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SYNTHESIS AND OPTIMIZATION OF DEMETHANIZER FLOWSHEETS FOR LOW TEMPERATURE SEPARATION PROCESSES

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Abstract
Low temperature distillation remains the most important route for the separation and purification of gas mixtures, especially when high throughputs are required. A demethanizer system is an industrially important example of such a process that involves interactions between the separation system, refrigeration system and the heat recovery system.

The number of alternative demethanizer flowsheets, both in theory and commercially available, is large. The assessment of all structural alternatives and their operating conditions is a time consuming task requiring many simulations to select the most economic options. Therefore, a systematic approach for synthesis is required to generate effective and economic designs with minimal time and effort.

This research extends an existing platform for the design of heat integrated separation systems to address the demethanizer subsystem, characterized by interactions between the complex distillation column and other flowsheet components, including the turbo-expander, flash units, multistream exchangers and external refrigeration system. Heat recovery opportunities are identified to improve the economics of the process. Case studies illustrate that the optimization framework allows energy-efficient and cost-effective gas separation flowsheets to be developed.

1 Introduction

Low temperature separations are characterized by important interactions between the separation and refrigeration systems. These interactions should be considered at the early stages of design to ensure the maximum exploitation of integration opportunities leading to reduced cost of the process. Among the low temperature separations, one of the important is the recovery of natural gas liquids (NGL). In addition to methane, natural gas also contains some other heavier hydrocarbons along with impurities such as carbon dioxide and nitrogen. These heavier hydrocarbons must be separated from the methane to provide pipeline quality methane and recover natural gas liquids. The increasing demand for natural gas liquids has led to the construction of turbo-expander plants that recover ethane from natural gas streams at cryogenic temperatures as low as $-95\,^{o}C$[1]. There are many process alternatives for NGL recovery based on gas expansion refrigeration. The different process schemes proposed in patents have usually been justified in terms of reduced energy consumption or increased recoveries.

The heart of NGL recovery is the demethanizer system for the separation of methane from the heavy hydrocarbons, for which technology licensors have different designs. The demethanizer system is characterized by interactions between the complex distillation column and other flowsheet components, including the turbo-expander, flash units, multistream exchangers and external refrigeration. There are many possible options to consider before the design of the complex demethanizer system is finalized. It may be beneficial to cool the feed, or to split the feed in multiple flash separators at different pressures before it enters the column on different stages. The feed cooling is normally done by heat exchange with the top product in a multistream exchanger. Similarly, the heat for distillation required by side reboilers can provide cooling to the feed stream, which helps to minimize the use of external refrigeration for feed pre-cooling. The separation requires very low temperatures; this need for refrigeration can be fulfilled by a turbo-expander.

A typical demethanizer system for NGL recovery is shown in Figure 1. The inlet gas is cooled by heat exchange with the sales gas and through the demethanizer side reboiler in a multistream exchanger. The partially condensed feed gas is sent to a flash separator. The resulting vapour is then split into two parts. The first part is expanded through the turbo-expander to obtain the low temperatures required for high ethane recovery and is then fed as the upper feed into the demethanizer column. The second part goes to a subcooler and is sent as an external reflux stream into the column. The liquid from the flash is fed directly into the demethanizer as the lower feed.

