Modelling and optimisation of a natural gas liquefaction process

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Abstract

The goal of this project was the development of a mathematical model for a multi-stream heat exchanger (MSHX) based on the Pinch Analysis, called Pinch model, and to use that model in fast optimisations of cryogenic processes.

Liquefaction of natural gas (LNG) reduces its volume making it easier and safer to transport. LNG is produced by refrigeration and a very important unit involved in the refrigeration cycles is the MSHX. In order to optimise LNG processes with economic objectives it is necessary to have costing models of the main units of the process.

The Pinch model determines heat balances, composite curves, minimum temperature approach between hot and cold streams and factors of duty over temperature difference that introduced in a correlation allow the estimation of the unit cost. It acted as expected which was validated with a heat integration software.

The Pinch model was integrated in a Single-stage Mixed Refrigerant cycle that was optimised with the objective of maximising the profit of the process. The optimisation results and time were compared with a reference case. The results were difficult to compare because the initialisation of the optimisations returned very divergent exchanger costs due to the different assumptions used in the distinct MSHX models. The optimisation increased the profit in 41%. The optimisation time reduction obtained with the Pinch model in comparison with the reference case was of 60% which infers a good potential in the use of the Pinch model in fast optimisations of cryogenic processes. It is important to notice that the calculations of the Foreign Object with the Pinch algorithm took only 0.5% of the total optimisation time.

Keywords: Pinch, Heat Integration, LNG, Multi-stream heat exchanger, Cryogenic

1. Introduction

An environmentally friendly and efficient energy source, natural gas is the cleanest-burning conventional fuel, producing lower levels of greenhouse gas emissions than the heavier hydrocarbon fuels, like coal and oil [1]. Historically, natural gas has also been one of the most economical energy sources, and gas plants are flexible both in technical and economic terms, so they can react quickly to demand peaks, and are ideally twinned with intermittent renewable options such as wind power.

Transportation and storage of NG is difficult because of its low energy density at ambient temperature and pressure. Liquefying natural gas reduces its volume for easier and safer storage and transport which increases the importance of LNG role in the natural gas market as it allows transoceanic shipment from any region of supply to any region of demand. Liquefaction serves to overcome the obstacles in pipeline transport, and permits transport over larger distances and more diverse application of the gas as an energy source, having thus brought many large remote gas fields to the gas markets that are unreachable by pipeline. LNG offers an opportunity to diversify energy supplies and with the decrease in its cost, it becomes more competitive in the gas markets. At a time of political instability, it can also be a more attractive option than international pipelines that cross multiple borders.

Natural gas accounts for 1/4 of global energy consumption. Over the last 20 years, the share of gas in the global energy mix has increased, while the share for oil has decreased [2]. This shift is driven by the generally lower price of natural gas compared to oil on an energy content basis and the relatively lower costs of new natural gas electric generators. Further, the reduced emissions associated with natural gas use are increasingly important as many countries impose tighter emission standards. This growth is supported by an increase in gas production potential and expansion of international trade based on a growing number of LNG facilities and high pressure pipelines and will continue for several decades. Natural gas is expected to continue its growth spurred by falling or stable prices, and thanks to the growing contribution of unconventional gas, such as shale gas [2].

LNG is now considered safe and less polluting than other energy sources which originated its increasing demand. The demand is to be met by an increase in liquefaction plants and these are to be built with higher efficiency and in an environmentally responsible manner. This implies a constant development to enhance existing processes and lower its costs. LNG facilities are potentially very expensive but advances in technology have been reducing the costs associated with liquefaction and regasification [3].

With the prediction of increasing growth in LNG demand, the efforts to optimise the liquefaction technologies increase intensively. LNG projects are inherently capital-intensive, with the liquefaction process representing 30 to 40% of the capital cost. The liquefaction stage is then the best field to approach to make the largest cost savings because it has a greater influence in the project viability.

Mathematical models are of great importance in chemical engineering because they can provide information about the variations in the measurable macroscopic properties of a physical system using output from microscopic equations which cannot usually be measured in a laboratory. Computer aided modelling, simulation and optimisation permit a better understanding of the chemical process behaviour, saves the time and money by providing the fewer configuration of the experimental work. In addition, computer simulation and optimisation can help to improve the performance and the quality of a process and represent a more flexible and cost effective approach in design and operation [4].

