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Framework for Work-Heat Exchange Network Synthesis

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Chemical industries consume most of the energy for heating and compression needs. This energy can be saved by synergizing the work and heat requirements of the processes. In this work, we propose a generalized framework for handling both heat and work integration simultaneously. A mixed-integer nonlinear programming (MINLP) model is developed for work-heat exchange network synthesis (WHENS). Stage-wise superstructure with fixed number of splits and isothermal mixing is used for heat integration. Work integration involves turbines and compressors on single shaft turbine compressor (SSTC). In this work, the individual streams are not classified as high or low-pressure streams. Hence, pressure changing streams can undergo either compression in compressor or expansion in turbine or valve depending upon the process needs and specified target operating conditions. Also, the pressure changing stream are not classified as hot or cold stream a priori in the heat integration. This provides more flexibility and generalization for work-heat integration. Starting with a set of streams with known inlet flows, temperatures and pressures, the network can be synthesized for any desired objective. The model can also handle unknown exit temperatures of some streams. Finally, we illustrate the applicability of this framework on a natural gas liquefaction process.

1. Introduction

Chemical industries are one of the largest industrial energy consumer. Most of this energy is used for compression and heating purposes. Furthermore, expensive cold utilities are used in cryogenic processes, such as liquefaction of natural gas. Considerable energy savings can be achieved by synergizing the work and heat requirements of the process streams. For example, a low-pressure stream in the process can be compressed and used as a hot utility rather than using an external hot utility. One such application is the vapor compression heat pump which transfers heat from a lower temperature to a higher one (Yang et al., 2014). Also, the compression and expansion requirements can be indirectly combined through a single-shaft-turbine-compressor (SSTC). This reduces the overall utility and power consumption, and hence the annual operating costs. Optimized design of such synergistic systems can be accomplished through work and heat exchange network synthesis (WHENS) with an objective of minimization of overall energy consumption or minimization of total annualized costs.

Wechsung et al. (2011) presented synthesis of heat exchanger networks with adjustment of pressure levels at sub-ambient conditions combining Pinch Analysis, exergy analysis and mathematical programming. Razib et al. (2012) proposed an MINLP formulation for work exchange network (WEN) synthesis of compressor-turbines on single shaft. Fu and Gundersen (2015) studied appropriate placement of compressors and expanders in above ambient processes for heat and work integration. Onishi et al. (2014) developed an MINLP formulation for WHENS with superstructure based optimization method. Later, Huang and Karimi (2016) presented a more efficient model for WHENS that considers constant pressure streams and allows optimized selection of end-heaters and coolers. We have improvised this model to consider broader number of streams. The streams are not classified as high or low-pressure streams and the stream can either undergo expansion or compression as per process needs. The same stream can undergo compression in one stage and expansion in the subsequent stage. It will depend upon the available utilities, energy demand and costs associated with it. Similarly, the pressure-changing streams are not classified as hot or cold a priori in heat integration. This provides a generalised framework for work-heat exchange network synthesis.

2. Problem statement

Consider a set of S streams $(s = 1, 2..., S)$ with flow F_s, inlet pressure PIN_s, and inlet temperature TIN_s for work-heat exchange network synthesis (WHENS). Either the temperature or both pressure and temperature of the stream should be changed. Let $POUT_s$ represent the known final pressure of the stream s. Exit temperatures of the stream may be known or unknown. Let $TOUT_s$ represent known final target temperatures of stream s. There are utilities available in case the streams are not able to meet the final specified conditions through heat and work exchange. The inlet and outlet temperatures of the utilities are known.
Given this set of streams with their physico-chemical properties, the objective is to synthesize a work-heat exchange network (WHEN) with minimum energy consumption or minimum total annualized cost (TAC). The assumptions in this WHENS are as follows:

- Process is at steady state.
- No pressure drop and heat loss in heat exchangers
- Only centrifugal pumps, compressors and turbines with known efficiencies are considered.
- All compressions and expansions except through valve are isentropic.
- Expansion through valve is adiabatic and irreversible with known Joule Thomson coefficient.
- Parallel work exchange units are not considered.
- Each gas stream behaves as an ideal gas and remains above its dew point and below their inversion temperatures.
- Known constant film heat transfer coefficient of each stream are considered.
- HEN employs 2-stream counter-current exchangers.