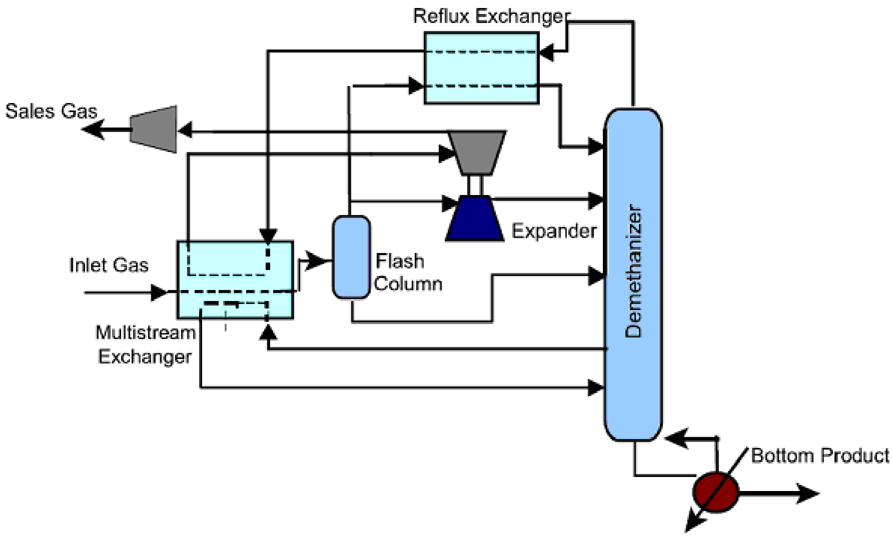

Figure 1. A typical demethanizer system

The top product from the demethanizer cools the inlet gas and is then recompressed to pipeline pressure and delivered as sales gas. The product from the demethanizer bottom can be further fractionated to produce pure ethane and heavier components, such as propane, butanes, and heavier hydrocarbons. When the fraction of condensable components present in the feed gas is relatively low, the plant can be operated without external refrigeration. Otherwise, mechanical refrigeration is required in addition to the refrigeration provided by the turbo-expansion process. Note that compression and refrigeration requirements dominate both capital and operating costs in this process[2].

2 Demethanizer Flowsheet Design and Simulation

The assessment of all possible flowsheets with numerous options is a time consuming task with a large number of simulations required to select the most economic option. There are many design alternatives that must be evaluated when selecting the ethane recovery process for a new gas processing facility. The current practice for design of the demethanizer flowsheets is based on previous experience, design heuristics and simulation of the flowsheet at different operating conditions[3]. The complex nature of these flowsheets makes their design challenging. However, no systematic procedure has been described in the literature to find the appropriate process technology and operating conditions to achieve an optimal design for a particular product specification. This work presents an approach to screen the various options and narrow the design options to viable schemes. A methodology is being developed for the design of a demethanizer system, ensuring that promising design options are identified at an early stage and all major design options are considered. The design objective is a high recovery of ethane with low shaft power demand for refrigeration and recompression. Good recovery of process 'cold' from the demethanizer in the multistream heat exchanger can minimize the shaft power requirement.

2.1. Sensitivity Analysis

Gas Subcooled Process[4] (GSP) for the recovery of NGL is simulated to highlight the design parameters affecting the process performance. The process is simulated in HYSYS 2006.5 (Figure 2) to determine the process power requirement and its sensitivity to selected variables.

The process performance is strongly dependent on the operating pressure of the distillation column. At medium to low pressures, i.e. 2000 kPa or lower, the recompression horsepower requirement will be so high that the process becomes uneconomic. However, at higher pressures the recovery of hydrocarbon liquids will be significantly reduced due to the less favourable separation conditions, i.e., lower relative volatility inside the distillation column. The selection of appropriate operating pressure is thus a key variable in NGL recovery plant design.

