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Automated Optimisation of Multi Stage Refrigeration Systems within a Multi-Objective Optimisation Framework

Ishan Sharma[a*], Andrew Hoadley[b], Sanjay M. Mahajani[c], Anuradda Ganesh[d]

[a] IITB-Monash Research Academy, Indian Institute of Technology Bombay, Powai, Mumbai, 400076, India
[b] Department of Chemical Engineering, Monash University, Clayton, VIC-3168, Australia
[c] Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, 400076, India
[d] Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, 400076, India
114174001@iitb.ac.in

This work demonstrates an automated optimisation of a two stage refrigeration system, which is embedded into an Excel-based Multi-Objective Optimisation (EMOO) framework. The proposed framework has been demonstrated using the Rectisol™ process with CO_2 capture as an example. The automated optimisation procedure assesses any opportunities to exploit “pockets” in the process Grand Composite Curve (GCC), besides analysing the GCC for two discrete refrigeration temperature levels. The program uses a Co-efficient of Performance (COP) approximation to estimate the required electrical duty. The results of this sub-program are analysed as part of the wider Multi-Objective Optimisation (MOO) which sets the process decision variables such as the solvent flow-rates and solvent regeneration pressure levels in order to minimise the total electrical power consumption and maximise CO_2 capture rate. Two options for increasing the pressure of the captured CO_2, i.e. by condensation and pumping of CO_2 up to 100 bar (Case-I) and by compression up to 100 bar (Case-II) have also been compared by assessing their respective Pareto plots. This is interesting as the condensation case adds an additional refrigeration duty.

1. Introduction

Process plants working in the sub-ambient temperature range require some kind of refrigeration system. Refrigeration systems, because of their high capital and operating costs, are known to dominate the technical and economic aspects of many chemical processes. Process integration methodology may play a significant role in the optimisation of such systems. Most of the industrial refrigeration systems employ vapour compression cycles, where the compressor shaft work is often considered to dominate the operating cost of the system (Lee, 2002). One such process is the acid gas physical absorption process, known as Rectisol™ which uses refrigerated methanol as a solvent to absorb impurities from synthesis gas. The cost of the Rectisol™ process is tightly coupled to the associated refrigeration system.

In recent years, there has been a surge in research articles dealing with Multi-Objective Optimisation (MOO) applications in chemical engineering (Rangaiah, 2009). A major milestone was achieved by Bhutani et al. (2007) when they demonstrated the integration of a MOO algorithm with commercial simulation softwares like, Aspen Hysys™ and Aspen Plus™. Sharma et al. (2012) implemented this strategy in a Microsoft Excel-based MOO framework, which was extended by Harkin et al. (2012) to incorporate heat pinch analysis. In this work, further addition to this framework is developed which incorporates the optimisation of vapour compression refrigeration systems. This addition is demonstrated using the Rectisol™ process with CO_2 capture as an example. Rectisol™ process is typically used to produce a very high purity hydrogen product, which is required for applications such as the synthesis of ammonia. Rectisol™ uses chilled methanol at temperatures between -20 and -70 °C (Sun and Smith, 2013) to physically absorb CO_2. Gatti et al. (2013) looked at the role of energy integration in optimization of chilled methanol based CO_2 capture process. Their analysis was however confined to a particular CO_2 capture level, which doesn’t provide the opportunity to analyse the trade-off involved between energy