With the motivation in LNG growth and the importance of process modelling, the purpose of this work was to develop a mathematical model for multi-stream heat exchangers that predicts the cost of the unit using the Pinch Analysis algorithm. There is an existing model for this unit in gPROMS libraries that determines the mass and heat balances but it lacks a tool for the cost calculation. This calculation was essential to use the model in optimisation problems with economical objective functions, like the LNG flowsheet used as case study in the present work.

2. Pinch analysis

Multi-stream heat exchangers are traditionally analysed using composite curves, a thermodynamic concept used in heat integration called Pinch analysis. This is a technique based on thermodynamic principles that offers a systematic approach to optimum energy integration in a process. Using the first and second laws of Thermodynamics and the concept of temperature approach, this technology is used to design networks of heat exchangers through the identification of energy cost and network cost targets. The minimum temperature approach is defined by the minimum temperature difference, ΔT_{min}, that determines how closely the hot and cold composite curves can be without violating the Second Law [5]. From the perspective of process modelling, MSHXs can be treated in the same way as heat exchangers networks through the use of high level targeting models [6].

The Pinch technology technique begins by predicting the minimum requirements of external energy (utilities), network area, and number of units (exchangers) for a given process at the pinch point. Then there is the construction of the network that satisfies the energy targets, and finally the optimisation of the network so that the total cost is minimised. The main steps of the Pinch analysis are:

- Identification of hot, cold and utility streams in the process;
- Thermal data extraction for process and utility streams;
- Selection of initial minimum temperature approach;
- Construction of composite curves and grand composite curve;
- Estimation of minimum energy cost targets;
- Estimation of capital cost targets;
- Determination of optimum temperature approach;
- Design of the Minimum Energy Requirements network;
- Optimisation of the network minimising total cost.

The input data required to perform the Pinch analysis for heat exchangers networks comprises inlet and outlet temperatures, flowrates, heat capacities and heat transfer coefficients for all the streams involved. The selection of the initial ΔT_{min} can be made using the typical industrial values for a specific case. The above mentioned data is required to build the composite curves. In composite curves all hot streams are merged into one pseudo-stream, the hot composite curve, while all cold streams are merged into the cold composite curve. Globally, the curves represent the cumulative heat content of all hot and cold streams (separately).

The composite curves allow the determination of the minimum utility requirements as well as the identification of the Pinch Point that is the most constrained point of the network, where ΔT_{min} happens. To determine the utility requirements in a more accurate way there is a numerical approach called Problem Table Algorithm, developed by Linnhoff & Flower (1978). The base idea of this method is to verify, for each interval of temperatures, the energy amount available between the process streams involved in the interval and transfer the excess of energy of a thermic level to the level below.

The composite curves can be used to evaluate the overall trade-off between energy and capital costs. An increase in ΔT_{min} causes the energy costs to increase, with the increase in utility requirements, but also provides larger driving forces for heat transfer, so smaller area, and accompanying reduced capital costs. The determination of the Pinch Point is essential in the construction of the network but it will not be covered in this work since the Pinch analysis is being applied to MSHXs and not to heat exchangers' networks. For the same reasons the last 3 steps of the above list are not relevant for this work.

The estimation of the capital costs involves the calculation of the equipment cost. This calculation is usually made with a correlation that depends on the type and material of the exchanger, and on the heat transfer area. The composite curves are also used to determine the minimum heat transfer area required to achieve the energy targets. For this the curves are further divided in enthalpy intervals such as in each interval neither curve changes slope.