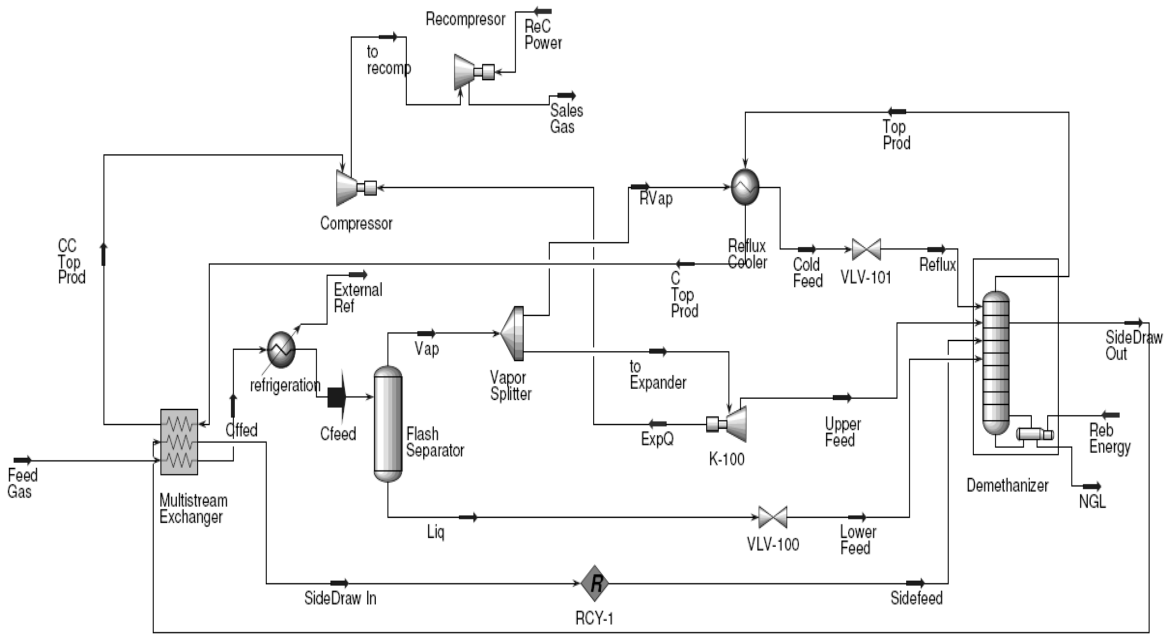

Figure 2. Flowsheet for simulation of a gas subcooled process (GSP) using HYSYS

A significant cost in NGL recovery processes is related to the refrigeration required to chill the inlet gas. Refrigeration for these low temperature recovery processes can be provided by external refrigeration systems using ethane or propane as refrigerants. In most cases, the refrigeration is provided by turbo-expansion of the compressed natural gas feed.

The amount of cold recovery by the side reboiler is also important: provision of refrigeration at temperatures lower than the temperature of the column reboiler can significantly reduce the refrigeration cost. Opportunities to add low-temperature heat to the side reboiler at different locations in the column are investigated.

The temperature of the high pressure separator has a significant effect as it affects the ratio of vapour to liquid leaving the flash separator, which in turn affects the performance of the column and the rest of the process. The minimum approach temperature criterion in the multistream heat exchanger is assumed to be 2°C.

2.2. Flowsheet simulation

The different unit operations of the demethanizer system are modelled in MATLAB 2007b. The complex distillation column is simulated using a modified boundary value method[5]. The column model in MATLAB is linked to HYSYS for calculation of physical properties using the Peng-Robinson equation of state. A new design method[6] based on the boundary value method is employed for generating the column design, verifying the separation performance and calculating energy requirements. In the new boundary value method, the feed and product compositions, column pressure and reflux or reboil ratio must be specified as design parameters. The boundary value method is extended to allow the design of the demethanizer column which is a double-feed column with side reboilers and an external reflux stream separating a multicomponent mixture. The simplified model is computationally efficient and predicts process behaviour satisfactorily.

Pinch analysis is applied to calculate the heat recovered in the multistream exchanger from the column top product and side reboiler. The methodology begins with the construction of the hot and cold composite curves and determination of enthalpy intervals. When the two curves are superimposed, the overlap between them indicates the amount of heat that can be recovered within the process, whereas the overshoot on each end indicates the amount of external heating and cooling required for the process to be in thermal balance. Enthalpy intervals are defined for the given composite curves; these are characterized by a temperature difference, a heat load and a stream population[7].

The simulation of the process begins with the flash, for which the temperature and pressure are assumed. The refrigeration required to meet these operating conditions is evaluated based on the overall energy balance over the whole flowsheet. If the total refrigeration provided by the cold recovery from the top product and the side reboilers is insufficient to achieve the flash temperature at the selected pressure, the amount of external refrigeration is computed. Refrigeration power demand is estimated using a simple vapour compression cycle and equation (1)[8].

$$W = \left(\frac{n}{n-1}\right)\frac{P_{in}F_{in}}{\eta_P}\left[1-\varepsilon^{\frac{n-1}{n}}\right] \qquad (1)$$

where $$\eta_P = 0.017 \ln F + 0.7 \qquad (2)$$

W	power required for compression (W)
E	pressure ratio, P_{out}/P_{in} (-)
P_{in}, P_{out}	inlet and outlet pressure (Pa)
F_{in}	inlet volumetric flowrate ($m^3 \cdot s^{-1}$)
n	polytropic coefficient(-)
η_P	polytropic efficiency (-)

The flowsheet model is validated for an industrially relevant case[9]. The process separates ethane and heavier components, from natural gas (NG). The lean methane-rich sales gas is used as fuel whereas the NGL product serves as feed to ethylene plants. The feed gas is at 25 ^oC with a pressure of 60 bar and a molar flow rate of 36000 kmol/h. The composition of the feed is given in Table 1. The demethanizer operates at a pressure of 30 bar.

Table 1. Feed Gas Composition

Component	Mole Fraction
Methane	0.865
Ethane	0.075
Propane	0.035
i-Butane	0.015
n-Butane	0.006
i-Pentane	0.004

The model predicts the recovery of methane and ethane and compression power requirements. The process is also simulated in HYSYS to provide a more rigorous basis for model validation. The modelling results for the base case are in good agreement with those of the HYSYS, as shown in Table 2.