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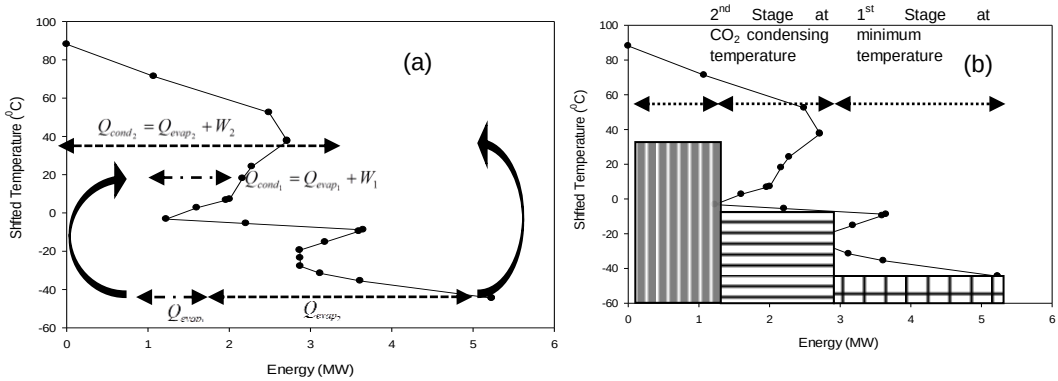

Figure 1: (a) Pocket Exploitation and (b) Extra refrigeration level at CO_2 condensation temperature

consumption and the extent of CO_2 capture. Although the authors are interested in the optimisation of the full coal to ammonia plant, in this study, the Rectisol™ plant with CO_2 capture is optimised as a stand-alone unit.

There are two options for increasing the pressure of the captured CO_2, i.e. by condensation and pumping of CO_2 up to 100 bar (Case-I) and by compression up to 100 bar (Case-II). These two cases are evaluated in this study, because of the interesting refrigeration synergy in Case I.

2. Refrigeration system optimisation strategy

Lee (2002) discussed a number of design options available to improve the performance of a refrigeration system. A typical GCC for the Rectisol™ process involving CO_2 condensation is shown in Figures 1(a) and (b). The flat portion in the GCC at around -10 °C corresponds to the CO_2 condensation stream. The GCC shows that the two most promising options available to optimise such a refrigeration system are "pocket exploitation", Figure 1a, and adding another refrigeration level at the CO_2 condensing temperature, Figure 1b.

Estimating shaftwork is a major challenge encountered while optimizing multi stage refrigeration systems with the help of process GCC. Linnhoff and Dhole (1989) first used the Exergy Grand Composite Curve (EGCC) to estimate the shaftwork requirements. This methodology of estimating shaftwork has been used by many researchers over the years. Recently, Hackl and Harvey (2012) used it, in conjunction with total site analysis, to reduce the shaftwork of the cooling systems in one of the industrial clusters in Sweden. Raei (2011) also used this approach to estimate shaftwork for an industrial case study. However, in this work, the shaftwork for the refrigeration section is estimated by using a simple COP-based formulation (Smith, 2005). An actual performance of 60 % of that of the ideal isentropic performance has been assumed for each stage of the refrigeration system.

The pocket exploitation, optimisation problem for the GCC shown in Figure 2(a) is formulated as follows:

$$\left(E_{AP/BP}\right)_i = Min\left\{ Q_{cond}\frac{\left(T_{cond_S} - T_{\min}\right)}{\left(273.15 + T_{cond_S} + 0.5 * \Delta T_{\min}\right)} + \left(Q_{tot} - Q_{CW} - Q_{cond} + Q_{cond}\frac{\left(T_{cond_S} - T_{\min}\right)}{\left(273.15 + T_{cond_S} + 0.5 * \Delta T_{\min}\right)} \right) * \left(\frac{T_{CWS} - T_{\min}}{\left(273.15 + T_{\min} + 0.5 * \Delta T_{\min}\right)} \right) \right\} \quad (1)$$

Where,

Q_{cond}: Heat being given to the pocket (MW), T_{cond_S}: Temperature (shifted) on the GCC corresponding to Q_{cond} $(°C)$, $T_{\min}$: Minimum temperature (shifted) on GCC $(°C)$, $\Delta T_{\min}$: Minimum temperature difference for the heat exchanger network $(°C)$, Q_{tot}: Total Cooling Utility (MW), Q_{CW}: Cooling Water Target (MW) and T_{CWS}: Cooling water temperature (shifted) $(°C)$

Q_{cond} and T_{cond_S} are linearly related and the exact relation can be deduced by the decomposition of the GCC.