This area target is based on the assumption that vertical heat exchange will be adopted between the hot and the cold composite curves across the whole enthalpy range. The area is calculated for each enthalpy interval and the total network area is considered to be the sum of all the areas, as explicit in equation 1, where i is the index for the intervals and j is the index for the streams.

$$A = \sum_i \left(\frac{1}{\Delta T_{ln,i}} \sum_j \frac{Q_{ji}}{h_{ji}} \right) \tag{1}$$

A is the total area, ΔT_{ln} is the mean logarithmic temperature difference (MLTD), Q is the heat transferred for each stream in each interval and h is the stream heat transfer coefficient or film coefficient. MLTD is calculated assuming countercurrent heat exchange, equation 2.

$$\Delta T_{ln} = \frac{(T_{HOT}^{in} - T_{COLD}^{out}) - (T_{HOT}^{out} - T_{COLD}^{in})}{ln\left[\frac{(T_{HOT}^{in} - T_{COLD}^{out})}{(T_{HOT}^{out} - T_{COLD}^{in})}\right]} \tag{2}$$

In summary the benefit of using Pinch analysis in this project is related to the fact that composite curves not only provide information about energy targets but also help predicting heat transfer area of the network, or in this case, the MSHX. Moreover this method is also capable of ensuring the minimum driving force criteria.

Heat integration technology relies on an assumption of constant heat capacity flowrate. Typically the heat capacity does not vary significantly with temperature in the subcooled and superheated regions, which are in a single phase, though when phase change occurs this assumption does not hold. A cryogenic process like LNG mainly utilises the vaporisation of mixed refrigerants to cool, liquefy and sub-cool natural gas. This is especially important for multi-component streams where the phase change occurs over a large temperature range.

To overcome this issue, a piecewise linearisation can be applied to the variation of enthalpy with temperature dividing this relation in small intervals which temperature, enthalpy pairs (T, H) contain the dew and bubble points to track the phase change. The variation of enthalpy with temperature is then assumed to be linear inside each interval [7]. As one of the objectives of this work is to build a model for a MSHX that is mainly used for cryogenic applications where change of phase occurs, this approach is used to increase the accuracy of the model regarding the physical properties of the streams.

The software used in the construction of the MSHX model was gPROMS, a platform for high-fidelity predictive modelling for the process industries developed by Process Systems Enterprise (PSE). gPROMS ProcessBuilder is an Advanced Process Simulation tool for model-based support of key design and operating decisions. Another feature of gPROMS ProcessBuilder is the optimisation tool which can be used to optimise steady-state and dynamic behaviour of continuous flowsheet, considering design and operation variables. The optimisation solver used by gPROMS was the NLPSQP solver that employs a sequential quadratic programming (SQP) method for the solution of a nonlinear programming (NLP) problem, as the optimisation problem in this work is non-linear.

gPROMS also allows the use of external software components, called Foreign Objects (FO), that provide certain computational services to gPROMS models. These include physical property packages, like Multiflash that was the package used in the present work to estimate the properties of the process streams, with the Peng-Robinson equation of state. Part of the MSHX model developed in this work was built as a FO in C++ language.

3. Multi-stream heat exchanger model

The model developed in the present work simulates a MSHX including a tool to estimate its cost based on the Pinch analysis. It is composed of 3 submodels, 2 written in gPROMS language and one FO written in C++, figure 1.

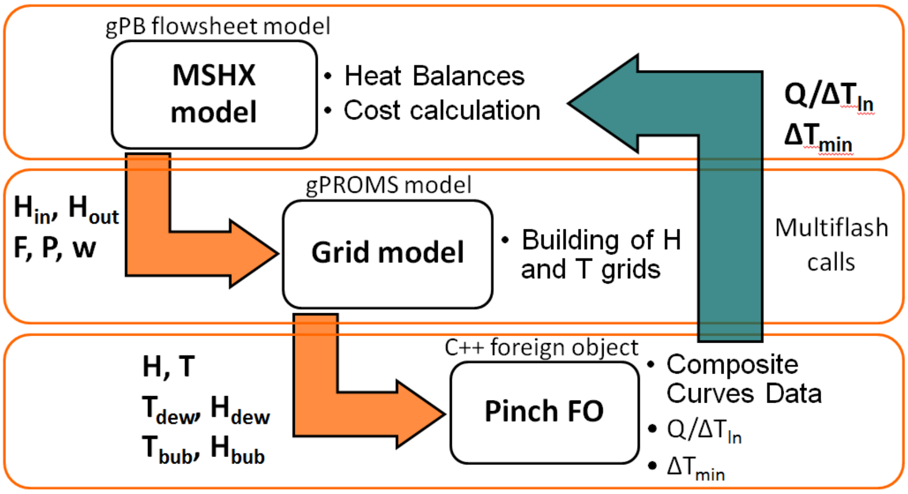

Figure 1: Schematics of the global MSHX model.

