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Operational optimisation of centrifugal compressors in multilevel refrigeration cycles

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ABSTRACT

Low-temperature energy systems are processes that require cooling at temperatures below ambient, which are accomplished using refrigeration cycles. Little research has addressed the operational optimisation of refrigeration cycles considering the performance of existing equipment. This work develops a methodology for operational optimisation of refrigerated processes, taking into account existing centrifugal compressors. For the optimisation of multilevel cycles, the evaporation temperatures of each level are varied to find a set of operating conditions that minimise shaft work demand. The optimisation takes into account equipment constraints, including compressors on a common shaft, minimum and maximum allowable inlet flow rates, etc. Two examples are presented; the first represents a three-level refrigeration cycle and the second a cascade cycle. For the two examples, the conditions of the base case are optimised, identifying improvements of around 3% in shaft work demand. In addition, both cycles were also optimised for a range of process cooling demands.

1. Introduction

Low-temperature energy systems are processes that need to operate below ambient temperature and thus require the use of refrigeration cycles. Very-low-temperature energy systems, such as ethylene separation processes or liquefied natural gas (LNG) plants, operate at temperatures of around −150 °C or below, and are also known as cryogenic processes (Timmerhaus and Reed, 2007, Ch. 1). In a simple closed refrigeration cycle, the refrigerant is vaporised (by removing heat from the process streams), compressed, condensed at the discharge pressure by a cold utility or heat sink, and expanded to the vaporisation pressure. If the cooling temperature range of the process streams is wide, then cycles with several evaporation temperatures can be implemented (e.g. multilevel cycles, cascade cycles) (Dinçer and Kanoğlu, 2010, Ch. 5). One of the main issues with refrigeration cycles in cryogenic processes is that their associated costs tend to be very high because of the capital cost of the compression trains and the operating cost of the shaft work required to drive them (Mokhatab et al., 2014, Ch. 3.2). Once the refrigeration cycle has been designed and put in operation, the compression shaft work dominates the processeconomics; thus the shaft work is typically used (and is used in this work) as a key performance indicator for the design and operational optimisation of refrigeration cycles.

The synthesis (design) of refrigeration cycles is a subject of much interest because of its economic importance. It is a challenging problem that considers complex interactions between the process that requires cooling, the heat exchanger network (HEN) and the refrigeration cycle. While the synthesis of refrigeration cycles has been widely researched, the operational optimisation of refrigeration cycles is an important subject that has not been as extensively investigated. The target of operational optimisation of refrigeration cycles is to minimise operating costs of a cycle that has already been designed and is already in operation. Minimising the operational costs can lead to higher energy efficiency, improved process economics and reduced carbon emissions to the environment. The publications that have, so far, addressed the operational optimisation of refrigeration cycles (discussed further in Section 3) do not include the performance of the existing equipment nor its limitations. Thus, the optimised results from these publications could overestimate the real achievable savings, which are restricted by the operation of the existing equipment. Furthermore, few of the published models are able to predict the performance of centrifugal compressors for different operating conditions, and no published work was found that considered the physical and/or operational limitations of compressors (e.g. minimum or maximum allowable volumetric flow rates).

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Nomenclature

$\%H_p$	polytropic head correction factor (1)
$\%Q$	inlet volumetric flow rate correction factor (1)
f_p	polytropic head factor (1)
g	acceleration due to gravity (m s^{-2})
I	total number of cooling levels
H_p	polytropic head (ft)
h	specific enthalpy (kJ kg^{-1})
lb	vector of lower bounds (K, °C)
M	number of compression stages
m	mass flow rate (kg s^{-1})
N	rotational speed of compressor (rpm)
n_p	polytropic coefficient (1)
n_s	isentropic coefficient (1)
P	pressure (Pa)
Q	heat duty (MW)
Q^V	actual volumetric flow rate (ACFM)
T	temperature (K, °C)
ub	vector of upper bounds (K, °C)
v	specific volume (m^3 kg^{-1})
W_p	polytropic work (kW)
γ	ratio of the inlet gas heat capacities
$\Delta T_{\min}$	minimum temperature difference (K, °C)
η_m	mechanical efficiency of the compressor (1)
η_p	polytropic efficiency (1)
Θ	vector of evaporation temperatures and ΔT_{min} (K, °C)

Subscripts

cond	condensation
est	estimated
evap	evaporation
i	cooling level
in	inlet
m	compression stage
out	outlet
p	polytropic
r	reference
req	required
s	isentropic

Abbreviations

ACFM	actual cubic feet per minute
C3-MR	propane precooled mixed refrigerant cycle
GA	genetic algorithm
GCC	grand composite curve
HEN	heat exchanger network
LNG	liquefied natural gas
MINLP	mixed-integer non-linear programming
NLP	non-linear programming

This paper proposes a model for the optimisation of the operating conditions of an existing refrigeration cycle for a given cooling requirement, arising from process needs, taking into consideration the operational limits of the existing centrifugal compressors (e.g. lower and upper volumetric flow rate limits). In particular, the physical properties and the cooling requirements of the process streams are taken as given, i.e. the cooling duties are known, as are their physical properties. The proposed model extends previous work on synthesis and operational optimisation of refrigeration cycles (presented in Section 3) to model the part-load performance of multistage compressors in multilevel refrigeration cycles. The model finds a set of operating conditions (evaporation temperatures, cooling duties, refrigerant flow rates and rotational speed of compressors) that minimise the shaft work demand of the refrigeration cycle. A multistart optimisation algorithm, which uses a gradient-based non-linear programming (NLP) solver together with a scatter search algorithm, is applied to search for such set. This optimisation algorithm is implemented to avoid getting trapped in locally optimal solutions, which are due to the highly non-linear nature of the model, and to find an approximation to a globally optimum solution.

First, an overview related to the basic thermodynamic theory of refrigeration cycles and centrifugal compressors is presented, followed by a literature review on the design and operational optimisation of refrigeration cycles, focusing on works that address the modelling of centrifugal compressors in these cycles. Section 4 introduces the models for estimating the performance of centrifugal compressors and for the optimisation of their operating conditions in refrigeration cycles. Finally, the benefits of the use of the proposed models are illustrated by means of two different examples in Section 5, a multilevel cycle and a cascade cycle.

2. Centrifugal compressors in refrigeration cycles

2.1. Introduction to refrigeration cycles

A simple vapour-compression cycle with a pure refrigerant, illustrated in Fig. 1, comprises a compressor (where the pressure of the vapour is raised), a condenser (where the superheated vapour is cooled and condensed to its bubble point), an expansion valve (where the liquid is expanded through an isenthalpic valve) and an evaporator (where the process stream rejects heat to the refrigerant and the refrigerant is vaporised to saturation conditions) (Dinçer and Kanoğlu, 2010, Ch. 4.2). Note that pressure drops in the heat exchangers and piping are assumed to be negligible in this work.

A more complex refrigeration cycle may provide cooling at multiple temperature levels (known as a multilevel cycle). For example, in the two-level cycle illustrated in Fig. 2, the cooling duty is satisfied at two different evaporation temperatures using a single refrigerant expanded to two different pressure levels. The use of two cooling levels reduces the refrigerant flow through the low-pressure compressor, which in turn reduces the overall shaft work demand of the cycle, compared to a simple refrigeration cycle (Smith, 2005, Ch. 24.6). In this simple cycle, the cooling duty is provided at the lowest cooling level of the two-level cycle and the condensing pressure and cooling duty are the same for both cycles. However, with increasing number of cooling levels, the capital costs of the cycle may also rise, as a higher number of exchangers and compression stages are needed; thus, the final design of the refrigeration cycles is a trade-off between shaft work demand and capital costs.

Cascade cycles consist of two or more cycles, where each cycle uses a different refrigerant, and are normally implemented when cooling is required at low temperatures and a single refrigerant

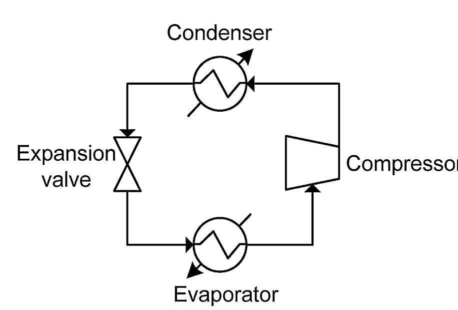

Fig. 1. Simple refrigeration cycle.

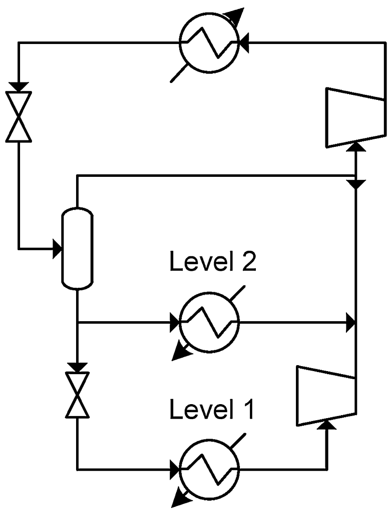

Fig. 2. Two-level refrigeration cycle.

