. At 75% and 95% DOC, a similar CO$_2$ network topology with higher pipeline capacities (i.e., 406 mm (16 in) and 507 mm (20 in) trunk lines instead of 324 mm (12 in) and 406 mm (16 in) trunk respectively) was built.

Another important observation of the results shown in Table 6.5 is that the cost-optimum degree of capture from the selected CO$_2$ sources depends on site-specific factors in addition to the techno-economic interconnectedness between CCTS components. Thus, the deployment of a compression plant at the steel plant with the highest degree of capture (i.e., 100%) is expected as it has a pure stream of CO$_2$ that only needs to be compressed and dried for transportation. However, a higher CO$_2$ content in the boiler fired power plant compared to the CCGT does not mean that this source needs to be exploited completely as can be seen in the results in Table 6.5. These results highlight the complexity of deploying an interconnected network to meet a specific reduction target. It also emphasizes the need to explicitly account for the effect of optimal degree of CO$_2$ capture from different sources as this is a site specific factor that is highly interconnected with the availability and the cost of pipeline networks.

The detailed design variables listed in Table 6.6 highlight the usefulness of using a multiscale modelling approach as a design tool to find the optimal sizes of the major units of the CO$_2$ capture plant and compression train including cost-optimal bypass ratio and DOC for the remaining flue gas. Further, optimal operating or control variables such as amine lean loading need to be sustained to ensure cost-optimal operation of the CCTS system. The flexibility in
the level of detail outlined in the multi-scale modelling approach allows it to be expandable in that it can be modified to account for uncertainty and in that it can be developed to a dynamic model, which can be used to assess the operability and controllability of the system.

![Figure 6.8](image)

**Figure 6.8:** Levelized cost of establishing CCTS network that meet reduction targets at 25%, 50%, 75% and 95% out of the 4 CO\(_2\) sources announced in Abu Dhabi for phase 1.

Figure 6.8 presents the total levelized cost of CO\(_2\) capture, compression and transport to a geological storage site that has a specific CO\(_2\) demand for EOR while assuming four reduction targets. The cost of capture and compression increases gradually with higher reduction targets because more expensive sources need to be connected to the system. This increases the total cost of the network as the cost of capture and compression contributes to more than 90% of total cost. The cost of transportation, however, decreases with larger CO\(_2\) reduction targets as a result of aggregating CO\(_2\) flows into larger diameter pipelines and hence exploiting economies of scale.

It is worth noting that the total cost of CCTS shown in Figure 6.8 is lower than CO\(_2\) capture and compression cost from CCGT plant shown in Figure 4.1. This is due to the low cost associated with capture and compression from the steel plant, which lowered the overall CCTS network cost for this case study.
6.4 Concluding remarks

CCTS is an essential technology for CO₂ reductions, which will allow us to continue consuming fossil fuels in the short to medium term. Although the technologies involved in CCTS have been proved independently, the remaining challenge facing governments and industries is to implement the whole system safely and at the minimum cost on a large scale that makes a material effect in global warming mitigation. To tackle this challenge, an integrated whole-system model of a CO₂ capture, transport and storage (CCTS) network was developed in order to design the cost-optimal network linking CO₂ sources (e.g., power stations) with potential sinks (e.g., depleted oil reservoirs). This work is multi-scale in nature, employing models describing system behaviour and interactions through a range of length and timescales. The multiscale CCTS network model was used to determine the optimum location and operating conditions of each CO₂ capture process while giving full consideration to the whole-system behaviour. A key result of our study was that the cost-optimal degree of capture is a function of several site-specific factors, including exhaust gas characteristics, proximity to transportation networks and adequate geological storage capacity. This conclusion serves to underscore the need to comprehend the science governing the behaviour at different scales and the importance of a whole-system analysis of potential CCTS networks.
7 CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