3.1. MSHX model

The MSHX model represents a heat exchanger with more than two streams exchanging heat. Its inputs are: inlet temperatures and pressures, flowrate and composition of all streams, outlet temperatures for $N-1$ streams (being N the number of streams), and pressure drop or outlet pressure of all streams. With heat balances the model calculated the heat transferred for every stream and one outlet temperature.

This model is an adaptation of an existing gPROMS ProcessBuilder model with two main additions: composite curves building and cost correlation. The composite curves are built with data returned by the Pinch FO. The correlation used for the calculation of the exchanger cost is called C Value Method [8] represented in equation 3. In this method, C is defined as the cost per unit of $Q/\Delta T_{ln}$ (calculated in the Pinch FO) avoiding difficulties in defining area and heat transfer coefficients.

$$Cost = C \times \left(\frac{Q}{\Delta T_{ln}}\right) \tag{3}$$

The determination of the C value for different conditions is done by logarithmic interpolation using two pairs of tabulated C-($Q/\Delta T_{ln}$) as interpolation limits [8].

In Pinch Analysis the area is calculated for each enthalpy interval and the total area is estimated to be the sum all the intervals areas, equation 1. Similarly, the C value is calculated for each stream in each interval, as well as $Q/\Delta T_{ln}$ and the total cost is considered to be the sum of the costs of all the parcels, equation 4 where j and i represent streams and intervals, respectively.

$$\text{Exchanger cost} = \sum_{j}\sum_{i} C_{ji} \times \left(\frac{Q}{\Delta T_{ln}}\right)_{ji} \tag{4}$$

3.2. Grid model

The Grid model developed in this work is responsible for the determination of the enthalpy and temperature grids that are passed to the Pinch FO. Its inputs are: number of streams N, number of intervals that divide the enthalpy sets Z_j (user defined), inlet and outlet enthalpies, pressure, flowrate and composition of all the streams, and arrays to define if streams are condensable ($cond_j$) and volatile (vol_j). These last 2 parameters are required because in many cryogenic processes, the streams are in the critical stage and Multiflash may not be able to calculate the dew or bubble points and that would cause the simulation to fail.

The Grid model uses the input Z to develop a set of enthalpy equidistant points from the inlet to the outlet enthalpy. These enthalpy sets are grouped in a grid being each row correspondent to a different stream, and the correspondent temperature is built using a pressure/enthalpy flash calculation in Multiflash. With these sets of points it is viable to assume that in each interval (between two points) the enthalpy changes linearly with temperature. Dew and bubble temperatures and enthalpies are calculated in this model using Multiflash. Outputs of the Grid model are inputs of the Pinch FO.

3.3. Pinch FO

The inputs and outputs of the Pinch FO developed in this work are defined in tables 1 and 2.

N is the number of streams and M is the maximum number of points of the enthalpy sets defined in the Grid model, meaning it is the number of columns of the H and T grids. The $DewPoint$ and

Table 1: Inputs of the Pinch FO.

Input	Size	Variable type	Definition
H	$N \times M$	Real	Enthalpy grid
T	$N \times M$	Real	Temperature grid
$DewPoint$	$2 \times N$	Real	Dew point data
$BubblePoint$	$2 \times N$	Real	Bubble point data

Table 2: Outputs of the Pinch FO.

Output	Size	Variable type	Definition
ΔH_{ac}	$Sz + 1$	Real	Accumulated enthalpy (composite curves)
T_{HOT}	$Sz + 1$	Real	Hot curve temperature
T_{COLD}	$Sz + 1$	Real	Cold curve temperature
$Q/\Delta T_{ln}$	$N \times Sz$	Real	Duty over mean logarithmic temperature difference
ΔT_{min}	1	Real	Minimum approach temperature

$BubblePoint$ arrays store the dew and bubble temperatures and enthalpies (from the Grid model) of the streams, respectively.