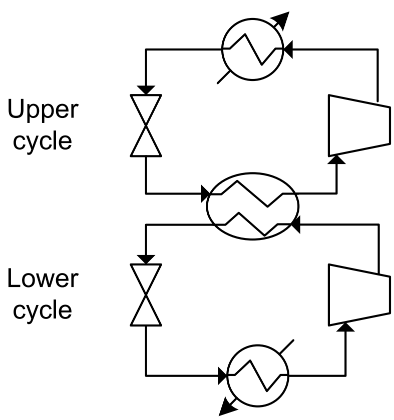

Fig. 3. Simple cascade refrigeration cycle.

cannot operate at such temperature range (Dinçer and Kanoğlu, 2010, Ch. 5). A simple cascade cycle is shown in Fig. 3. The lower cycle cools the process stream and rejects the heat absorbed to an upper cycle, while the upper cycle usually rejects the heat absorbed from the lower cycle to an external utility (e.g. cooling water) in the condenser, or could also be heat integrated with any cold stream from the associated process. Furthermore, each cycle of the cascade can have several cooling levels, increasing the complexity of the cycle. One of the most important parameters in cascade refrigeration cycles is the partition temperature, which is the temperature of the evaporator of the upper cycle (Smith, 2005, Ch. 24.6). The partition temperature determines the evaporation temperatures and total shaft work demand of the cycle.

2.2. Centrifugal compressors

In centrifugal compressors, a constant gas flow passes through a rapidly rotating impeller, where the kinetic energy is transformed to pressure energy, also known as 'head'. The head developed by a centrifugal compressor can be defined as the height to which a column of gas can be raised at the compressor discharge; the head depends in great measure on the flow rate that passes through the compressor (Davidson and Von Bertele, 1996, p. 24). Centrifugal compressors are used in many industrial refrigeration applications because of their reliability, their capacity to handle high volumetric flow rates at medium pressures, and because they can be driven by steam turbines (Bloch, 2006, Ch. 3; Ludwig, 2001, Ch. 12). In order to identify the best set of operating conditions in a refrigeration cycle, the compressor and associated cycle need to be appropriately modelled.

2.2.1. Compression process model

Two different thermodynamic compression processes can be described: adiabatic and polytropic. In adiabatic compression, no heat is transferred to or from the process and an isentropic (ideal) path is followed during compression (Ludwig, 2001, Ch. 12). In polytropic compression, the entropy of the gas changes as it is being compressed (Ludwig, 2001, Ch. 12). For an ideal adiabatic compression process Pv^{γ} remains constant, where P is the pressure, v is the specific volume and γ is the ratio of the inlet gas heat capacities. However, this ideal relation is normally valid only when the compressor is internally cooled and is mostly used as a theoretical model (Ludwig, 2001, Ch. 12). Centrifugal compressors are often modelled in terms of polytropic compression, where Pv^{n_p} remains constant and n_p is the polytropic coefficient, which depends on the actual inlet and outlet conditions of the gas (Ferguson, 1963, Ch. 2.7).

Head and efficiency characterise the performance of centrifugal compressors. The polytropic head, which is the same head that was previously defined but following a polytropic path, is defined as (Ferguson, 1963, Ch. 2.7):

$$H_p = P_{in} v_{in} \frac{n_p}{n_p - 1} \left[\left(\frac{P_{out}}{P_{in}} \right)^{(n_p-1)/n_p} - 1 \right] \tag{1}$$

where H_p is the polytropic head, P_{in} is the inlet pressure, v_{in} is the specific actual inlet volume, n_p is the polytropic coefficient, and P_{out} is the discharge pressure. The polytropic coefficient can be calculated knowing the inlet and outlet conditions of a stage (Ludwig, 2001, Ch. 12):

$$n_p = \frac{\ln(P_{out}/P_{in})}{\ln(v_{in}/v_{out})} \tag{2}$$

where v_{out} is the specific outlet volume of the gas.

The polytropic efficiency is the ratio of the theoretical polytropic work required by the compressor and the real polytropic work at the compressor shaft. The polytropic efficiency (η_p) can be estimated from (Ferguson, 1963, Ch. 2.7):

$$\eta_p = \frac{\gamma - 1}{\gamma} \frac{n_p}{n_p - 1} \tag{3}$$

Finally, the actual polytropic work (W_p) required by the compressor is (Ludwig, 2001, Ch. 12):

$$W_p = \frac{mgH_p}{\eta_p \eta_m} \tag{4}$$

where m is the mass flow rate and η_m is the mechanical efficiency of the compressor, which takes into account the losses caused by the friction of the wheel, the fluid friction, gas turbulence and the friction of the seals.

2.2.2. Part-load performance prediction of centrifugal compressors

To predict the part-load performance of an operating centrifugal compressor, away from the design point, manufacturers provide performance curves, an example of which is presented in Fig. 4. In these curves, the design point marks the original operating conditions for which the compressor was initially designed (inlet volumetric flow rate, discharge pressure and rotational speed). The solid lines predict the performance at lower or higher rotational speeds, and for different inlet flow rates. Two limits are presented on these curves: the surge limit (the lowest allowable inlet flow rate) and the choke limit (the maximum allowable inlet flow rate).

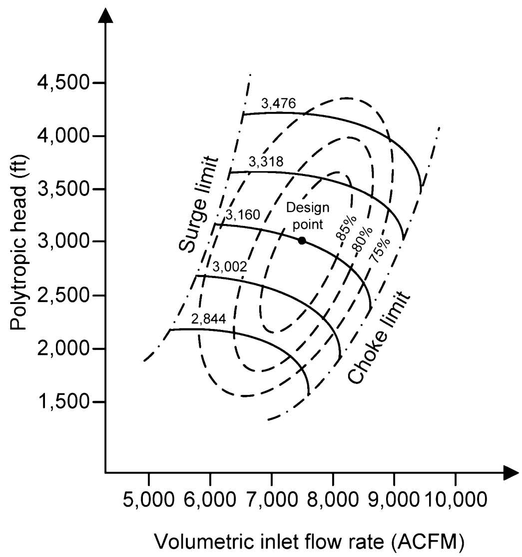

Fig. 4. Example of a compressor performance curve.

If the operation of the compressor is beyond any of these limits, it becomes unstable, potentially causing serious damage to the compressor (Hanlon, 2001, Ch. 4). For multistage compressors, the performance curves can either be represented by the curves of each individual compression stage or by a global compressor curve that takes into account all the stages of the compressor. Rigorous simulation software (e.g. Aspen HYSYS, Aspen Plus) needs the information given by these curves regressed in polynomial form or tabulated (Aspen Technology Inc, 2013a,b).

Performance curves are not the only way to predict the performance of centrifugal compressors: mathematical expressions for geometrically similar centrifugal compressors (called fan laws) can also be used. The fan laws have low deviations as long as the difference of the rotational speed between the two operating conditions is not large (Lapina, 1982). These interdependent fan laws express the relationship between the head, flow rate, speed and size (impeller diameter) of centrifugal compressors. The first law, for a fixed compressor diameter, can be expressed as (Ludwig, 2001, Ch. 12):

$$Q_A^V = Q_B^V \left(\frac{N_A}{N_B}\right) \tag{5}$$

where Q^V is the volumetric flow rate, N is the rotational speed of the compressor, and A and B are two different operational points. The second and third laws state that, for a given compressor diameter, the head varies with the speed squared (Eq. (6)) and the work varies with the speed cubed (Eq. (7)), respectively.

$$H_{p,A} = H_{p,B} \left(\frac{N_A}{N_B}\right)^2 \tag{6}$$

$$W_{p,A} = W_{p,B} \left(\frac{N_A}{N_B}\right)^3 \tag{7}$$

The performance curves or the fan laws can be used to predict the part-load performance of centrifugal compressors. For example, the volumetric flow rate, head and shaft work of operational point A can be predicted with Eqs. (5)–(7), and knowing the rotational speed at A and the volumetric flow rate, head, shaft work and rotational speed of operational point B. To predict the performance of centrifugal compressors when operating at different conditions, rigorous simulation software may use several performance curves, but not the fan laws, or they may only use the data from one of the performance curves and the second fan law (Eq. (6)) (Aspen Technology Inc, 2013a,b). Each prediction method has its own limitations; the model proposed in this paper aims to reduce the inaccuracies incurred by allowing the use of more than one reference curve from the performance curves together with the fan laws. The model is then included in an optimisation framework to address changes in the operation of the refrigeration cycle due to changes in the process conditions (e.g. cooling duty, temperatures).

