Simultaneous Refrigeration Cycle Synthesis and Refrigerant Selection

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Abstract

This paper proposes a unified framework for the simultaneous synthesis of refrigeration system topologies and selection of refrigerants to seamlessly match a set of process cooling requirements. An optimization-based approach is described that simultaneously selects refrigerants and synthesizes refrigeration structures by minimizing a weighted sum of investment and operating costs. The proposed description is a superstructure representation which considers the majority of refrigeration cycle features encountered in complex multistage refrigeration cycles. A novel theoretical treatment of modeling representations and algorithmic improvements is introduced. Results for examples involving multiple refrigerants, cooling loads are obtained. Complex, non-intuitive topologies typically emerge as the optimal refrigeration configurations. These configurations are better than the ones obtained when the optimal refrigeration topology is determined after refrigerant selection is finalized.

Background and Objectives

Refrigeration systems in chemical process plants are complex, energy and capital intensive utility systems which remove heat from low temperature process streams and reject it to process streams at higher temperature or cooling water at the expense of mechanical work. Most research work in refrigeration systems addresses the refrigeration cycle synthesis problem in isolation of the refrigerant selection. In this work we show that significant cost reductions can be realized by encompassing both objectives within the same unified framework. A simple vapor compression refrigeration cycle consists of a sequence of evaporation, compression, condensation, and expansion steps. In most cases, refrigeration needs arise simultaneously for multiple cooling loads at different temperature ranges. This necessitates the need for staged refrigeration cycles with multiple compressors and evaporators to meet the cooling loads. This complexity of the topology of refrigeration cycles and the diversity in the selection of refrigerant molecules coupled with the high investment and energy intensive nature of refrigeration cycles motivates the need for the development of systematic procedures for the efficient synthesis of refrigeration cycles.

Notable contributions to the refrigeration synthesis problem include the work of (Barnes and King, 1974; Cheng and Mah, 1980; Townsend and Linnhoff, 1983; Shelton and Grossmann, 1986; Colmenares and Seider, 1989; Swaney, 1989). A detailed literature overview is provided in (Vaidyaraman and Maranas, 1999). Research results so far indicate that minimum cost refrigeration systems typically involve complex, counter-intuitive topologies. This complexity is not an artifact of the employed modeling features and solution methods. Patented refrigeration configurations share the same complexities. The need to replace CFC refrigerants with environmentally benign ones of comparable performance has also sparked research efforts on the molecular design of refrigerant molecules (Joback and Stephanopoulos, 1989; Gani *et al.*, 1991; Duvedi and Achenie, 1996).

Nevertheless, the present state of the art involves a gap between the refrigeration cycle synthesis and the refrigerant design or even selection problem. This work attempts to narrow this gap by considering a simplified version of the problem. Instead of designing refrigerant molecules

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(see above paragraph), the best refrigerants are selected from a prespecified list of candidate refrigerants and at the same time the refrigeration topology is designed. The starting point of our developments is the generalized network representation of Shelton and Grossmann (1986). This superstructure representation is extended to account for more elaborate refrigeration features and allow the automatic selection of refrigerants from a list of available ones.

Problem Definition

The problem addressed in this work is described as follows:

Given a set of process cooling loads, heat sinks at different temperatures and a set of available refrigerants, find the refrigeration cycle topology, operating conditions and refrigerants that optimize a weighted sum of the investment and operating costs for the refrigeration system.

The proposed model involves a superstructure representation for both the synthesis and the refrigerant selection problems. The model allows for the identification of the number of stages, their operating temperature ranges, the type of refrigerant participating in a stage, the temperature where a switch between two refrigerants occurs, the use of economizers, presaturators or heat exchangers between intermediate stages. The objective to be optimized considers both investment and operating costs.