Sz is the number of enthalpy intervals of the composite curves resulting from the Pinch calculations. ΔT_{min} is directly related to the effectiveness of the exchanger and will be used as optimisation constraint. The rest of the data returned from the Pinch FO is passed to the MSHX model where the composite curves are built and $Q/\Delta T_{ln}$ values are used to estimate the cost of the exchanger.

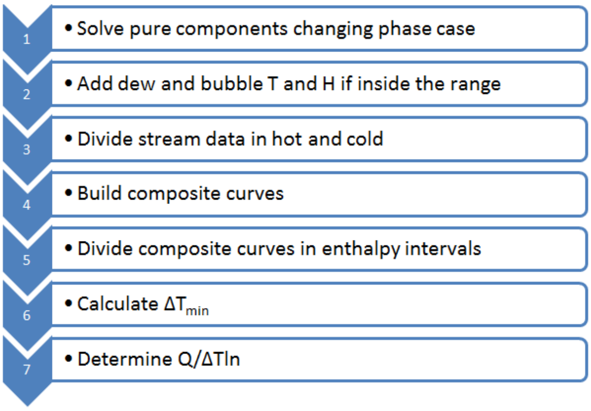

Figure 2: Pinch algorithm list of steps.

Figure 2 contains the steps followed by the Pinch FO. The first step of the list regards the possibility of a stream composed of a pure component changing phase in which case the temperature is constant while the enthalpy changes. This situation is not favourable since the enthalpies of the streams will be summed for each temperature level. In the Pinch Analysis this situation is usually dealt with a small temperature variation, δ. The duplicate temperatures are replaced by a range from $T - \delta$ to $T + \delta$.

Step 2 is to introduce the dew and bubble points in the grids if they are inside the stream range. This improves the linearisation assumed for each interval as these are the points of more abrupt change in the curve temperature vs. enthalpy.

In step 3 the enthalpy and temperature grids are divided in hot and cold to facilitate the construction of the composite curves, hot and cold separately. The hot and cold composite curves are built in parallel, step 4, thus only the hot curve is regarded in the following exposition. The temperature points of all hot streams are placed in one single array, $allT_{HOT}$, and the corresponding enthalpies are determined for all streams and placed in a new enthalpy grid, $allH_{HOT}$.

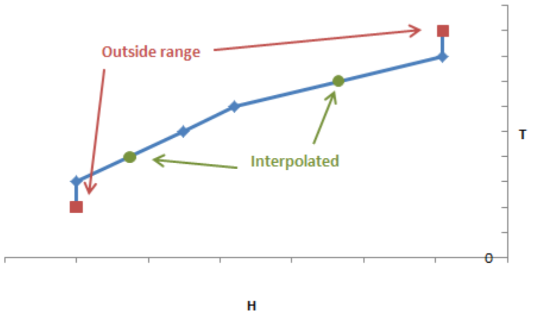

Figure 3: Assignment method used to complete new matrices or arrays.

The extra points of the new enthalpy grid are determined by interpolation when inside the stream range. When new temperature points in $allT_{HOT}$ are outside the initial enthalpy range, the first or last enthalpy values of the stream are assigned. If the temperature is lesser than the first of the range (smaller of the range) it is assigned the first enthalpy point (smaller of the range) to the $allH_{HOT}$

point. Similarly, if the temperature is higher than the last temperature of the stream range it is assigned the last enthalpy to the correspondent point of the new grid. Figure 3 exemplifies this assignment method.

In figure 3 the original range is represented in blue; in green the new points inside the range, determined by interpolation; and in red the points outside the range, to which the first/last value of the range is assigned. This way when the heat load of the interval is calculated, the contribution of a stream for temperatures outside its original range will be zero.