3. Literature review

Early works on the synthesis of refrigeration cycles applied pinch analysis (Linnhoff and Dhole, 1992) or mathematical programming (Barnés and King, 1974; Shelton and Grossmann, 1986). Pinch analysis allows to evaluate the economic performance of energy targets (i.e. external utility consumption), without the need of detailed HEN designs (Linnhoff and Dhole, 1992; Smith, 2005, Ch. 16). Linnhoff and Dhole (1992) used a method in which the shaft work demand at different refrigeration temperature levels can be easily evaluated by graphically representing the temperature–enthalpy profile of the process streams and assuming constant exergetic efficiency (defined as the ratio of the exergy supplied by the refrigeration cycle to its shaft work demand). However, it may not be sound to assume constant exergetic efficiency. In addition, the savings achieved by considering features that reduce shaft work demand (e.g. use of economisers, presaturators, aftercoolers) cannot be taken into account as the effect of their use (i.e. less shaft work consumption) cannot be represented in the temperature–enthalpy profile of the process streams.

On the other hand, Barnés and King (1974) proposed a model that combines the use of heuristics and mathematical programming to find a refrigeration cycle design that has minimum annualised costs. The model includes the use of features that reduce shaft work demand and implements a sequential approach to determine the number of cooling levels. This sequential approach consists of adding new cooling levels to the refrigeration cycle and optimising the new design, until the costs of this new cycle are not further decreased, compared to the previous cycle design. The evaporation temperatures of the refrigeration cycles are chosen using the following interpolation formula:

$$\frac{1/T_i - 1/T_{evap}}{1/T_{cond} - 1/T_{evap}} = \frac{i-1}{I} + 0.5\left(\frac{i-1}{I}\right)\left(1 - \frac{i-1}{I}\right) \tag{8}$$

where T_i is the evaporation temperature of ith cooling level, T_{evap} is the evaporation temperature of the coldest cooling level, T_{cond} is the temperature at which the refrigerant is being condensed, and I is the number of cooling levels. Their results show that applying process analysis (using the heuristics) prior to optimisation considerably reduces the search for the optimum design. However, the sequential approach to determine the number of cooling levels limits the evaluation of design options when complex refrigeration cycles (e.g. multilevel cascade cycles) are designed.

The model developed by Shelton and Grossmann (1986) generates feasible designs for multilevel refrigeration cycles to minimise utility costs, capital costs or total annualised costs. The problem is formulated as a mixed integer linear programming model, where the integer variables account for the possible cooling levels. Although the designs presented are feasible, the simple model formulation only considers presaturators as possible design options, uses a linear compressor model and ignores the number and costs of heat exchangers, which limits the usefulness of the model in practical applications.

Later works integrate the two approaches proposed by Linnhoff and Dhole (1992) and Shelton and Grossmann (1986): Wu (2000) developed a model that divides the temperature range into intervals to address the heat integration between the process and the refrigeration cycle. In addition, the major refrigeration design options and the costs of heat exchangers are considered, which helps to generate more realistic designs. Nonetheless, one of the main problems with the models of Shelton and Grossmann (1986) and Wu (2000) is that it is necessary to divide the temperature range into intervals to find the optimal refrigeration temperature levels. By dividing the temperature range into intervals, each interval is considered as a potential cooling level. To try to account for all possible evaporation temperatures, the temperature range must be finely discretised. This discrete number of intervals involves a large number of binary variables, resulting in the need to implement complex optimisation algorithms that demand long computational running times.

Lee (2001) improved the model of Wu (2000) by using grand composite curves (Linnhoff and Thomas, 1994) and treating the evaporation temperatures and cooling duties of each level as continuous variables, reducing the reliance on binary variables. In the model of Lee (2001), the implementation of a methodology for optimising the shaft work demand, using an enhanced disjunctive programming model, reduces the computational running time. In this optimisation model, the active evaporating levels (i.e. total number of cooling levels) are found by modelling the grand composite curves (GCC) as a series of linear functions, from which the temperature and cooling duty of each level can be directly read. Furthermore, two different options for 'exploiting the pockets' of the GCC (i.e. additional heat integration between process streams and the refrigeration cycle rather than exchanging all the possible heat between process streams) are considered for further reducing shaft work demand: adding heat rejection levels or subcooling the refrigerant. Once the evaporation temperatures are found, the inlet and outlet pressures and outlet temperatures of each compression stage are estimated, and the shaft work demand is found by making an energy balance around the stages. This shaft work optimisation model is formulated as a mixed-integer non-linear programming (MINLP) model, where the only integer variables are the number of cooling levels. The objective function is to minimise the operating cost of compression or to minimise the sum of the operating costs and annualised capital cost of the compressors and HEN. Additionally, the use of features that reduce shaft work demand (e.g. use of economisers, presaturators, aftercoolers) is also considered. However, the main drawback of the model is that the cycle configuration (i.e. use of presaturators, economisers, etc.) cannot be evaluated simultaneously with the number of cooling levels.

Vaidyaraman and Maranas (2002) proposed a methodology for the synthesis of mixed refrigerant cascade cycles. Since evaporation and condensation of refrigerant mixtures take place over a temperature range, substreams with different compositions can be obtained by partially condensing such mixtures. Vaidyaraman and Maranas (2002) proposed to partially condense the mixture to different vapour fractions, cooling the process or another mixed refrigerant stream over a temperature range but at the same pressure. They formulate the problem as a NLP model, where the objective function is minimisation of shaft work demand and the variables are the pressure levels, mixed refrigerant composition and vapour fraction after each partial condensation. However, in this work the temperature–enthalpy profiles of the process stream and mixed refrigerant stream are only compared at the end of the exchanger, so it is not possible to ensure during the optimisation that there are no temperature crosses along the exchanger length.

Del Nogal et al. (2008) optimised the design of mixed refrigerant cycles (single and cascade cycles) using a genetic algorithm (GA). The optimisation routine includes the calculation of the composite curves from the process and refrigerant streams, dividing the whole cooling demand into enthalpy intervals, and making checks within every enthalpy interval to ensure there is no temperature cross between streams. The optimisation objective can be set to different scenarios, which include minimisation of total annualised capital costs (including the cost of heat exchangers) or minimisation of shaft work demand.

So far, the literature review has addressed the synthesis of refrigeration cycles. Although the synthesis of refrigeration cycles is important, plants that are already in operation need to be revamped or operated in a better way to improve their energy consumption. Optimisation of the operating conditions can address various objectives; for example to find a different set of operating conditions for the refrigeration cycle that can improve the energy efficiency for the current plant capacity, or to find a new set of operating conditions for the refrigeration cycle for a different plant capacity or different process operating conditions (e.g. change in process stream temperatures, physical properties). Just as the design problem is complex due to the interactions between the process, the HEN and the refrigeration cycle, operational optimisation is also very complex, because of the additional interactions between the operational variables (mainly the refrigerant flow rates and the rotational speed of compressors) within the refrigeration cycle.

Alabdulkarem et al. (2011) optimised the operating conditions of a propane precooled mixed refrigerant (C3-MR) LNG plant, simulated in Aspen HYSYS, by means of a GA model coded in MATLAB. The variables considered are the refrigerant flow rates, mixed refrigerant composition and pressure levels; the objective function is the minimisation of shaft work consumption. Their results achieved power savings between 7% and 14%, compared to other works. Wang et al. (2013) also optimised a C3-MR process to find process improvements for different optimisation objectives, which are: minimisation of shaft work demand, improvement of exergy efficiency and minimisation of operating costs. The model varies the refrigerant flow rates, mixed refrigerant composition and pressure levels. The simulation and optimisation is carried out in Aspen HYSYS and the best results for the system (i.e. lowest power demand per tonne of LNG produced) were found when optimising for highest exergy efficiency.

Hasan et al. (2009b) proposed a MINLP model to optimise the operation of compressor trains of AP-X LNG plants (Air Products and Chemicals Inc., 2002). The AP-X refrigeration cycle has three cascades: a propane cycle, a mixed refrigerant cycle and a subcooling nitrogen cycle (Air Products and Chemicals Inc., 2002). This model is able to address the complex interactions between the different refrigeration cycles and minimises shaft work consumption by varying the cooling loads and evaporation temperatures of the refrigerant cycles. A first set of binary variables represents the operation (or not) of a compressor in a cycle, while a second set determines if either the inlet or outlet pressure to each compressor train is used as a continuous variable for the optimisation. The shaft work consumption of each compressor train is calculated as a function of its polytropic efficiency and coefficient, and of the refrigerant inlet temperatures and flow rates. Once the pressures are known, the model calculates the refrigerant flow rates and process temperatures from energy balances around the units. However, the model does not incorporate the part-load performance of compressors. The only limit associated with the operating compressors that this work accounts for is the range of allowable pressures; flow rate limits and the rotational speed of compressors are not considered.