Specifically, the model accounts for vapor compression cycles with only pure refrigerants. The condenser outlet is assumed to be saturated liquid and the evaporator outlet saturated vapor. Expansion valves are treated as isoenthalpic and the refrigerant vapor heat capacities are assumed to remain constant within a simple compression cycle but they may change value for different cycles. Liquid heat capacities and heats of vaporization can be explicitly treated as temperature dependent. Refrigerant switches are allowed only in the direction of decreased volatility. Compressor investment cost is described with a fixed-charge term and a variable term linearly related to work input. These costing parameters are assumed to be dependent only on the compressor suction-side temperature and independent of the compression ratio. A discussion and justification of these modeling features and assumptions can be found in (Vaidyaraman and Maranas, 1999).

A *multistage refrigeration system* is a series-parallel combination of simple vapor compression cycles (simple cycles or stages). A heat exchanger is used only when heat is removed from a process stream or if a simple cycle rejects heat to another simple cycle involving a different refrigerant. If the same refrigerant operates between two adjacent simple cycles then a presaturator or an economizer is used instead. The temperature at which the (pure) refrigerant in a simple cycle evaporates or condenses is referred to as a *temperature level.* The refrigerants used in a refrigeration system are constrained by the temperature range over which they can operate. This range of temperatures is referred to as the *allowable operating temperature range* of the refrigerant.

Superstructure Description

A superstructure-based model is proposed whose optimal solution directly answers which refrigerants will operate in the refrigeration system, how many stages are needed and whether a presaturator, economizer or a combination is utilized at a particular temperature level. This superstructure superimposes all feasible and allowable refrigeration configurations and refrigerants. The superstructure description defines a hierarchy where at the top the refrigerants which may participate in the system are prepostulated. For each such refrigerant, all possible refrigeration stages (i.e., number of levels and operating temperatures) are postulated. Finally for each stage (temperature level) all possible configurations (topologies) involving heat exchangers, economizers and/or presaturators are constructed. Instead of treating the stage temperatures as variables (Colmenares and Seider, 1989), a discretization of the temperature scale of each allowed refrigerant (Shelton and Grossmann, 1986) which provides candidate temperature levels for refrigeration stages is employed. Energy flow between two different temperature levels operating with the same refrigerant defines a

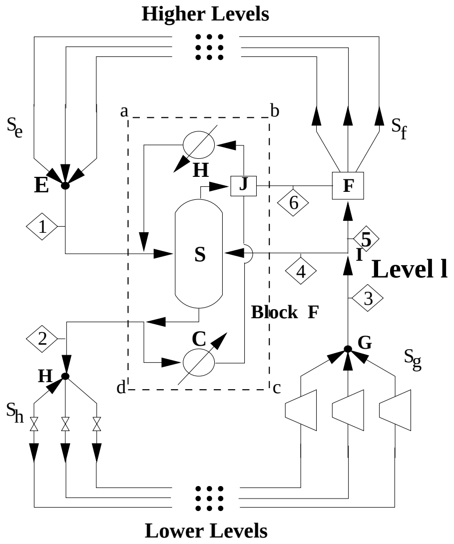


Figure 1: Single level l refrigeration superstructure

simple cycle. Also energy from a temperature level of one refrigerant can be rejected to a temperature level of another refrigerant at a lower temperature. This accounts for all possible energy flow patterns in the refrigeration system. The advantage of this approach is that nonlinearities resulting from treating temperatures as variables are avoided. The disadvantage is that a fine temperature discretization is needed to ensure that no good solutions are overlooked due to coarseness of the discretization.

A convenient way to represent the allowed energy flows in the system is through a network representation $\mathcal{G}(\mathcal{L}, \mathcal{A})$. Node set $\mathcal{L} = \{l\}$ contains all the candidate temperature levels in the refrigeration system. Arc-set $\mathcal{A} = \{(l, m)\}$ denotes the set of all possible energy flows between any two temperature intervals. This set is further partitioned into subset $\mathcal{A}_i$ which is the set of all energy flows forming a simple cycle, and $\mathcal{A}_e$ which is the set of all energy flows representing energy transfer to or from a process stream or denoting a switch between refrigerants.