The aim of this thesis has been to develop a multiscale modelling and optimization approach that integrates all the components of CCTS to enable us to provide decision makers with a systematic tool which will help them find and analyse the cost optimal deployment of CCTS infrastructure meeting reduction mandates at the national or regional level. This was achieved by developing detailed sub-process models of the post-combustion capture plant, compression train and pipelines. These models were validated to ensure a reliable prediction of the behaviour of the system across the integrated scales. The effects of key operating parameters on the performance of the post-combustion capture plant and compression train coupled with a potential CO$_2$ source plant were analysed using selected key economic and environmental performance indicators. An optimization-oriented model of the post-combustion capture plant and compression train was then used to find the cost-optimal design variables in addition to operating parameters, which were modified to avoid harmful effects on the environment. Further, an optimization-oriented model of the transportation system (i.e., pipeline, compression train, booster pump) was also used to find the cost-optimal design and operating variables of the transportation system. The results obtained by these fine scale optimization models are then passed to the macro scale models through the development of meta-models, which summarize their behaviour in terms of a small number of key variables. This macro model was then used to design the cost-optimum network linking CO$_2$ sources (e.g., power stations) with potential sinks (e.g., depleted oil reservoirs). The results obtained included the optimum location and operating conditions of each CO$_2$ capture process, compression train and pipeline while giving full consideration to the whole-system behaviour.

The remainder of this chapter is outlined as follows: an extended summary that discuss the key results, limitations and implications of developing different models and performing different analyses was outlined. After this, directions for future work were suggested.
7.1 Extended summary

This section is subdivided into three sections: techno-economic analysis of post combustion CO₂ capture plant and compression train model; cost optimal CO₂ transportation model; and multiscale CO₂ network model.

7.1.1 Techno-economic analyses of post-combustion CO₂ capture plant and compression train model

A mathematical model of the MEA-based post-combustion capture plant with compression system was proposed and implemented in gPROMS. The model was then used to study the effects of key operating parameters on the capital cost, operating cost, and environmental impact of CO₂ capture plant applied to a case study of an exhaust gas typical of a 400 MW CCGT power plant in hot countries where the availability of low temperature cooling water is severely limited, using selected KPIs.

It was observed that operating at low amine lean loading is not favourable because of increased specific reboiler duty resulting from high heat of vaporization needed to maintain the driving force at the bottom of the stripper column. The optimum amine lean loading that minimized the specific reboiler duty, which represents the balance between sensible heat needed to heat the solvent circulated into the system and the heat of vaporization linked to the steam generated to maintain the driving force of CO₂ transfer in the stripper column, was obtained at value of 0.31. This however, required a higher volume of packing linked with more solvent circulating into the system and hence higher blower power consumption linked with higher-pressure drops in a taller column.

It was noticed that the degree of capture did not affect the specific reboiler duty obtained in earlier studies because the amine lean loading, which represents the relation between the liquid circulation rate and the net CO₂ loading, was fixed in this study. Further, there was dramatic increase in volume of packing at higher than 85% rate of CO₂ capture leading to an increase in the blower power consumption leading to bottlenecks associated with economies
of scale. An increased rate of amine vaporization was also observed at high capture rates as a result of gas exiting the absorber at high temperature.

It was also observed that operating the stripper and reboiler at high pressure reduces reboiler duty, volume of packing and power consumption of the whole capture and compression plant but it should be run at lower than degradation temperature. This is due to the attained increase of operating temperature of the stripper and reboiler at high pressure, which reduced heat of vaporization dominating the specific reboiler duty as a result of increased driving force of CO$_2$ transfer in the stripper column and hence less steam was generated to maintain the driving force. It was also noticed that it is not favourable to operate the MEA-based CO$_2$ capture plant and compression train at vacuum pressure due to increased reboiler duty, power consumption and cooling duty. This is linked to decreased driving force of CO$_2$ in the stripper column at low operating temperature leading to an increase of heat of vaporization and packing volume of the stripper column to maintain the driving force. Further, a higher compression power was required to pressurize the low pressure gas exiting from the stripper column.

It was also observed that while reducing flue gas temperature or lean amine temperature reduces amine vaporization and reboiler duty slightly, it increases the volume of packing, blower consumption and cooling duty. This was a result of decreased solubility and reaction rate of the solvent that outweighed the increased driving force of CO$_2$ transfer in the absorber column leading to an increase in volume of packing and hence higher blower power. The reduction in reboiler duty was linked to the increase of amine rich loading, which decreased the solvent circulation rate.