Sun and Ding (2014) optimised the operating conditions of a PRICO LNG process (Black & Veatch Corporation, 2014), taking into consideration speed changes to the compressors. The PRICO LNG process consists of a single mixed refrigerant cycle (Black & Veatch Corporation, 2014). Various load scenarios (percentage of cooling load compared to base case) are presented and optimised, where the optimisations evaluate the use of three possible adjustable variables, namely, the mixed refrigerant composition, the use of a throttle valve before the compressor (to reduce the density of the suction gas) and the use of a variable-speed compressor. The optimisation objective is minimisation of shaft work consumption.

The performance curves of the compressor are provided for its two stages, from which both the discharge pressure and the polytropic efficiency can be read. Minimum shaft work demand is obtained for the case when the mixed refrigerant composition and speed of the compressor are changed simultaneously. If the plant has no load adjustment facilities (no throttle valve and no variable-speed compressor), considerable savings can still be achieved by changing the mixed refrigerant composition for the different load scenarios. Although speed changes were considered for the compressor, the authors assume for the optimisation that the existing heat exchanger is able to achieve the design outlet temperatures. However, the temperatures of the streams can be higher or lower than the design conditions, depending on the effect that changes to the natural gas flow rate and mixed refrigerant flow rate and composition have on the performance, i.e. changes to the overall heat transfer coefficient of the operating heat exchanger.

In the present work, the shaft work estimation method developed by Lee (2001) is used as a base, given the similarities between the two problems, i.e. to find the set of evaporation temperatures and cooling duties that lead to minimum shaft work consumption. However, the optimisation algorithm used in this paper is different from that used by Lee (2001). In addition, the goal of this paper – to develop an operational optimisation model – is different to that of Lee (2001), who proposed a design model; therefore, the variables involved in the two models are different. Furthermore, different constraints need to be implemented in the model to address the operational limits of compressors and other constraints that only concern the synthesis problem need to be removed (e.g. integer variables for each cooling level).

4. Model formulation for operational optimisation of multilevel refrigeration cycles

For the synthesis of refrigeration cycles, the most important parameters to be estimated are the number of cooling levels, their respective cooling duties and the cycle configuration (e.g. use of features that reduce shaft work demand). On the other hand, for operational optimisation, the flowsheet and number of cooling levels are already set. In addition, various constraints arise due to the physical limits of the equipment in operation. If the operating conditions of the refrigeration cycle need to be changed, then it is necessary to know whether the equipment in operation is able to operate, without problems, at this new set of conditions (refrigerant flow rates, rotational speed of compressors, etc.). Problems may arise because of the presence of liquid droplets at the inlet of the compressor, or because the compressor operation is beyond its surge or choke limits.

For centrifugal compressors, a key operational variable is the rotational speed. Shaft work and hence operating costs can be saved if the rotational speed is decreased and vice versa. When finding a new set of operating conditions for the refrigeration cycle (combinations of refrigerant flow rates, evaporation temperatures and rotational speeds of the compressors), isolated changes to the rotational speed of compressors cannot be considered, as the total cooling duty of the process must be satisfied; therefore, changes to the refrigerant flow rates must also be considered. The effects that variations of the refrigerant flow rates have on shaft work demand are not easily predicted, as the change depends on the volumetric flow rate and the inlet conditions of the gas. These simultaneous changes of refrigerant flow rates and rotational speed can generate a large number of possible solutions (i.e. the solution space), where each solution could have a different shaft work demand for the same total cooling duty. Out of this large solution space, the objective is to find a set of operating conditions for the refrigeration cycle that consumes the least shaft work. Thus, this work proposes a new optimisation approach for shaft work minimisation of refrigeration cycles, which considers all these simultaneous changes, together with its relevant operational constraints.

4.1. Model for estimating the part-load performance of centrifugal compressors

Schultz (1962) developed a centrifugal compressor model that takes into account the actual behaviour of the gas that is being compressed by making use of the polytropic head factor, which corrects the assumption that the polytropic coefficient is constant throughout the compression process. The polytropic head factor (f_p) is defined as (Schultz, 1962):

$$f_p = \left(\frac{h_{s,out} - h_{in}}{P_{out} v_{s,out} - P_{in} v_{in}} \right) \left(\frac{n_s - 1}{n_s} \right) \tag{9}$$

where $h_{s,out}$ is the specific isentropic discharge enthalpy, h_{in} is the specific inlet enthalpy, $v_{s,out}$ is the specific isentropic discharge volume and n_s is the isentropic coefficient. The isentropic coefficient is calculated as:

$$n_s = \frac{\ln (P_{out}/P_{in})}{\ln (v_{in}/v_{s,out})} \tag{10}$$

Finally, the polytropic head can be calculated by multiplying Eq. (1) and Eq. (9). This compressor model (Schultz, 1962), also known as the ASME model (Eq. (11)), is used in the present work. The use of this model improves the accuracy of the design and testing of centrifugal compressors by assuming the behaviour of the gas as real instead of ideal (Schultz, 1962).

$$H_p = f_p P_{in} v_{in} \frac{n_p}{n_p - 1} \left[\left(\frac{P_{out}}{P_{in}} \right)^{(n_p - 1)/n_p} - 1 \right] \tag{11}$$

In multistage compressors the discharge of the first stage is the suction of the second stage, and the discharge of the second stage is the suction of the third, and so on. So, when the inlet conditions of the first stage of a multistage compressor change, this effect can have an impact on the downstream stages. This cascaded effect, known as the volume-ratio effect (Lapina, 1989), makes predicting the performance of multistage compressors a difficult task. The volume-ratio effect can be of major importance if any changes in the inlet operating conditions of the first stage cause the gas density at its discharge to change from the design conditions. For example, if the discharge volumetric flow rate of the first stage decreases (compared to design conditions), then the discharge volumetric flow of the second stage also decreases (again, compared to design conditions); this decreased volumetric flow could, at some stage, cause surge problems and make the operational point infeasible.

In this work it is assumed that the polytropic head remains approximately constant, for a given inlet volumetric flow rate and speed, independent of its inlet conditions since it is only a function of the tip speed of the impeller (Lapina, 1982). By making this assumption, the performance of centrifugal compressors for changes in the inlet conditions of the gas can be predicted by making use of the original performance curves provided by the manufacturers.

Since the present work makes use of the fan laws to estimate the performance of compressors, it is necessary to make some corrections to account for their use. As mentioned in Section 2.2.2, the fan laws act in an interlinked way, which means that they must be used simultaneously. Given that both Eqs. (5) and (6) estimate changes in flow rate, it is necessary to ensure that the flow rate ratios of both equations are the same, considering simultaneous changes to the speed and head.

To calculate the part-load performance of a compressor using the fan laws, the methodology proposed by Lapina (1982) is implemented in this work. The methodology proposed is described below:

1. Find the reference polytropic head ($H_{p,r}$), based on the design operating conditions (refrigerant inlet flow rate, temperature and pressure and compressor rotational speed) and reference performance curves.
2. Given the new operating conditions of the process, calculate the required polytropic head ($H_{p,req}$) corresponding to the new required pressure ratio of the compressor using Eq. (11).
3. For the required pressure ratio, calculate the new rotational speed using the second fan law (Eq. (6)).
4. According to the second fan law, to find the new rotational speed, the volumetric flow rate is affected as per Eq. (5), which causes a deviation from the required pressure ratio. To take into consideration the simultaneous use of the fan laws, a factor that determines the head variation due to volumetric flow changes is introduced (Lapina, 1982):

$$\%Q^V = \frac{Q^V_{req}/N_{est}}{Q^V_r/N_r} \tag{12}$$

where $\%Q^V$ is the inlet volumetric flow rate correction factor, N_{est} is the estimated speed found in step 3, $Q^V{}_{req}$ is the required inlet volumetric flow rate, N_r is the reference rotational speed and $Q^V{}_r$ is the reference inlet volumetric flow rate found in step 1.
5. The percentage of polytropic head change is calculated, similarly, as (Lapina, 1982):

$$\%H_p = \frac{H_{p,\%Q^V}}{H_{p,r}} \tag{13}$$

where $\%H_p$ is the polytropic head correction factor, $H_{p,\%Q^V}$ is the polytropic head for the reference inlet volumetric flow rate multiplied by $\%Q^V$ (read from the performance curves).
6. The required rotational speed is then found by modifying the second fan law, accounting for the simultaneous use of Eqs. (5) and (6):

$$N_{req} = N_r\sqrt{\frac{H_{p,req}}{H_{p,r}\cdot\%H_p}} \tag{14}$$

where N_{req} is the final required speed.

Thus, when a different rotational speed for a compressor is needed during the operational optimisation to achieve a required pressure ratio, Eqs. (5), (12)–(14) are used together with a reference curve, which can be any of the performance curves provided by the manufacturers. As recommended by Lapina (1982), to avoid inaccuracies, the difference between the required and reference speed in every iteration of the proposed optimisation model is set to be less than or equal to 2.5%.