In absence of a pocket below the pinch, the total cooling duty can be provided at two different temperature levels, as shown in Figure 2(b). Such a situation is expected in Case II, i.e. the case in which CO_2 is being compressed up to 100 bar. In this case, the optimum intermediate temperature level, T_{evap_S}, can be estimated by solving Eq(2), to minimise the refrigeration compressor work.

$$E_{WP} = Min\left\{ Q_{evap}\left(\frac{T_{CWS} - T_{evap_S}}{273.15 + T_{evap_S} + 0.5 * \Delta T_{\min}} \right) + \left(Q_{tot} - Q_{evap}\right) * \left(\frac{T_{CWS} - T_{\min}}{273.15 + T_{\min} + 0.5 * \Delta T_{\min}} \right) \right\} \quad (2)$$

Where,

T_{evap_S} : Intermediate temperature (shifted) level $\left({}^0C\right)$, Q_{evap} : Duty corresponding to T_{evap_S} (MW)

In Case I, a separate refrigeration level can also be provided at the CO_2 condensing temperature. The corresponding shaft work is termed as E_T. The Optimum shaftwork is thus the minimum value among $\left(E_{AP}\right)_i$'s, $\left(E_{BP}\right)_i$'s, E_{WP} and E_T ; i.e. $E_{ref,opt} = Min\left[\left(E_{AP}\right)_i, \left(E_{BP}\right)_i, E_{WP}, E_T\right]$.

It is important to note here that exploiting pocket 2 will require an additional refrigeration stage to be introduced in order to satisfy the cooling requirement of the heat source within the pocket. Therefore, in such a case, a three stage refrigeration system would be required. In this work, however, we have restricted our analysis only to two stage refrigeration systems. The proposed MOO framework is depicted in Figure 3. The optimisation algorithm used in this study is Nondominated Sorting Genetic Algorithm-II (NSGA-II) proposed by Deb et al. (2002).

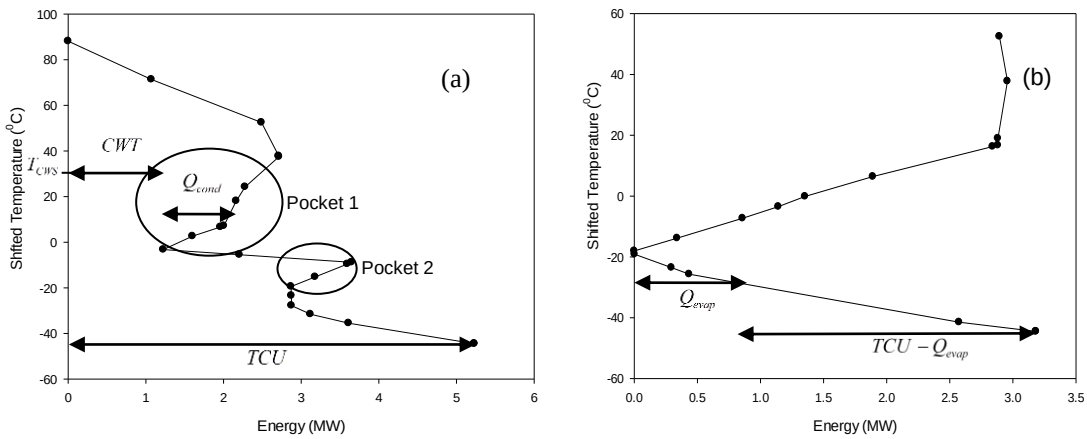

Figure 2: (a) Pocket exploitation optimisation and (b) Two stage refrigeration system optimisation in absence of a pocket below pinch