New arrays are then created to sum the enthalpies of all streams for each temperature point, represented in equation 5 where p and j represent points and streams, respectively.

$$SumH_p = \sum_j H_{jp} \tag{5}$$

So far, all values where points of temperature and enthalpy. Next there is the calculation of the accumulated enthalpy that refers to an interval, comprised by two consecutive enthalpy points. The accumulated enthalpy is calculated using equation 6 where i represents intervals and 1 corresponds to the first position of the array.

$$\Delta H_{ac,i} = SumH_p - SumH_1 \tag{6}$$

The hot composite curve is composed by pairs of enthalpy/temperature points where the enthalpy is the accumulated enthalpy calculated with equation 6 and the temperatures are in the $allT_{HOT}$ array. The cold composite curve is calculated in parallel with the exact same procedure.

In step 5 the composite curves are further divided in enthalpy intervals so that in each interval none of the curves changes slope. Array ΔH_{ac} is then completed to contain all enthalpy points of both composite curves and becomes $areaH$. The completion of the temperature arrays $areaT_{HOT}$ and $areaT_{COLD}$ to correspond to the enthalpy points in $areaH$ is done with the assignment method explained above, figure 3. The resulting composite curves, constituted by the data contained in the arrays $areaT_{HOT}$, $areaT_{COLD}$ and $areaH$, are represented in figure 4. In step 6 the minimum temperature difference between hot and cold streams is identified.

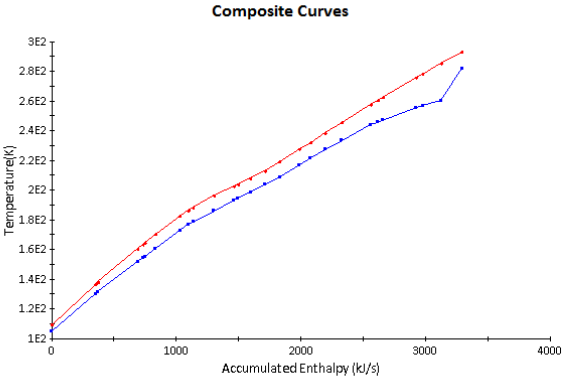

Figure 4: Composite curves representation.

Step 7 comprises the calculation of the MLTD using the data of arrays $areaT_{HOT}$ and $areaT_{COLD}$ in equation 2.

Finally, it is calculated the duty of the streams. Taking the arrays $areaT_{HOT}$ and $areaT_{COLD}$ from the composite curves division, the correspondent enthalpies are calculated for each stream with the assignment method mentioned before, using and interpolating values from the initial enthalpy grid. The resulting grid is $auxH$ and by making the difference between the heat of two consecutive points of this matrix, the duty matrix Q is obtained. Q is the heat transferred by each stream in each enthalpy interval. At last $Q/\Delta T_{ln}$ is determined and passed to the upper level model.

Resuming, the MSHX model calculates the mass and heat balances providing the properties like enthalpy and temperature for all the inlets and outlets of the exchanger; the Grid model builds enthalpy and temperature grids for the streams and makes calls to the Pinch FO (PinchMS method); Pinch FO uses the Pinch algorithm to build the composite curves, calculate the MLTD, the heat load (Q) for every stream in each enthalpy interval and the minimum temperature approach between hot and cold streams, ΔT_{min}. The $Q/\Delta T_{ln}$ factor is then used to estimate the exchanger cost using the C value method[8] in the MSHX model.

3.4. Algorithm validation

the Pinch model was not validated with experimental data due to the difficulty in finding public data. Thus, a validation of the model is done by comparison with a heat integration software, Hint, to verify the accuracy of the calculations. With the same inputs, the results obtained from the software Hint were compared to the results in the Pinch model and the final error obtained was irrelevant. The Pinch analysis method can be used to determine the heat transfer area within 10% of the actual minimum [9], so it can be inferred that the model has a good accuracy in terms of area prediction.