The results of the study have also highlighted the challenges in applying post combustion capture technologies in hot countries. It indicates a dramatic increase of cooling water requirements in regions where the cooling water temperature is higher than 25°C most of the year. Further, a higher compression power is required in hot countries due to higher exit pressure required to maintain single-phase flow compared to cold countries. Another
The challenge that needs to be overcome is the higher amount of cooling water needed in the washing water system to minimize the environmental impact of amine slippage. This abovementioned model was extended with an optimization-oriented model in gPROMS. This model was then used to find the cost optimal amine lean loading, flue gas and lean solvent temperature, reboiler and stripper pressure, temperature differences in heat exchangers and flue gas feed fraction ratio (FFR) for different CO₂ reduction targets for a post combustion capture plant and compression train applied to typical flue gas of 400 MW NGCC power plant. There was consistency on most of the abovementioned variables for a range of degrees of capture. The cost optimum amine lean loading has an average value of 0.28, which is the balance between the OPEX represented in the reboiler duty and the CAPEX represented by the height of the columns. Operating the capture plant at a flue gas temperature of 50°C and lean solvent temperature of 45°C minimized the total levelized cost because of the reduction of the height of the columns associated with enhanced reaction rate and solubility. It was also found that operating the reboiler and stripper at 0.2 MPa was the cost optimal solution as a result of enhanced driving force in the stripper column and hence reduced stripper column height. The optimal temperature difference for the rich lean heat exchangers was observed to be 20°C. Similarly, the temperature difference for the DCC cooler, and the scrubber cooler were 14.7°C and 15°C respectively. The flue gas bypass option was observed to be the cost optimum choice for lower than 60% overall DOC because capturing the remaining flue gas at higher than 60% DOC results in an increase in volume of packing and hence higher blower power.

The order of main components contribution in CAPEX, OPEX and utilities were the same for varying degrees of capture. The orders of contribution in CAPEX are as follows: absorber; compressor train; stripper; rich lean heat exchanger. The orders for of contribution in OPEX are as follows: reboiler; compressor; amine make-up. The order of their contributions in the total utility cost from higher to lower are as follows: steam; electricity; cooling water; MEA make-up.
It was also observed that the carbon price has a clear impact on the cost optimal DOC: at $0/ton CO₂, there is a shallow minimum between 55%-80% DOC; at $4/ton CO₂, there is shallow minimum between 70%-80% DOC; at $23/ton CO₂, there is shallow minimum between 85%-90% DOC. The assumed carbon prices are lower than the minimum cost of CO₂ capture and compression cost (i.e., $60/ton CO₂). Thus, it would be cheaper to vent the CO₂ rather than investing in CCS with current carbon prices. At a sufficiently high carbon price (i.e. higher than $60/ton CO₂), which covers the cost of CO₂ capture and compression, there will be sufficient incentive to capture the CO₂ at higher than 95% DOC.

7.1.2 COST OPTIMAL CO₂ TRANSPORT SYSTEM MODEL

A detailed optimization-based model of the whole CO₂ transport system including compression train, booster pump and pipeline was developed and implemented in gPROMS™. This model was successfully used to simultaneously find the cost optimum pipeline diameter in addition to design and control variables (i.e., compressor output pressure and rating power, pipeline operating velocity, compressibility and pressure drop) that were overlooked or assumed to be at constant values in the literature. Further, the thermophysical properties that behave non-linearly at pipeline operating conditions were obtained simultaneously using SAFT-VR equations of state and thus improve the accuracy of the obtained results.

The developed model was used to find the optimum control and design variables of the transport system considering a case study of capturing 83% of the CO₂ emitted from a natural gas fired power plant located in the UAE under variability in seasonal temperature between the summer and winter and uncertainty in the flow CO₂ content. It was shown that the optimal design should be made for the worst-case scenarios which involves the lowest CO₂ content flow and the highest operating summer temperature due to the fact that operating capacity is minimum at these conditions. The manipulating control variables such as operating velocity and rating power can then be reduced accordingly in cool temperatures and while transporting purer CO₂ flow in order to minimize cost. It was also observed that
transportation companies should levy a charge to discourage transporting flow from low CO$_2$ content sources in order to cover the charges associated with higher compression power required to maintain flow capacity.