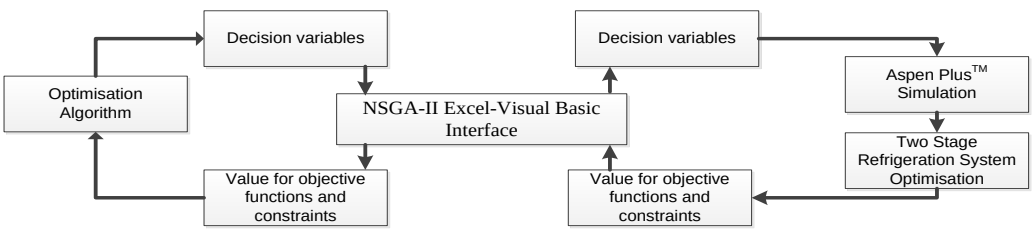

Figure 3: Proposed MOO framework

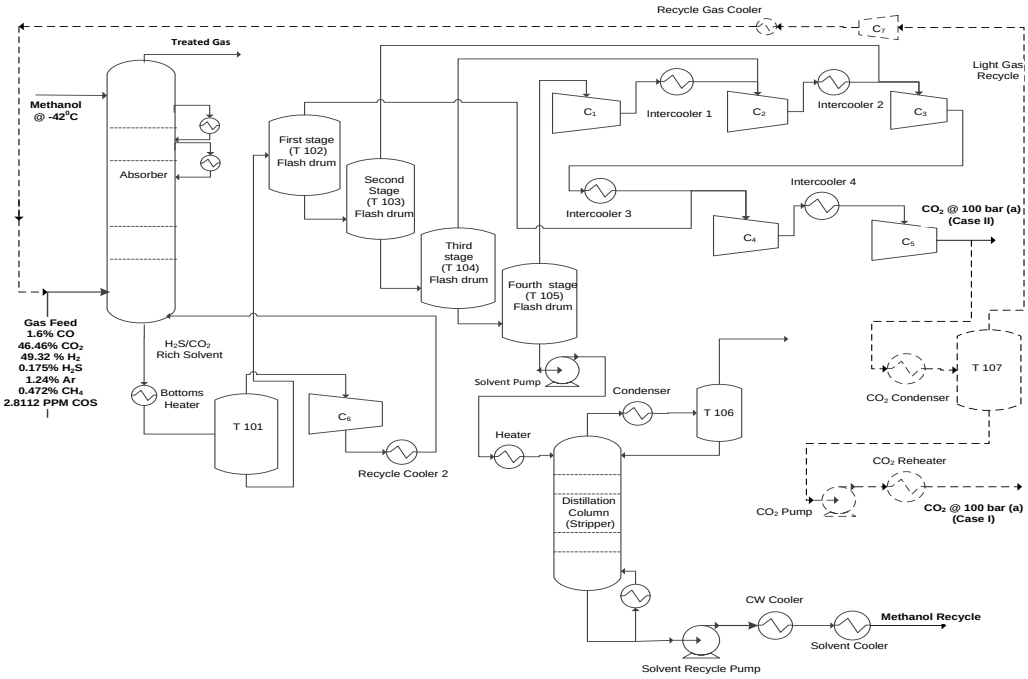

Figure 4: Process flowsheet for Case I and Case II (The dotted section represents the additional unit operations for Case I)

3. Process Description

Figure 4 shows the two Rectisol™ configurations considered in this work. Methanol solvent at -42 °C is fed to the absorber where it absorbs the acid gas components from the raw syngas, being fed at -21 °C. The absorber has two liquid side-draw cooling loops. The CO_2 rich solvent is heated and flashed to recover the co-absorbed H_2 and CO. The flashed gases are then compressed and recycled back to the column. The solvent is then flashed in a series of drums in order to recover CO_2 at different pressure levels. A stripper is used downstream in order to complete the regeneration of the solvent with the help of steam to remove H_2S.