4.2. Calculation procedure for the operational optimisation of multilevel refrigeration cycles

For the operational optimisation of refrigeration cycles it is first assumed that the process cooling requirements can be represented appropriately using a temperature–enthalpy profile for the process streams and that the evaporation temperatures can be adjusted according to this profile. The temperature–enthalpy profile is used to identify the total cooling duty and lowest refrigeration temperature level. In this work, the temperature–enthalpy profile chosen is the GCC and it is assumed that the process is designed for maximum heat recovery. Additionally, the heat exchangers are assumed to meet the process target temperatures and to have no pressure drop, i.e. the evaporation of the refrigerant is isothermal.

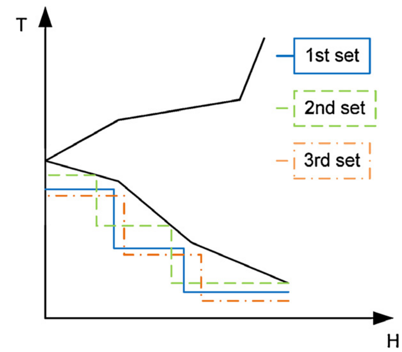

Fig. 5. Adjustment of cooling duties for different evaporation temperatures sets.

In multilevel refrigeration cycles, the evaporation temperatures may be varied, and the cooling duties of each cooling level adjusted accordingly, so that the total cooling requirement is satisfied. The evaporation temperatures (and associated pressure levels in the refrigeration cycle) are therefore degrees of freedom. For example, in Fig. 5, it can be seen how the cooling duties of every cooling level of a three-level refrigeration cycle are adjusted accordingly depending on the evaporation temperatures and minimum temperature ($\Delta T_{\min}$) difference using the GCC.

In Fig. 5, it can be seen that when the operating conditions are changed from the first to the second set, $\Delta T_{\min}$ is reduced and the evaporation temperatures increase. In addition, the cooling duties of the lower-temperature levels are increased, whereas the cooling duty of the highest-temperature level is decreased. The opposite happens when the operating conditions are changed from the first to the third set.

Two situations can be tested in multilevel refrigeration cycles to minimise shaft work consumption for a given cooling duty and condenser pressure: reduce or increase refrigerant flow rate. If the refrigerant flow rate of a lower-temperature cooling level is reduced, then shaft work could be saved at this cooling level. However, the rotational speed of the higher-temperature cooling levels must be increased in order to meet the condenser pressure. So, the shaft work demand of the higher-temperature cooling levels increases due to the increase in rotational speed. The opposite situation happens if the refrigerant flow rate of a lower cooling level is increased. Thus, the final shaft work consumption is a trade-off between changes in the flow rates and rotational speeds.

The higher the number of cooling levels and compression stages, the more complex the interactions between the variables become in a multilevel refrigeration cycle. If the refrigerant flow rate of one cooling level changes, the refrigerant flow rate of the other levels must be adjusted such that all the constraints are met and the total cooling duty is satisfied. To meet the constraints, the other refrigerant flow rates can either increase or decrease, which in turn causes changes in the rotational speed of those stages. Thus, even if shaft work could be initially saved at a particular low-temperature cooling level by reducing its refrigerant flow rate, the effect of the corresponding increase in the refrigerant flow rate at a higher-temperature cooling level, together with the change in rotational speed of the corresponding compression stage, could cancel the initial saving. These complex interactions make the optimisation problem difficult to address, as the optimiser could get trapped in local minima or not converge because of the non-linearity of the model.

The optimisation model inputs are: the process stream data (cooling duties, target and supply temperatures and heat capacities) and the design operating conditions (to be used as an initial guess for the optimisation). Since the calculation procedure is based on the GCC, once the evaporation temperatures are known, the refrigerant flow rates and rotational speed of compressors can be found. Therefore, the independent variables for the optimisation are the evaporation temperatures and $\Delta T_{\min}$; the dependent variables are the refrigerant flow rates and cooling duties, and rotational speed of the compressors. For the optimisation, the model varies the evaporation temperatures at which the cycle provides cooling and $\Delta T_{\min}$ of the exchangers. Finally, the model gives as outputs: the evaporation temperature, refrigerant flow rate and cooling duty of each level and the rotational speed of compressors.

To find the optimal refrigeration levels, the MINLP model developed by Lee (2001) for estimating the shaft work demand of refrigeration cycles is used as a basis – but without employing binary variables and with added constraints that take into account the physical limits of the compressors (surge and choke). The optimisation problem can be stated as:

$$\min W(\Theta) = \sum_{m=1}^{M} W_m(\Theta) \tag{15}$$

Subject to:

$$m_m(h_{out} - h_{in})_m - \frac{m_m g H_{p,m}}{\eta_{p,m}} = 0 \tag{16}$$

$$H_{p,m} g - f_{p,m} P_{in,m} v_{in,m} \frac{n_{p,m}}{n_{p,m}-1} \left[\left(\frac{P_{out,m}}{P_{in,m}} \right)^{(n_{p,m}-1)/n_{p,m}} - 1 \right] = 0 \tag{17}$$

$$s_{out,m} - s_{s,in,m} = 0 \tag{18}$$

$$m_m v_{out,m} - Q^V_{in,m} \left(\frac{P_{in,m}}{P_{out,m}} \right)^{1/n_{p,m}} = 0 \tag{19}$$

$$Q^V_m \geq Q^{V,Surge}_m \tag{20}$$

$$Q^V_m \leq Q^{V,Choke}_m \tag{21}$$

$$lb \leq \Theta \leq ub \tag{22}$$

where W is the total shaft work demand of the refrigeration cycle, Θ is the vector of evaporation temperatures and $\Delta T_{\min}$, M is the number of compression stages, W_m is the shaft work demand of the mth compression stage, $s_{out,m}$ is the outlet specific entropy of the mth stage, $s_{s,in,m}$ is the isentropic inlet specific entropy of the mth stage, Q^V_m is the inlet volumetric flow rate to the mth compression stage, $Q^{V,Surge}_m$ is the volumetric surge limit of the mth compression stage, $Q^{V,Choke}_m$ is the volumetric choke limit of the mth compression, lb is the vector of lower bounds, and ub is the vector of upper bounds. Eqs. (16)–(19) represent the energy balance around the compressors. To ensure that the compressor does not surge (Eq. (20)) or choke (Eq. (21)) at the new required rotational speed, the surge and choke limits must also be corrected to this new speed using the first fan law (Eq. (5)). Eq. (22) keeps the evaporation temperatures within certain bounds. Additional constraints relate to the same rotational speed for the compression stages that are placed on the same shaft and for the part-load compression model (Eqs. (12)–(14)).

Due to the non-linear nature of the model and the fact that the solution space is large, traditional gradient-based NLP solvers can get trapped in different local minima depending on the starting point used for optimisation. To make the optimisation more robust and to look for an approximation to a global minimum rather than a local one, an optimisation algorithm based on the one developed by Ugray et al. (2007) is used. This algorithm consists of a combination of scatter search and traditional gradient-based NLP solvers, where the different points generated by a scatter search algorithm are used as potential starting points for a gradient-based NLP solver.

In this optimisation methodology (Ugray et al., 2007), not all the points (which are generated based on the upper and lower bounds of the variables) are selected to run the gradient-based NLP solver. To determine which points are selected to initialise optimisation runs, the objective function and constraints are evaluated for each point to calculate its penalty function, which is the summation of the objective function and the absolute amount by which the constraints are violated. Filters are then used to exclude points that are within a certain distance of a previously found optimal solutions or points for which the value of the penalty function is above a certain threshold. The use of these filters helps to avoid finding the same optimal solution several times or starting the optimisation from low quality points. However, the use of these filters does not hinder the algorithm from finding an approximation to a globally optimal solution.

In addition, the computational time required to find a global minimum is relatively low, due to the small number of times that the gradient-based NLP solver is started. The main benefit of using this kind of hybrid form of optimisation is that it combines the main advantages of each optimisation method (Ugray et al., 2007). Scatter search optimisation can locate different optimal solutions of a large solution space, but it has problems satisfying the constraints (especially the non-linear ones). Conversely, gradient-based NLP solvers are able to find optimal solutions that meet the constraints with high accuracy, relatively fast, but they tend to get trapped in locally optimal solutions.

4.3. Calculation procedure for the operational optimisation of cascade refrigeration cycles

For the optimisation of cascade cycles, additional steps need to be taken compared to a multilevel cycle. In cascade refrigeration cycles, the cooling duty of the upper cycle has to take into consideration the duty of the condenser of the lower cycle. This means that the operating conditions of the lower cycle can be determined independently of its upper cycle; however, the operating conditions of the upper cycle are determined based on the ones from its lower cycle. By assuming that the total condensing duty of the lower cycle is satisfied by the upper cycle, the integration of this condensing duty with the process does not need to be considered. So, it is necessary to implement a methodology that considers the integration between the cycles of a cascade refrigeration cycle, but that does not affect the heating and cooling requirements of the process streams.