The developed model was also used to identify the cost optimum operating capacity in addition to control and design variables for each NPS diameter considering a delivery pressure of 8.7 MPa and a storage site within 100 km. The results indicate a lower operating velocity (i.e., 1-2 m/s) and pressure compared to the ones reported in the literature. They also highlighted that the increase in pipeline thickness obtained for safety reasons does not necessitate a higher operating pressure. This study underscores the importance of incorporating all CO$_2$ transport system performance indicators such as CAPEX and OPEX driven by higher operating pressure, which might be neglected while considering the diameter of the pipeline alone or fixing a decision variable such as operating velocity.

### 7.1.3 Multiscale CO$_2$ Network Model

A detailed multiscale model that describes a complex CCTS system using a series of interacting scale specific models has been developed to design and analyse the optimal deployment of a CO$_2$ network. It takes into account the limits that physical material represented by a solvent poses in the performance of the capture plant and in the system as a whole. Thus, the optimum network design obtained for the whole system incorporates the potential interactions between models at different scales. This goal was achieved by analysing and identifying the key operating parameters of the system and then setting them at their optimal conditions while generating the data (e.g., levelized cost of capture and compression) needed for high-level analysis. This was also used to obtain the optimum operating, control and design variables including flue gas bypass ratio, degree of capture and unit sizes.

The model was successfully demonstrated for a case study in the UAE that includes 4 major CO$_2$ sources and three potential oil recovery sites amenable to CO$_2$ flooding. Although the results obtained are specific to the case study, a number of general observations can be
summarized including: the most promising CO$_2$ sources for CCTS implementation are the high CO$_2$ content sources within a reasonable distance to sinks; the deployment of large scale CCTS networks that meet high CO$_2$ reduction mandate increases the CCTS levelized cost as a result of capturing CO$_2$ from increasingly more expensive sources, which outweigh the benefits gained from aggregating CO$_2$ flows into larger pipelines; the uncertainty in reported pipeline construction costs did not affect the optimum layout of the network because the lion’s share of the total CCTS cost is associated with the capture plant and compression train. Further, the study emphasizes the need to explicitly account for the effect of degree of capture, and site-specific factors such as flue gas characteristics in planning future CO$_2$ reduction targets. Higher CO$_2$ content does not necessarily indicate that the source needs to be exploited completely. Other factors such as the location of the CO$_2$ source plant in the path of CO$_2$ network is another important factor that may be overlooked by policy makers. The results of this study indicated optimal capture rates lower than the ones obtained by taking into account the economies of the capture plant alone. This is due to a higher marginal cost of transporting extra CO$_2$ when capturing at higher level, which requires a larger diameter pipeline. Thus it competes with benefits of capturing CO$_2$ at the optimal rate considering the single CO$_2$ source alone. This conclusion underscores the importance of a whole-system analysis of potential CCTS networks, and serves to highlight that plant level details should be used to inform the design of CO$_2$ capture, transport and storage networks.

### 7.2 Future work

Further research needs to be undertaken to capture the effects of components details that were not looked at in this work on the overall system performance. More research is also required to examine the influence of the wider system in which the CCTS components serve on the operation of the whole CCTS system. This can be achieved by extending the multiscale CCTS network model and sub-process models.
7.2.1 Development of multiscale CCTS network

This area can be divided into the following research activities: Integration with EOR model; Integration with power plant model; Expanding the CCTS network model to be complex, stochastic and temporal; Development of dynamic CO\textsubscript{2} network model; CCTS network model implementation for the whole GCC region, development of smart transportation network. These are described below.

7.2.1.1 Integration with EOR Model

This activity involves developing detailed storage site models that capture the science governing CO\textsubscript{2} behaviour in each prospective oil reservoir amenable to CO\textsubscript{2} flooding. An important variable that needs to be quantified is the amount of CO\textsubscript{2} required throughout the lifetime of EOR implementation. This should include both the CO\textsubscript{2} captured from the CO\textsubscript{2} source plant and the CO\textsubscript{2} recycled from the processing surface facilities on site. This model will affect many non-trivial decisions that need to be made with regards to the optimal design and operation of the whole CCTS network.