4. MOO problem

The overall MOO problem for the two cases is formulated as follows:

Case I : $Maximise\ \ CR_{CO_2}(\%)\ \ \&\ \ Minimise\ \ PP = \sum_{i=1}^{6} E_{Ci} + E_{ref} + E_{RP} + E_{SP} + E_{SS}(kW)$ (3)

$$w.r.t.: P_{T102}, P_{T105}, F_{Sol}\ and\ VF_{BH}\ ; subject\ \ to:\ x_{CO_2}^{TG} \le 10\ \ PPM, R_{CO} \ge 98\ \%\ and\ \ R_{H_2} \ge 99.8\ \%$$

Case II: $Maximise\ CR_{CO_2}(\%)\ \&\ Minimise\ \ PP = \sum_{i=1}^{7} E_{Ci} + E_{ref} + E_{RP} + E_{CO2P} + E_{SP} + E_{SS}(kW)$ (4)

$$w.r.t.: P_{T102}, P_{T105}, F_{Sol}\ , VF_{BH}\ and\ P_{cond}\ ; subject\ \ to:\ x_{CO_2}^{TG} \le 10\ \ PPM, R_{CO} \ge 98\ \%\ and\ \ R_{H_2} \ge 99.8\ \%$$

Where; CR_{CO_2} : CO_2 capture rate $(\%)$, PP : Total power penalty associated with CO_2 capture (kW), E_{Ci}: Electrical power consumed by compressor $C_i\ (kW)$, E_{ref}: Optimum electrical power consumed by refrigeration compressor (kW), E_{RP} : Electrical power consumed by Solvent Recycle pump (kW) , E_{CO2P} : Electrical power consumed by CO_2 pump (kW), E_{SP} : Electrical power consumed by Solvent pump (kW), E_{SS}: Approximate electrical power sacrificed by using LP steam in stripper reboiler (kW), P_{T102}: First stage flash pressure (bar), P_{T105}: Last stage flash pressure (bar), F_{Sol}: Solvent (methanol) flow rate $(kmol/h)$, VF_{BH} : Outlet vapour fraction of Bottoms Heater, P_{cond}: Pressure at which CO_2 condensation

Table 1: Decision variable range for optimisation of Case I and Case II

Decision Variable	Case I	Case II
P_{T102}	10-30 (bar)	10-38 (bar)
P_{T105}	0.1-10 (bar)	0.1-10 (bar)
F_{Sol}	2,000-2,900 $(kmol/h)$	2,000-2,900 $(kmol/h)$
VF_{BH}	0.005-0.035	0.005-0.035
P_{cond}	30-65 (bar)	Not Applicable

takes place (bar), $x_{CO_2}^{TG}$: Mole fraction of CO_2 in treated gas, R_{CO}: Overall recovery of CO $(\%)$ and R_{H_2} : Overall recovery of H_2 $(\%)$. The electrical power sacrificed by using LP steam in stripper reboiler has been estimated using the Salisbury approximation (Salisbury, 1942). The range for each decision variable is given in Table 1.

Results and Discussion

The approximate Pareto front for Case I, obtained after 50 generations is shown in Figure 5(a). The fourth stage flash pressure (P_{T105}) had the most significant effect on the final Pareto front. P_{T105}values corresponding to the optimum objective function values are shown in Figure 5(b).
The optimum specific energy penalty (electricity consumed per unit mole of CO_2 captured) is an important measure that often gives useful insights in such situations. The optimum specific energy penalty, SEP_{opt} is the ratio of the total power to molar flowrate of captured CO2. Figure 6 shows SEP_{opt} for different CO_2 capture rates shown in Figure 5(a), with a minimum at around 75 % capture rate. The total power penalty