In the present work, the steps proposed by Lee (2001) are followed to take into consideration the condensing duty of the lower cycle. First, the evaporation temperatures and cooling duties of the lower cycle are set, so that its condensing duty can also be calculated. Then the condensing duty of the lower cycle is incorporated into the GCC of the process to produce an ‘effective’ GCC. With this effective GCC, the upper cycle calculations can account for the performance of the lower cycle, as well as that of the process. To integrate the condensing duty of the lower cycle into the GCC, the total condensing duty is assumed to be satisfied at the lower cycle condensation temperature (i.e. isothermal condensation), and then the GCC of the process is recalculated.

An example of these steps is shown in Fig. 6. In Fig. 6a, the evaporation temperatures and cooling duties of the lower cycle are set using the GCC. Knowing the evaporation temperatures and cooling duties of the lower cycle and the partition temperature, its condenser duty is calculated. This condenser duty is added as an additional hot stream at its condensation temperature, so that the effective GCC can be built, as seen in Fig. 6b. Once the condenser

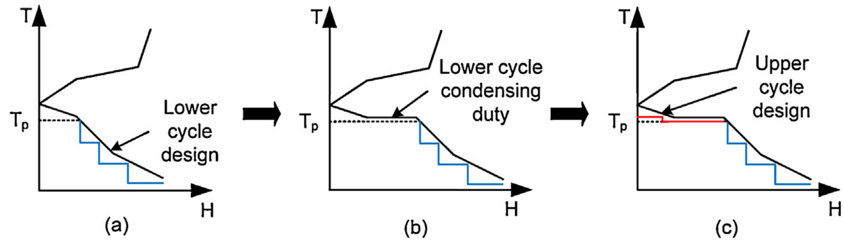

Fig. 6. Example of an effective GCC for the optimisation of cascade refrigeration cycles.

duty of the lower cycle has been added to the effective GCC, the evaporation temperatures and cooling duties of the upper cycle can be set, as shown in Fig. 6c.

Although the total condensing duty of the lower cycle includes both latent and sensible heat, for the calculation of the effective GCC, the supply temperature of the condensing stream is assumed to be the condensation temperature and not the compression discharge temperature. By making this assumption the profile of the process composite curve is not affected, i.e. the lower cycle condensing duty is not integrated with the process.

Once the effective GCC is built, the rest of the optimisation approach follows the same procedure proposed for multilevel cycles and uses the same model described in Section 4.2. Since this optimisation approach simultaneously optimises the operating conditions of the lower and upper cycles, all the variables and constraints must be considered in a single model.

4.4. Benefits of the proposed optimisation approach

While rigorous simulation software provides powerful tools for simulating existing refrigeration cycles, their optimisation capabilities are limited, and the energy flows cannot be expressed in terms of the GCC. The use of this optimisation model, instead of rigorous simulation software, is beneficial because it is specially developed from the process GCC. Thus, if the process cooling demand or temperatures changes, the new cooling duty that needs to be satisfied, using cooling water and refrigeration, and the new operating conditions of the refrigeration cycle are found without the need to implement complex optimisation routines in a rigorous simulation software.

Although the GCC is useful for selecting the evaporation temperatures of refrigeration cycles, the GCC assumes maximum heat recovery between process streams, i.e. an ideal, rather than actual, operating condition. HENs designed for maximum energy recovery have the lowest possible utility costs, but tend to have high capital costs due to the number of heat exchangers required (Smith, 2005, Ch. 18). On the other hand, designs that aim for minimum capital cost tend to have higher utility costs compared to maximum heat recovery designs (Smith, 2005, Ch. 18). The final HEN design tends to be an intermediate solution where the total annualised costs are the lowest, but it does not necessarily maximise energy recovery. So, in the cases where the energy recovery is not maximised, the GCC is no longer relevant; instead, another temperature–enthalpy profile should be used as a basis for the optimisation.

5. Example case: application of the proposed methodology

Two examples illustrate the application of the model proposed in this work. In the first example, a C3-MR refrigeration cycle of a LNG plant is presented. The main focus of the example is the propane precooled cycle. The second example, presented as Supplementary information, considers an ethylene-propylene cascade refrigeration cycle from the cold-end process of an ethylene plant.

5.1. Example 1: propane precooled mixed-refrigerant cycle

The process streams shown in Table 1 are part of a complex cascade refrigeration cycle of a LNG plant. In this example, both the natural gas stream and the mixed refrigerant of a lower cycle need to be precooled by propane; this cooling takes place at three temperature levels. Furthermore, both the natural gas and mixed refrigerant stream are divided into two or more segments to account for changes in the heat capacity flow rates in different temperature ranges. ΔT_{min} for the design is 5 °C; cooling water is available at 25 °C and returned at 30 °C.

The fluid properties are estimated using the Peng–Robinson equation of state. This equation of state is widely used in industrial applications for gas processing and is relatively simple to implement in programming models. All the equations and constraints are implemented in an optimisation model coded in MATLAB (The MathWorks Inc., 2014). The gradient-based NLP solver *fmincon* from the Optimisation Toolbox is used as the gradient-based NLP solver and the *GlobalSearch* algorithm from the Global Optimisation Toolbox is used as the global optimising solver. The optimisation parameters used in MATLAB are presented in Table 2. These parameters were chosen based on the results of several tests and using various scaling factors, where the latter are used to ensure the same order of magnitude for the constraints.

The *fmincon* solver, with the *interior-point* algorithm, is chosen due its capacity to handle medium and large-scale smooth problems, variable bounds and inequality and equality non-linear constraints. The *GlobalSearch* algorithm is the implementation of the optimisation methodology proposed by Ugray et al. (2007) in MATLAB, as discussed in Section 4.2. Information about these algorithms is presented by The MathWorks Inc. (2014).

Table 1
C3-MR process stream data.

Stream	Segment	Temperatures (°C)		Enthalpy change (MW)	Heat capacity flow rate (MW/°C)
		Supply	Target		
Natural gas	1	30.0	−6.0	1.630	0.453
	2	−6.0	−34.1	1.485	0.528
Mixed refrigerant	1	30.0	10.0	2.966	1.483
	2	10.0	−10.0	2.812	1.406
	3	−10.0	−34.1	3.184	1.321

Table 2
MATLAB optimisation parameters.

	Description	Value
fmincon algorithm	Algorithm used	Interior-point
fmincon MaxFunEvals	Maximum number of function evaluations	5000
fmincon TolFun	Tolerance on the objective function	1×10^{-2}
fmincon TolX	Tolerance on the variables	1×10^{-4}
fmincon TolCon	Tolerance on the constraints	1×10^{-3}
GlobalSearch NumTrialPoints	Number of trial points	2000

The design evaporation temperatures of the three-level propane refrigeration cycle are set following the interpolation formula (Eq. (8)) proposed by Barnés and King (1974). The design of the compressors is performed following the methodology suggested and information provided by Ludwig (2001, Ch. 12). Each compression level uses a single-stage centrifugal compressor without interstage cooling and has its own driver; the details of the compression stages can be seen in Table S13 (see Supplementary Information). The design conditions of the refrigeration cycle can be seen in Table 3. The balanced grand composite curve for the process is shown in Fig. 7, where T_i is the evaporation temperature of the ith level and Q_i is its corresponding cooling duty. The flowsheet configuration of the cycle can be seen in Fig. 8.

For simulation purposes, the proposed model takes as inputs the evaporation temperatures, refrigerant flow rates and speed of the compressors, and gives as outputs the cooling duty and shaft work consumption of each cooling level.

As explained in Section 4.2, the optimisation model varies the independent variables and evaluates the dependent variables to find a set of operating conditions that minimise shaft work demand. The optimisation model has three independent variables and 18 dependent variables. In this work, the condenser pressure is fixed during optimisation, but can be varied in an outer loop; and ΔT_{min} of all the exchangers is assumed to be the same. The computer used in this work has an Intel Core i5-3570 processor of 3.40 GHz and

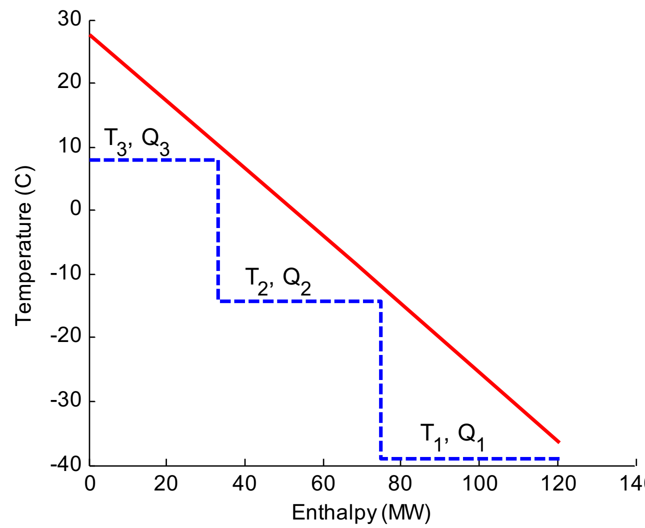

Fig. 7. Balanced grand composite curve for Example 1.