7.2.1.2 Integration with detailed power plant model

This involves developing detailed models of the power plant such as NGCC in gPROMS. This model will be integrated with the CCTS network model, which will then help us perform further analysis with regard to the effects of gas prices, carbon prices and electricity market on the performance of the whole CCTS system. Consequently, this power plant model can be developed to a dynamic model, which can be used to test the operability and controllability of the system.

7.2.1.3 Expanding the CO\textsubscript{2} network model to be stochastic and temporal

The current multiscale CO\textsubscript{2} network model should be extended to be stochastic and temporal. The complex stochastic approach presents uncertainties spanning a continuous space arising in the market (e.g., utility price), legal issues (e.g., CO\textsubscript{2} reduction target) and behaviour (oil reservoir response to CO\textsubscript{2} flooding). These can be organized into discrete plausible scenarios
with estimated probabilities of occurrence. The optimal robust designs in the presence of these impurities are then obtained from the optimization model.

The temporal model will be used to find the optimal CCTS network configuration, which evolves as a function of time. This will address the need to find the optimal design for the whole time period while implementing CO₂ reduction targets into phases.

### 7.2.1.4 Development of dynamic CO₂ network model

This involves developing dynamic models of CCTS components, which are able to capture their transient behaviour. The dynamic model of the whole CCTS system will be used to understand the dynamic behaviour of the whole system. This will help us identify any operational problems and understand the system’s ability to buffer against any disturbances. This is driven by the fact that the CCTS components will be serving wider systems. For example, source plants such as power plants may be running in a transient way in response to power demand changes. Furthermore, storage sites represented by CO₂ flooding for EOR will be serving the operational procedures implemented to maximize oil production. Thus, disturbances that might arise from CO₂ source or storage sites will be propagated to the whole CCTS network operation and performance. Thus, we need to find the optimal control strategy that sustains a safe performance of the whole CCTS model. This can be achieved by developing model predictive control methods for the whole dynamic CCTS system.

### 7.2.1.5 CCS network implementation for the whole GCC region

This involves generating data of the CO₂ sources and CO₂ storage sites from the whole GCC region. This will help us identify any potential of utilizing a common CO₂ network and policy for the whole region. This is driven by the proximity of the CO₂ sources and sinks within this region. Further, there might be a lot of carbon intensive industries within a country, which might exceed its potential for utilization and storage within its borders. Therefore, implementing CCS for the whole region will add flexibility of implementation and operation.
7.2.1.6 Development of smart transportation network

This activity is based on that the next future pipeline should be run in a smart way. The use of the term "smart" involves the ability to transport more than one flow in both directions to meet different objectives. For example, it has been considered in the literature to reuse existing high-pressure gas pipelines to transfer the CO$_2$ back to the storage site. This opens the door for further research on redesigning the gas networks that are going to be built in that region to be smart. The first step that needs to be taken is to perform a feasibility study quantifying the potential of utilizing smart pipelines in the region. Then, detailed network models of the smart pipelines system can be developed.

7.2.2 DEVELOPMENT OF SUB-PROCESS MODELS

This area can be divided into two main research activities: the development of thermodynamic models; and the development of hydrodynamic models.

7.2.2.1 Development of SAFT-VR thermodynamic models

This activity involves the development of thermodynamic SAFT-VR models for different innovative solvents and flue gas impurities, which were not covered in the current thermodynamic model such as oxygen and acidic components (e.g., H$_2$S). Further, the presence of oxygen, hydrogen and other impurities are expected in future pipelines as a result of advancements in CO$_2$ capture technologies (e.g., oxy-fuel, pre-combustion). Thus, there is a need to develop detailed thermodynamic models that take into account the presence of these components in the flow. This will help us evaluate their effects on the design and operation of the whole CCTS system.

7.2.2.2 Development of hydrodynamic model

This activity involves development of mass transfer coefficient models for new structured packing that is expensive but has a lower pressure drop. This will help us analyse the performance of different type of packing on the performance of the whole CCTS network design and operation.
DISSEMINATION RECORD

Journal articles:


Conference papers:


Talks:


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