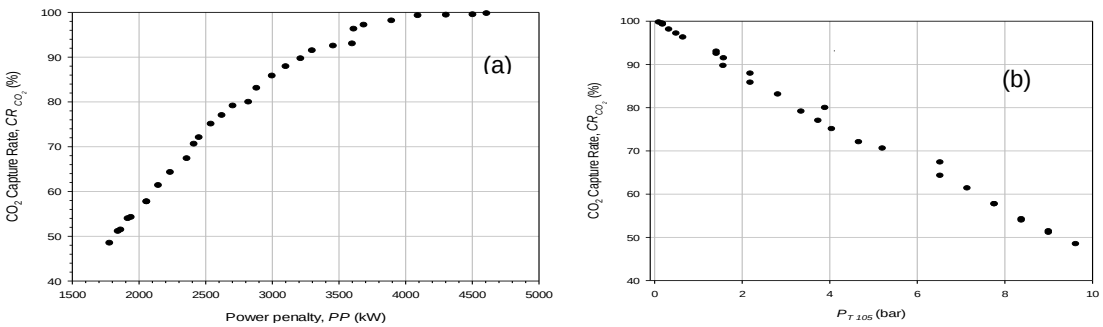

Figure 5: (a) Approximate Pareto front obtained for Case I and (b) P_{T105}values corresponding to optimum objective function values

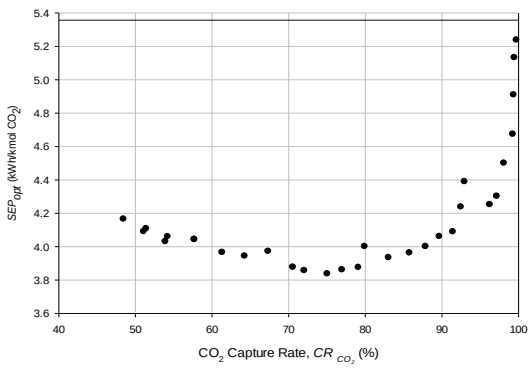

Figure 6: Minimum specific energy penalty at different CO_2 capture rates

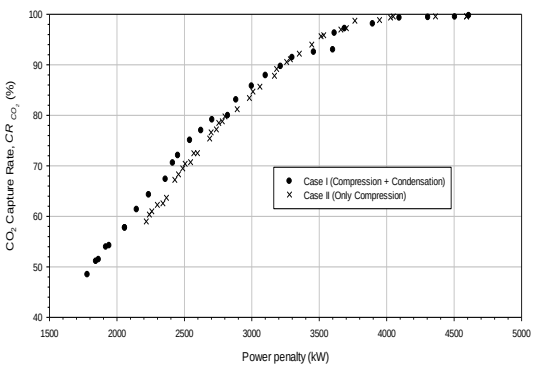

Figure 7: Pareto fronts obtained for two alternate CO_2 pressurisation mechanisms

associated with CO_2 capture is composed of the compression and refrigeration penalty. The refrigeration penalty is in turn composed of solvent refrigeration and CO_2 condensation. With decreasing CO_2 capture rate, the solvent refrigeration requirements remain the same due to the constant solvent flow rate required in order to achieve the quality constraint ($x_{CO_2}^{TG}$≤10 PPM) for the treated syngas, which in turn explains the trend observed in Figure 6. A comparison between the Pareto fronts obtained for Case I and Case II is shown in Figure 7. Case I had a slightly lower energy penalty for low capture rates, but the relative difference between the Cases decreased with increasing capture rates.

For all the Pareto optimal points obtained for Case I, the optimiser selected a two stage refrigeration system, with refrigeration temperature levels at (1) the CO_2 condensation temperature and (2) the minimum temperature on the GCC (i.e. T_{min}). By contrast, for every Pareto optimal point obtained in Case II, pocket exploitation was the preferred design option. This demonstrates the value in allowing the software to select the specific method of GCC optimization, rather than selecting it a priori.

5. Conclusions

An automated optimisation of a two stage refrigeration system, embedded into an Excel based Multi-Objective Optimisation (EMOO) framework has been proposed. The proposed framework has been applied to a Rectisol™ unit that absorbs and captures CO_2 from a water gas shifted syngas stream. The minimum electrical power penalty is thus obtained for different CO_2 capture rates, along with the corresponding operating parameters. Two options for increasing the pressure of the captured CO_2 have also been compared. The results show that the condensation case performs slightly better than the compression case. However, the relative performance of the condensation case declines with an increase in the CO_2 capture rate.

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