The superstructure representation of a single temperature level is shown in Figure 1. This figure pictorially illustrates the superimposition of all possible process choices for node l in the network $\mathcal{G}(\mathcal{L}, \mathcal{A})$. The entire refrigeration system is thus composed of a cascade of single level superstructures linked through energy and mass flows. Level $l \in \mathcal{L}$, shown in Figure 1, superimposes heat exchanger C which accepts energy from other refrigerants/process streams, heat exchanger H which rejects heat to other refrigerants/process streams and the vapor-liquid (V-L) separator S along with all the necessary mass and energy flows. The streams constituting sets S_e and S_f correspond to arcs $(l, m) \in \mathcal{A}_i$ forming simple cycles between l and m. Similarly, the sets S_h and S_g correspond to arcs $(m, l) \in \mathcal{A}_i$ forming cycles between m and l. Other streams include stream 4 which enters into the V-L separator and stream 5 which bypasses the V-L separator. Block J is a junction which represents a mixing or a splitting point. Block F is a superstructure representation of the splitting and mixing of streams 5 and 6 as they form the streams of set S_f. This superstructure representation is utilized within an optimization framework to solve for the optimal values of the energy flows in the network.

Model Formulation

A detailed analysis and derivation of the modeling equations describing the superstructure is provided in (Vaidyaraman and Maranas, 1999). These modeling equations involve nonlinearities in the form of flowrate/enthalpy products. This adversely affects solution tractability and prohibits the setting of optimality guarantees. We remedy this shortcoming by *recasting the problem so that nonlinearities appear only within a single nonlinear constraint set and then identify conditions un-*

der which this nonlinear constraint set is redundant at the optimal solution. This is accomplished by projecting the feasible region of the original modeling equations onto the reduced space of a set of key variables. These key variables include refrigerant flowrates μ_{lm} within simple cycles operating between levels l and m, energy flows D_{lm}, and work input W_{lm} to a simple cycle. This set of variables unambiguously describes the energy flow interactions of a given level with the entire refrigeration superstructure. This projection reduces the total number of variables but more importantly, after careful manipulation, "aggregates" all nonlinearities into a single constraint set in formulation (P). A detailed description of the sets, parameters and variables can be found in (Vaidyaraman and Maranas, 1999).

$$\min \; z = \sum_{(l,m)\in\mathcal{A}_i} \left[C_f y_{lm} + (C_v + C_e) W_{lm}\right]$$

subject to (P)

$$\begin{aligned} &\sum_{m:(m,l)\in\mathcal{A}_i} (D_{ml} + W_{ml}) + \sum_{m:(m,l)\in\mathcal{A}_e} D_{ml} \\ = &\sum_{m:(l,m)\in\mathcal{A}_i} D_{lm} + \sum_{m:(l,m)\in\mathcal{A}_e} D_{lm}, \;\; \forall\, l \in \mathcal{L}^{int} \end{aligned} \tag{1}$$

$$\begin{aligned} &\sum_{m:(l,m)\in\mathcal{A}_i} \mu_{lm}[\Delta H_l^{vap} - c_{pl}^{liq}(T_m - T_l)] + \sum_{m:(l,m)\in\mathcal{A}_e} D_{lm} \\ \geq &\sum_{m:(m,l)\in\mathcal{A}_i} \mu_{ml}\Delta H_l^{vap} + \sum_{m:(m,l)\in\mathcal{A}_e} D_{ml}, \;\; \forall\, l \in \mathcal{L}^{int} \end{aligned} \tag{2}$$

$$\frac{\sum\limits_{m:(m,l)\in\mathcal{A}_i} (D_{ml} + W_{ml})}{\sum\limits_{m:(m,l)\in\mathcal{A}_i} \mu_{ml}} \geq \frac{D_{lm}}{\mu_{lm}} + c_{pl}^{liq}(T_m - T_l), \;\; \forall \;\; (l,m) \in \mathcal{A}_i \tag{3}$$

$$D_{lm} \;\geq\; \mu_{lm}[\Delta H_l^{vap} - c_{pl}^{liq}(T_m - T_l)], \;\; \forall\, (l,m) \in \mathcal{A}_i \tag{4}$$