Table 2. Simulation results of new model and HYSYS

	New model	**HYSYS**
Methane recovery in Sales Gas	99.4 %	99.7 %
Ethane recovery in NGL	90.2 %	90.4 %
Reboiler Duty (MW)	15.95	16.35
Total Shaft Power (MW)	28.12	28.46

3 Demethanizer Flowsheet Optimization

3.1. Optimization framework

The optimization procedure considers the interaction of the demethanizer column with the upstream units such as the flash separator, the turbo-expander and the multistream exchanger. In a typical demethanizer process the power requirement constitutes the highest percentage of the operating cost[10]. This includes the power requirement in the recompressor for sales gas and shaft work requirement in the external refrigeration. The determination of the optimum operating conditions is formulated as a nonlinear programming (NLP) problem for a fixed flowsheet configuration. The objective function is to minimize the total power requirement for the process, given the feed composition, the inlet pressure, the sales gas pressure and maximum methane/ethane ratio in the bottom product.

The input variables to the model are the column operating pressure, the temperature of the flash, the duty of the side reboiler and the ratio of the reflux to upper feed in the demethanizer column. These variables affect the total power requirement for the process through mass balance, the energy balance and the composition profile calculation in the column. The derivative of the objective function with respect to the process variables is not straightforward, and the differentiation of the function involves complex mathematical formulation. Therefore a finite difference method is used to approximate the derivative of the objective function. Nonlinear inequality constraints represent the capacity limits of the main process units and process specifications, such as heat exchanger duties, purity specifications in the demethanizer bottom product and a lower bound on ethane recovery.

3.2. Optimization Algorithm

The algorithm for the demethanizer system optimization is based on the successive quadratic programming (SQP) method. The method is a type of recursive optimization procedure that minimizes a smooth non-linear objective function approximated by quadratic functions and constrained by linear functions, subject to equality or inequality constraints of the variables. The method is able to converge to a solution even if the initial variables are far from the optimum[11]. To apply this optimization method into our framework the derivative of the objective function and the initial estimates of the variables for the optimization are needed. Multiple initial estimates of the input variables to the optimization procedure are employed that allows the solution space to be thoroughly searched at the expense of computation time. In the present work, the optimization problem solved by the SQP algorithm is carried out in MATLAB using the function ‘fmincon’.

4 Case Study

The total shaft power required for the compressor and refrigeration need to be optimized. The base case presented in Section 2.2 is chosen for optimization. The ethane recovery in the bottom product is specified to be higher than 90%, with the constraint of methane to ethane ratio in the bottom product to be 0.015. The process is sensitive to the following independent variables, for which upper and lower bounds are:

- 1000 kPa ≤ Column operating pressure ≤ 5000 kPa
- - 20 ^{o}C ≤ Flash separator temperature ≤ -40 ^{o}C
- 0 ≤ Side reboiler duty ≤ 6000 kW
- 0.2 ≤ Upper feed to reflux ratio ≤ 0.8

The optimization process shows that the shaft power is reduced from 28.12 MW to 25.38 MW (i.e. 10 %) by choosing the optimal value of the independent process variables. These optimal values are presented in Table 3.

Table 3. Optimization results

	Base case[9]	**Optimized system**
Column pressure (bar)	30	36
Side reboiler duty (kW)	1800	2350
Flash column temperature (^oC)	-20	-28
Upper feed to reflux ratio	0.8	0.6
Compressor power demand (MW)	15.66	14.84
Refrigeration system power demand (MW)	12.46	10.54
Total power demand	28.12	25.38

Thus the optimization can be seen to address the four variables, taking into account their interactions, to improve the process performance. The results indicate that both the refrigeration and the compression power are reduced by operating at the optimal values of the independent variables. It can be seen that the optimal flash temperature is lower than the base case, which essentially requires more refrigeration, but the additional requirement can be provided by improved cold recovery in the side reboiler. The optimization results also show that proper exploitation of the interactions between unit operations and the process variables can lead to energy efficient and cost effective flowsheets.

5 Conclusions

This work applied short cut models to the components of a complex demethanizer system, including addressing the heat recovery with multistream exchangers. A base case design of the flowsheet is simulated using the simplified models allowing their validation against HYSYS simulation results. Key degrees of freedom for the system are identified from the sensitivity analysis. The optimization methodology adopted is based on sequential quadratic programming, with the derivatives of the objective function and the constraints approximated using finite difference methods. Process optimization identified the operating conditions that minimize the overall power requirements for the process.

The design and optimization methodology will be implemented in a broader framework for the synthesis of the demethanizer flowsheets by also including the structural optimization parameters. The methodology will also help to develop a benchmarking tool to screen, evaluate and optimize licensed flowsheets.

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