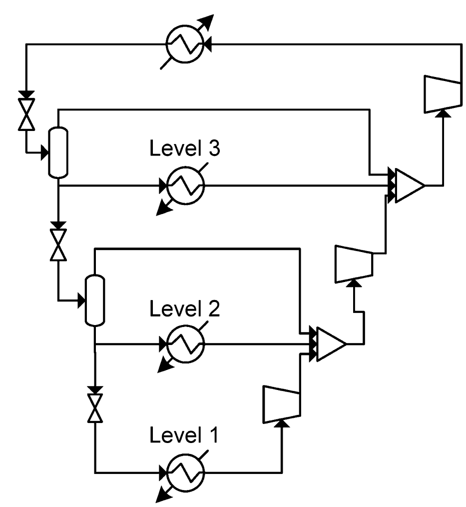

Fig. 8. Flowsheet configuration for Example 1.

Table 3
Example 1 base case simulation results.

		Design	Model	Aspen plus	Difference[c]
Level 1	Molar flow rate (kmol/s)	2.839	2.839[a]	2.839[b]	–
	Rotational speed (rpm)	3160	3160[a]	3160[b]	–
	Discharge pressure (bar)	2.98	2.96	2.98	0.01 bar
	Total shaft work (MW)	6.72	6.71	6.71	0%
	Evaporation temperature (°C)	−39.1	−39.1[a]	−39.1[b]	0.0 °C
	Cooling duty (MW)	45.79	45.83	45.52	−0.7%
Level 2	Molar flow rate (kmol/s)	3.248	3.248[a]	3.248[b]	–
	Rotational speed (rpm)	3,160	3,160[a]	3,160[b]	–
	Discharge pressure (bar)	5.99	5.93	6.00	0.06 bar
	Total shaft work (MW)	11.36	11.33	11.37	0.3%
	Evaporation temperature (°C)	−14.4	−14.5	−14.4	0.1 °C
	Cooling duty (MW)	41.87	42.04	41.63	−1%
Level 3	Molar flow rate (kmol/s)	4.146	4.146[a]	4.146[b]	–
	Rotational speed (rpm)	3,160	3,160[a]	3,160[b]	–
	Discharge pressure (bar)	12.21	12.00	12.21	0.22 bar
	Total shaft work (MW)	19.91	19.82	19.93	1%
	Evaporation temperature (°C)	7.9	7.6	7.9	0.4 °C
	Cooling duty (MW)	33.11	33.76	33.11	−2%
	Total shaft work (MW)	37.99	37.87	38.01	0.4%

[a] Denotes inputs to the model.
[b] Denotes inputs to Aspen Plus simulation.
[c] Difference between the results of the proposed model and those of Aspen Plus.

Table 4
Example 1 base case optimisation results.

		Base case	Optimised case		Difference[c]
			Model	Aspen Plus	
Level 1	Molar flow rate (kmol/s)	2.839	2.702	2.702[b]	–
	Rotational speed (rpm)	3160	3039	3039[b]	–
	Discharge pressure (bar)	2.98	2.99	3.00	0.01 bar
	Total shaft work (MW)	6.72	6.05	6.04	−0.2%
	Evaporation temperature (°C)	−39.1	−37.9[a]	−37.9[b]	0.0 °C
	Cooling duty (MW)	45.79	43.71	43.45	−0.6%
Level 2	Molar flow rate (kmol/s)	3.248	3.287	3.287[b]	–
	Rotational speed (rpm)	3160	3164	3164[b]	–
	Discharge pressure (bar)	5.99	6.08	6.05	−0.03 bar
	Total shaft work (MW)	11.36	11.31	11.30	−0.1%
	Evaporation temperature (°C)	−14.4	−14.2[a]	−14.2	0.1 °C
	Cooling duty (MW)	41.87	42.51	42.45	−0.1%
Level 3	Molar flow rate (kmol/s)	4.146	4.198	4.198[b]	–
	Rotational speed (rpm)	3160	3126	3126[b]	–
	Discharge pressure (bar)	12.21	12.21[a]	12.17	−0.04 bar
	Total shaft work (MW)	19.91	19.40	19.44	0.2%
	Evaporation temperature (°C)	7.9	8.4[a]	8.2	−0.2 °C
	Cooling duty (MW)	33.11	34.55	34.50	−0.1%
	Total shaft work (MW)	37.99	36.76	36.77	0.0%
	Savings relative to base case (%)	–	3	3	–
	ΔT_{min} (°C)	5.0	2.5	2.2	−0.3 °C

[a] Denotes inputs to the model.
[b] Denotes inputs to Aspen Plus simulation.
[c] Difference between the results of the proposed model and those of Aspen Plus.

8.00 GB of RAM memory. On average, the evaluation of the objective function and constraints of the 2000 points takes 0.6 s.

5.1.1. Comparison of the proposed model vs. a rigorous simulation software

Due to the lack of real operational data against which to compare the results of the proposed model, the results found by a rigorous simulation software are assumed to be an accurate description of the real cycle and used for comparison purposes (i.e. test the accuracy of the results of the proposed model). So, in order to compare the results of the model proposed in this work, the base case (design cooling demand) is simulated in Aspen Plus and its results are compared against those given by the proposed model in Table 3. In addition, Table 3 also presents the design operating conditions.

In the Aspen Plus simulation, where the Peng–Robinson equation of state is used for modelling the physical properties, the inputs are the refrigerant flow rates, pressure levels and rotational speed of compressors; the outputs are the cooling duty and shaft work consumption of each cooling level. The polynomial regressions from the performance curves are found by reading from these curves the head developed, and its respective efficiency, for a series of inlet flow rates at a given rotational speed (i.e. head as a function of flow rate and efficiency as a function of flow rate), where each rotational speed has its own regressions. The proposed model and Aspen Plus use the information from each of the performance curves of the compressors in the form of a third degree polynomial, as this is the form that is normally used. The information regarding the performance curves used and their regression can be seen in Tables S16–S21 (see Supplementary Information). Table 3 shows good agreement between the results of the proposed model and those of Aspen Plus, where the difference between the results is only 0.4% of the total shaft work demand.

If the results from the proposed model were to be compared against real operational data, then the operational data has to be pre-processed, i.e. cleaned and reduced, as in the work of Hasan et al. (2009a). In data cleaning, missing values are filled, noisy data are smoothed and outliers are identified (Han et al., 2011, Ch. 3). Data reduction is used to decrease the volume of the data set without altering the analytical results (Han et al., 2011, Ch. 3). The data can be reduced by organising it in clusters, so that 'similar' data are grouped and separated from other groups of data. One way of clustering data is by minimising the 'distance' between the data points in a given cluster.

5.1.2. Optimisation of operating conditions for Example 1

To illustrate the use of the proposed optimisation approach, the base case operating conditions are firstly optimised and then two scenarios are addressed: (1) the cooling duty of the process is reduced to 95% of the base case cooling duty; (2) the cooling duty is increased to 105%. The two scenarios are presented to show the complex interaction between the variables in a multilevel refrigeration cycle, and to account for plausible operational changes in an existing plant: a decrease in the production rate of the plant or an increase, respectively. For scenarios 1 and 2, the new base cases are found by assuming the same evaporation temperatures of the design and varying the refrigerant flow rates and rotational speed of the compressors to satisfy the required cooling demand.

The optimisation results for the base case can be seen in Table 4, while the optimisation results for scenario 1 can be seen in Table 5 and for scenario 2 in Table 6. In addition, the results obtained from the proposed optimisation approach are compared with those of Aspen Plus. The behaviour of the objective function during optimisation, for each case, can be seen in Figs. S4–S6 (see Supplementary Information).

The results in Table 4 show that the results from the proposed model are in good agreement with the results from a rigorous simulation software, the maximum difference between the results being 2%. The few differences found (e.g. cooling duties, discharge pressures) could be due to differences between the part-load performance model of compressors used in the present work (described in Section 4.1) and the one used by Aspen Plus (Aspen Technology Inc, 2013b). For the optimised base case shown in Table 4, the reduction in shaft work demand is around 3%.

The savings arise mainly from the smaller ΔT_{min}, which was reduced from 5 °C in the base case to 2.5 °C by optimisation. In addition, the cooling duty of the evaporator of Level 1 is reduced, as is its refrigerant flow rate, while the cooling duties of the evaporators and refrigerant flow rates of Level 2 and Level 3 are increased to

Table 5
Example 1 scenario 1 optimisation results.