$$W_{lm} \;=\; \left(\frac{WC_{lm}}{c_{pl}^{vap}}\right)\left[D_{lm} - \mu_{lm}(\Delta H_l^{vap} - c_{pl}^{liq}(T_m - T_l) - c_{pl}^{vap} T_l)\right], \;\; \forall\, (l,m) \in \mathcal{A}_i \tag{5}$$

$$Q_l^{load} \;=\; \sum_{m:(l,m)\in\mathcal{A}_e} D_{lm}, \;\; \forall\, l \in \mathcal{L}^{load} \tag{6}$$

$$Q_l^{sink} \;=\; \sum_{m:(m,l)\in\mathcal{A}_e} D_{ml}, \;\; \forall\, l \in \mathcal{L}^{sink} \tag{7}$$

$$D_{lm} \;\leq\; D_{lm}^{U} y_{lm}, \;\; \forall\, (l,m) \in \mathcal{A}_i \tag{8}$$

$$\sum_{m:(m,l)\in\mathcal{A}_e} D_{ml} \;\leq\; \sum_{m:(l,m)\in\mathcal{A}_i} D_{lm}, \quad \sum_{m:(l,m)\in\mathcal{A}_e} D_{lm} \;\leq\; \sum_{m:(m,l)\in\mathcal{A}_i} (D_{ml} + W_{ml}) \;\; \forall \;\; l \in \mathcal{L}' \tag{9}$$

$$D_{lm}, W_{lm}, \mu_{lm} \;\geq\; 0, \;\; y_{lm} \in \{0,1\} \tag{10}$$

The objective function is composed of the sum of the compressor investment and operating costs. Constraint set 1 is the overall energy balance for a given level. Constraint set 2 describes the energy balance around area abcd shown in Figure 1. The nonconvex constraint set 3 maintains consistency of the mass and energy balances at the mixing block F. The refrigerant stream operating in a cycle between levels l and m is formed by mixing portion of the superheated vapor stream 5 with part of the saturated vapor stream 6. The nonconvex constraint ensures that the resulting stream from this mixing (belonging to set S_f) is less superheated than stream 5. Inequality 4 ensures that the compressor inlet is either saturated or superheated vapor. Constraint 5 relates compression work to energy flows, temperature levels and refrigerant mass flows. Constraint 6 ensures that the refrigeration system satisfies the cooling loads required by the process streams. Constraint 7 maintains that the energy requirements for process streams to be heated are satisfied by the refrigeration system. Logical constraint set 8 sets the energy flow in a simple cycle to zero if the cycle does not exist. Constraints 9 ensure that consecutive refrigerant switches without a compression cycle operating between them are do not occur. Finally, constraint 10 imposes a nonnegativity restriction on the variables and declares y_{lm} as binary.

Formulation (P) corresponds to a nonconvex MINLP. Nevertheless, all nonlinear terms are "isolated" within a single constraint set (3). In (Vaidyaraman and Maranas, 1999), it is shown that if at least one of the following two properties hold at the optimal solution of the MILP then constraint set 3 is redundant and thus can be eliminated.

Property 1: *The destination of all energy flows emanating from level l is a single level located higher in the refrigeration structure.*

Property 2: *The optimal solution of formulation P does not include any economizers.*

A sufficient condition for satisfying Properties 1 and 2 is that they are no economizers and a single heat sink in the refrigeration topology.

Additional modeling improvements aiming at tractability, such as replacement of level-to-level binary variables y_{lm} with much fewer level-activation binary variables z_l, a priori selection between a presaturator or economizer, and identification of tight bounds on the energy flows have been explored (see (Vaidyaraman and Maranas, 1999) for details).

Example

This example explores the use of the proposed methodology for synthesizing optimal refrigeration systems when multiple loads are present and refrigerants are selected from an extensive list. The objective here is to refrigerate four process streams whose temperatures and cooling loads are given in Figure 2a. The refrigerants are grouped together in blocks of decreasing volatility as shown in Figure 2b. Four different levels of discretization (i.e., 8K, 4K, 2K, and 1K) are considered to study the effect of discretization on the trade off between accuracy versus computational requirements. Finer discretizations, as expected, by providing more choices for intermediate levels result in improved objective function values. However, this improvement comes at the expense of a significant increase in the CPU requirements (see Table 1).