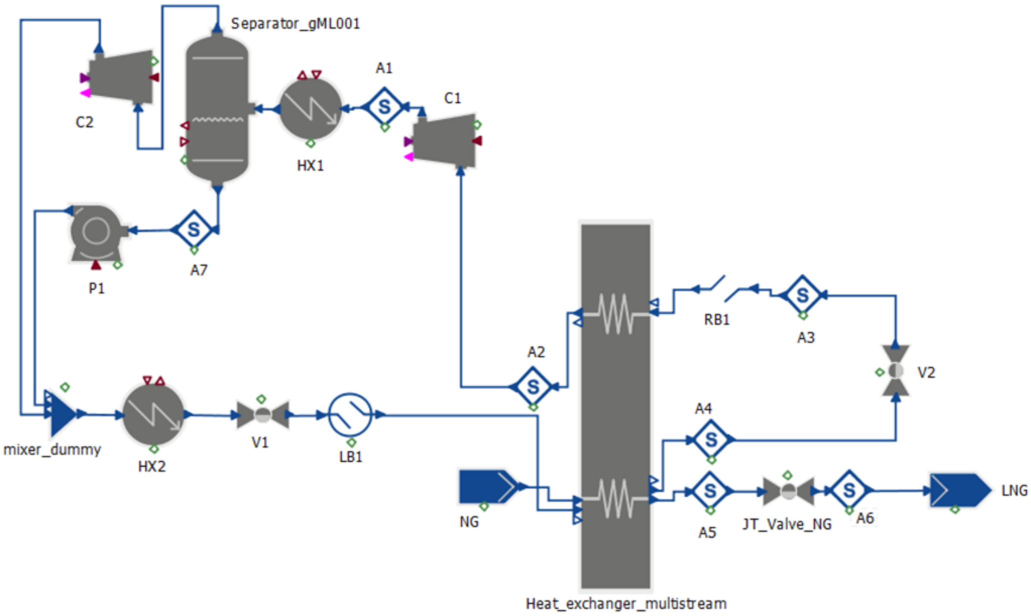

Figure 5: SMR process used in optimisation.

4. Single-stage mixed refrigerant process optimisation

The global Pinch model was integrated in a PRICO process for NG liquefaction. This process was optimised to maximise the profit reproducing a reference case [10] optimisation with the purpose of comparing the optimisation times with 2 different models for the main cryogenic heat exchanger (MCHX). The process flowsheet (including economic section), the objective function, control variables and constraints were (most of them) taken from the reference case and reproduced in the present work using the Pinch model to simulate the MCHX.

This process is very energy consuming and uses a single-stage mixed refrigerant (SMR) cycle, figure 5. The objective function was the NPV (net present value) that represents the profit of the process regarding a 15 year life time for the process. NPV depends essentially on LNG production, NG cost, and utilities that depend on the compressor power and equipments cost.

To maximise the NPV the control variables used were: mixed refrigerants (MR) flowrate, composition, suction pressure and condensation pressure. Their initial guesses and optimisation limits are stated in table 3. The process constraints are in table 4.

Dew margin is the difference between the MR cold stream outlet of the MCHX and the dew temperature of that stream at its operating pressure. This variable was constrained with a lower bound to prevent liquid formation in the suction part of the compressor. A positive temperature difference between the two curves is required to avoid temperature crossing hence a decrease in efficiency.

The simulation base case presents relative deviations of 58% for the MCHX cost and consequent -121% for NPV. The optimisation performed in the present work increased the NPV from 4.20 to 5.92M$. The optimum values and relative deviation of controls with the reference case[10] are stated in table5.

The optimisation increased the NPV in 41% by decreasing the energy requirements in 6% and the MSHX cost in 12%.

It is difficult to compare the results on a fair basis since the optimisations did not start from the same initial point because the MSHX costs were so divergent. The model using the Pinch FO calculates the cost of each interval that divides the heat transfer of the streams (composite curves) while the reference case model used the total heat transferred determined in the heat balance and the global mean logarithmic temperature difference, besides other internal model calculations. This difference in the cost of the exchanger has a great influence in the objective function, NPV, that also regards a high relative difference. Other reason for the results to be difficult to compare is because neither optimisation case found the optimum values, in fact they ended due to lack of improvement, both in optimisation variables and in objective function, which

Table 3: Control variables, their bounds and initial guesses for optimisation.

Control variable	Initial value	Lower bound	Upper bound
Outlet pressure C1 (bar)	14	1	20
Outlet pressure C2 (bar)	52.37	10	60
Outlet pressure V2 (bar)	3.23	1	10
MR mass flowrate (kg/s)	4.669	1	15
MR components molar fraction			
Nitrogen	0.155	0	1
Methane	0.288	0	1
Ethane	0.345	0	1
Propane	0.022	0	1
Butane	0.19	0	1

Table 4: Constrained variables and their bounds in the optimisation problem.