		Base case	Optimised case		Difference[c]
			Model	Aspen Plus	
Level 1	Molar flow rate (kmol/s)	2.697	2.585	2.585[b]	–
	Rotational speed (rpm)	3137	3029	3029[b]	–
	Discharge pressure (bar)	2.98	3.01	3.02	0.01 bar
	Total shaft work (MW)	6.38	5.82	5.82	0.0%
	Evaporation temperature (°C)	−39.1	−37.9[a]	−37.9	0.0 °C
	Cooling duty (MW)	43.50	41.77	41.53	−0.6%
Level 2	Molar flow rate (kmol/s)	3.086	2.987	2.987[b]	–
	Rotational speed (rpm)	3,136	3,071	3,071[b]	–
	Discharge pressure (bar)	5.99	5.95	5.99	0.03 bar
	Total shaft work (MW)	10.78	10.10	10.09	−0.1%
	Evaporation temperature (°C)	−14.4	−14.1[a]	−14.0	0.1 °C
	Cooling duty (MW)	39.78	38.83	38.54	−0.7%
Level 3	Molar flow rate (kmol/s)	3.939	4.107	4.107[b]	–
	Rotational speed (rpm)	3136	3141	3141[b]	–
	Discharge pressure (bar)	12.21	12.21[a]	12.33	0.12 bar
	Total shaft work (MW)	18.90	18.91	18.97	0.3%
	Evaporation temperature (°C)	7.9	7.7	7.9	0.2 °C
	Cooling duty (MW)	31.46	34.14[a]	33.72	−1%
	Total shaft work (MW)	36.06	34.83	34.88	0.1%
	Savings relative to base case (%)	–	3	3	–
	ΔT_{min} (°C)	5.0	2.5	2.3	−0.2 °C

[a] Denotes inputs to the model.
[b] Denotes inputs to Aspen Plus simulation.
[c] Difference between the results of the proposed model and those of Aspen Plus.

Table 6
Example 1 scenario 2 optimisation results.

		Base case	Optimised case		Difference[c]
			Model	Aspen Plus	
Level 1	Molar flow rate (kmol/s)	2.981	2.783	2.783[b]	–
	Rotational speed (rpm)	3198	3033	3033[b]	–
	Discharge pressure (bar)	2.98	2.95	2.96	0.01 bar
	Total shaft work (MW)	7.16	6.14	6.13	−0.2%
	Evaporation temperature (°C)	−39.1	−37.9[a]	−37.9	0.0 °C
	Cooling duty (MW)	48.08	45.13	44.87	−0.6%
Level 2	Molar flow rate (kmol/s)	3.410	3.260	3.260[b]	–
	Rotational speed (rpm)	3,200	3,133	3,133[b]	–
	Discharge pressure (bar)	5.99	5.85	5.90	0.05 bar
	Total shaft work (MW)	12.12	11.02	11.07	0.5%
	Evaporation temperature (°C)	−14.4	−14.6[a]	−14.6	0.1 °C
	Cooling duty (MW)	43.96	42.66	42.32	−0.8%
Level 3	Molar flow rate (kmol/s)	4.354	4.655	4.655[b]	–
	Rotational speed (rpm)	3200	3265	3265[b]	–
	Discharge pressure (bar)	12.21	12.21[a]	12.51	0.30 bar
	Total shaft work (MW)	21.27	21.58	22.14	3%
	Evaporation temperature (°C)	7.9	7.1[a]	7.3	0.2 °C
	Cooling duty (MW)	34.77	39.01	37.70	−3%
	Total shaft work (MW)	40.55	38.74	39.34	2%
	Savings relative to base case (%)	–	4	3	–
	ΔT_{min} (°C)	5.0	2.5	2.2	−0.3

[a] Denotes inputs to the model.
[b] Denotes inputs to Aspen Plus simulation.
[c] Difference between the results of the proposed model and those of Aspen Plus.

satisfy the total cooling demand. Once the pressure ratio is determined, the rotational speed of compressors is then adjusted to meet the required pressure ratios. It is worth mentioning that for the present example, all the compressors were considered to be on independent shafts, i.e. each compressor has its own driver, which gives the system flexibility. A more restricted system, where all compressors are placed on the same shaft, can be evaluated by adding the necessary constraints into the model.

As mentioned in Section 4.2, the relation between the refrigerant flow rates and the rotational speed of compressors makes the optimisation problem complex. From Table 5 it can be seen that, for scenario 1 (95% of base case cooling demand), the shaft work demand of Level 3 is the same as that in the base case; this is due to the higher pressure ratio of the compressor. However, the overall shaft work reduction is achieved by reducing ΔT_{min}, refrigerant flow rates and rotational speeds of the compressors of Level 1 and Level 2. So, a 5% cooling load reduction results in 3% shaft work savings, compared to its base case.

For scenario 2 (105% of base case cooling demand), the cooling duties and refrigerant flow rates of Level 1 and Level 2 are reduced compared to the base case, as seen in Table 6. Because of these changes, the refrigerant flow rate and cooling duty of Level 3 are increased to satisfy the total cooling demand. So, a 5% cooling duty increase results in 4% shaft work savings, compared against its base case. These savings in shaft work demand are due to the optimally distributed cooling loads and evaporation temperatures, and the reduced $\Delta T_{\min}$. The main differences found between the results of proposed methodology and those of Aspen Plus are due to the different way the compressors are modelled. Given that the discharge temperatures and pressures of the compressors are different, the heat balances around the rest of the units in the refrigeration cycle are also affected. However, these differences are small for most of the parameters and, as also seen in Table 6, the difference in the total shaft work demand (2%) is less than the savings achieved (4%).

One of the advantages of using the optimisation approach proposed in this work is that changes to the operating conditions of the process (e.g. changes in flow rate) can be readily incorporated and evaluated; this capability has not been addressed by any other published work. Additionally, the hybrid optimisation methodology used in the proposed approach finds an approximation to a globally optimal solution. It is not possible to use this kind of optimisation methodology within rigorous simulation software.

Although the optimisation of the operating conditions of the base case and two scenarios is able to improve the shaft work demand of the refrigeration cycle, the savings achieved are relatively low. These low savings are a consequence of the constrained nature of the problem, which arises mainly from the operating compressors (allowable flow rate limits), the complex interactions between the variables and good design operating conditions.

5.2. Example 2: ethylene cold-end process

The cold-end process of an ethylene recovery plant comprises a refrigeration cycle that interacts with the separation process through the HEN. Due to space limitations the discussion and results of this example are presented in Section S1 of the Supplementary Information.

5.3. Summary of examples

The examples presented in this section show that the achievable savings in the operating conditions of refrigeration cycles, depend in great measure on the cycle configuration and in the capacity of the compressors to operate at different operating conditions without operational problems (e.g. operation beyond the surge or choke limit). In the case of Example 2, greater savings are achieved, compared to Example 1, for the case when the process throughput is increased by 5%. This better performance of Example 2 is mainly due to the fact that the cascade refrigeration cycle has more variables than the multilevel cycle, increasing the solution space.

Although 3% savings could be considered a small amount, if the electricity price to run the compressors is 0.082 £/kWh (U.K. Department of Energy & Climate Change, 2014) and considering that the average saving for all the scenarios is 1.22 MW, then annual savings of £0.86 million could be achieved if the suggested changes were implemented. Greater savings could be achieved if new equipment could be installed. However, the present work only optimised the operating conditions considering the limitations of the existing equipment.

6. Conclusions

A new approach has been proposed for modelling centrifugal compressors that are used in refrigeration cycles of cryogenic processes, and for optimising multilevel and cascade refrigeration cycles that make use of these compressors. The proposed model predicts the part-load performance of compressors by making use of performance curves provided by the manufacturers and the fan laws, together with details of the operating conditions of the refrigeration cycle.

Because of the complex interactions between the variables in the refrigeration cycle, different sets of operating conditions of the refrigeration cycle can achieve the same cooling duty and demand different amounts of shaft work. The new optimisation model finds an optimal set of operating conditions of the refrigeration cycle (for a given process cooling duty), taking into consideration the operational limits of the compressors, and minimising the shaft work demand. The optimisation approach combines the use of a scatter search algorithm, together with a gradient-based NLP solver, to find an approximation to a global minimum solution and avoid getting trapped in local optima. In addition, the new optimisation model is able to readily incorporate changes to the operating conditions of the process (e.g. changes in the supply temperatures, throughput) by using the GCC.

The benefits of using the new optimisation approach are illustrated using two different examples: one for a multilevel refrigeration cycle and one for a cascade refrigeration cycle. The results show that the achievable savings depend on the complexity of the cycle configuration (e.g. number of cooling levels, number of compressors' drivers), the complex interaction between the variables and the design operating conditions. In addition, the results also show that around 3% savings can be achieved by just changing the operating conditions and without having to invest in new equipment.

Although the present work is able to address the operational optimisation of refrigeration cycles considering operational variables (e.g. rotational speed of the compressors) and constraints (e.g. surge and choke limits) that had not been taken into account in other published works, the scope of the present work is limited as it does not include the simulation of heat exchangers and their corresponding constraints (e.g. temperature crosses along the exchanger length), the use of mixed refrigerants and other cycle configurations. Future work should address these subjects and be included in the optimisation approach.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compchemeng.2015.11.006.

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