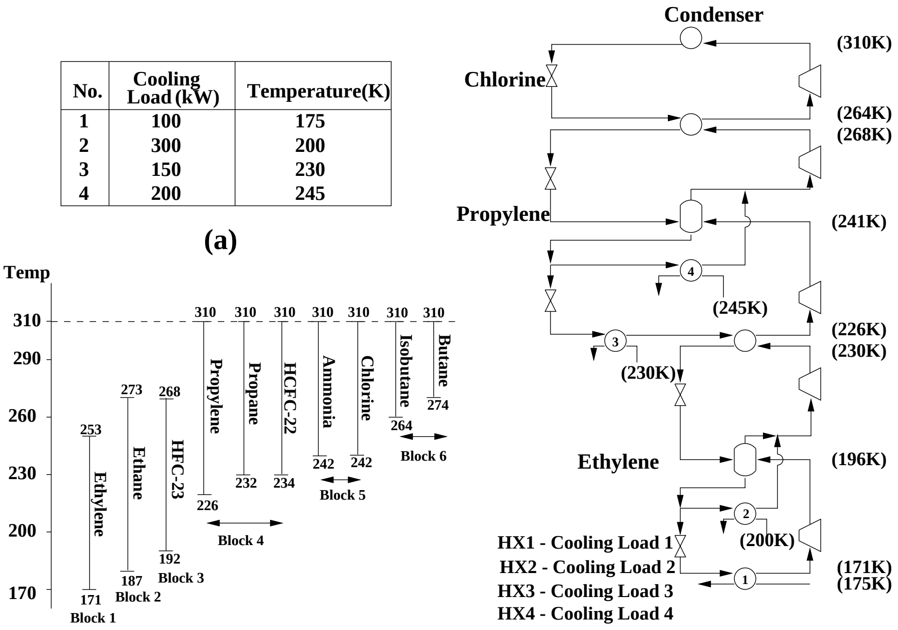
Table 1: Computational performance for different discretizations

No.	Total levels	Cost (\$/yr)	Relative Gap (%)	CPU (sec)
8K	96	1200084	0.98	8.33
4K	187	996528	0.92	18.23
2K	364	984187	1.00	796.91
1K	714	982448	5.12	10^4

The refrigeration system topologies for all four discretization schemes involve 5 stages and refrigerants ethylene, propylene and chlorine operating with only presaturators (see Figure 2c for the 1K solution). Note that even though ten refrigerants can potentially participate in the system, the optimal solution involves only three refrigerants. The topology of the refrigeration system for the 8K case is considerably different than that of the 4K case. In contrast, the topology for the 4K case is identical with that of the 2K case with only minor differences in the location of the intermediate levels. This and other examples (Vaidyaraman and Maranas, 1999) have revealed that complex, non-intuitive optimal topologies could be generated by the proposed methodology better than the ones obtained after heuristic-based refrigerant selection (Cheng and Mah, 1980).

Summary

A systematic methodology for finding the optimal refrigeration cycle topology incorporating refrigerant selection was proposed. The optimization formulation obtained was a nonconvex MINLP. Based on a variable projection technique all nonlinear terms were isolated within a single constraint set. Theoretical and modeling improvements were also proposed aimed at improving tractability. The approach was illustrated with one example problem involving selection of refrigerants and refrigeration system synthesis to meet multiple cooling loads at different temperatures. Currently,



No.	Cooling Load (kW)	Temperature(K)
1	100	175
2	300	200
3	150	230
4	200	245

(a) (b) (c)

Figure 2: Cooling loads and refrigeration temperatures, refrigerant operating ranges, and minimum cost refrigeration structure for 1K discretization

we are exploring decomposition approaches for solving problems with very fine discretizations and modeling extensions to account for refrigerant mixtures and group contribution based property prediction.

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