Constrained variable	Lower bound	Upper bound
Dew margin (K)	2	100
Compressor ratio C1	1.5	5
Compressor ratio C2	1.5	5
ΔT_{min} **(K)**	1.5	20

Table 5: Optimisation results of present work: controls and constrained variables.

Variable	Value after optimisation	Relative difference (%)
Outlet pressure C1	6.455 bar	-90.5
Outlet pressure C2	32.28 bar	-24.2
Outlet pressure V2	1.29 bar	-90.5
MR mass flowrate	3.851 kg/s	-5.3
Dew margin	42.8 K	-
Compressor ratio C1	5	-
Compressor ratio C2	5	-
ΔT_{min}	1.5 K	-
MCHX cost	0.76 M$	53.9
NPV	4.20 M$	-104.7
MR components molar fraction		
Nitrogen	0.051	-172.7
Methane	0.305	25.7
Ethane	0.310	18.0
Propane	0.105	100.0
Butane	0.229	-17.1

came from numerical issues.

In order to create a comparable environment for the optimisation cases it was necessary to limit the number of iterations performed during optimisation so that these could be similar in both cases. The optimisation of the present work used 94 major and 330 minor iterations while the reference case used 414 major and 833 minor. To approximate the number of iterations, the maximum line search step length and the maximum number of functions were reduced and both optimisations were performed again. Thereby the simulations were forced to end sooner and became comparable in terms of computational effort. For 49 major and 49 minor iterations the resulting optimisation CPU time was 29s for the present work and 72s for the reference case. Thus, the Pinch model produced a time reduction of 60%.

Table 6 contains the fraction of optimisation time spent by the Foreign Objects used by the MSHX

Pinch model. It is to be noticed that the time used during optimisation in Pinch FO calls represents only 0.5% of the total time while the PHflash calls take 30% of the time which means a significant amount of total time is spent building the temperature grid in the Grid model.

Table 6: Foreign objects statistics in optimisation with Pinch model.

Statistic parameter	PHflash	Pinch
No. of calls	10130	5
No. of calls for derivatives	3020	200
Time of calls (s)	7.36	0.02
Derivative call time (s)	1.15	0.14
Calls time fraction (%)	30	0.5

The objective of building a model for a MSHX that would allow for simpler and consequently faster optimisations was achieved and though the comparison of results was not fair, the model built in the present works presents potential to be used in optimisation of other cryogenic processes.

In the present work a mathematical model was built to simulate a multi-stream heat exchanger used in cryogenic applications. The model includes 2 gPROMS models to calculate mass and heat balances, build grids and determine streams' properties; and a FO with an adaptation of the Pinch Analysis for MSHXs. The model is working as expected which was confirmed by a comparison of results against a software of heat integration, named Hint, with the same input data.

The Pinch model was developed with a tool to calculate cost and/or heat transfer area. Like this it was used in optimisation of a SMR process, with an incorporated cost model, as the MCHX. The use of an exchanger with a cost option provided the possibility of optimisation of the process with economic objective functions.

The SMR gPROMS flowsheet was taken from a reference case [10] and the cryogenic exchanger was replaced with the model built in this project for optimisation time comparison. The MSHX cost of the initialisations were very divergent making the comparison of the optimisation results with the reference case much difficult as they did not start from the same point. The different prediction of area/cost is essentially due to the different assumptions and calculations used in the exchanger models. Besides, both optimisation run cases ended due to lack of improvement which means the global optimum was not found. Even so, the objective function, NPV improved 41% with the optimisation done in this work.

Despite the difficulty in comparison of results, a comparison of optimisation time was performed. The optimisation case implemented in the present work resulted in an optimisation time reduction of 60% for 98 iterations. It is then reasonable to state that the Pinch model has great potential for less time consuming optimisations. The distribution of the optimisation time in the present work was evaluated and the results demonstrated that the Pinch FO used only 0.5% of the total optimisation time, while PHFlash took 30%, both results including derivatives calculation times.

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