3. Model formulation

3.1 Framework

There are two broad categories of streams in this system; one with same initial and final pressures and the second with different initial and final pressures. Streams are classified as pressure change streams (*PC*) and no-pressure change streams (*NPC*)

$$PC = \{\text{Pressure-Change streams}\} = \{s \mid PIN_s \neq POUT_s\} \tag{1a}$$

$$NPC = \{\text{No-Pressure-Change streams}\} = \{s \mid PIN_s = POUT_s\} \tag{1b}$$

PC streams are further classified as pressure-change liquid (*PCL*) and pressure-change gases (*PCG*). Furthermore, these streams are not classified as high or low-pressure streams. This provides flexibility for a stream to either get expanded or compressed in intermediate stages. *PCL* streams can be considered when liquids require pumps, and their heat transfer properties change with pressure and temperature. Normally, liquids are incompressible and their specific heat capacity does not change considerably with pressure. Hence, liquid pressures are not considered in optimization as they are usually constant and specified by the process. But, in cases, when a liquid stream is pressurized to supercritical fluid via pump, its heat capacity and heat transfer coefficient can change considerably with pressure and temperature. In such cases, the outlet pressure of the pump is considered as an optimization variable.
As proposed by Huang and Karimi (2016), the overall work-heat exchange network (WHEN) will consist of two interconnected networks, the heat exchanger network (HEN) and work exchange network (WEN). HEN will have 2-stream heat exchangers which will bring about temperature change with no pressure change. WEN will consist of single-shaft-compressor-turbine (SSTC) which will bring about both temperature and pressure change. This is because temperature change accompanies pressure change for a stream. Other than the SSTC, there are valves, utility compressors and turbines for pressure change. Valves decrease the pressure of stream adiabatically and irreversibly without producing any useful work. Utility turbines and compressors use external utilities instead of process streams for pressure change.
The WHENS superstructure consists of alternate WEN and HEN configuration. All streams enter HEN whereas only *PC* streams enter WEN. Consider a pressure change stream $s \in PCG$ with K_s pressure changing stages. In the stage $k = 0$, each *PCG* stream will enter HEN at PIN_s, and TIN_s.This stream will be either heated or cooled in the $k = 0$ stage without any work exchange. Certain thermodynamic insights can be incorporated in the model. For example, a stream that should be pressurized in stage $k = 1$ will be cooled in the stage $k = 0$. This will reduce the power requirement in compressors. Similarly, streams that are expanded in $k = 1$ will be heated in stage $k = 0$. After exiting stage 0 at temperature TI_{s0} and pressure PIN_s, it will enter WEN followed by the HEN in stage $k = 1$. Before entering HEN, every *PCG* stream will split into two streams; one hot stream and one cold stream. The identity of this stream as hot or cold can be decided by the preceding WEN, except in stage $k = 0$. For example, if a stream is compressed, its temperature will rise and it will be used as a hot stream. Similarly, if

a stream has been expanded, its temperature will drop and it will be considered as a cold stream. The stream exiting last stage K_s will have flexibility to either use a utility heater or utility cooler in HEN to meet its final temperature requirement.

Each *PCG* stream in a WEN stage can enter a turbine, compressor, valve or bypass the stage. Hence, the WEN superstructure for a stage will have splitter before the stage and mixer after the stage. The splitter will split the streams into six substreams. The first five substreams will enter SSTC compressor, SSTC turbine, utility compressor, utility turbine, valve. The last substream is for bypassing the stage without entering any of the units. The SSTC consists of compressors, turbines, motor, and generator. The motor (generator) is for providing (using) deficit (excess) power. The *PCL* streams will have *M* stages in WEN. In these stages, it will have a chance to use a pump to increase its pressure before taking part in heat exchange. Thus, The HEN will have *NPC* streams, *PCL* streams and $2.(K_s+1).PCG$ streams. The *NPC* and *PCL* streams can be classified as hot and cold streams based on their inlet and outlet temperatures. The HEN superstructure adopted is stage wise superstructure with *L* stages and isothermal mixing (Yee and Grossmann, 1990). However, this HEN synthesis is different from traditional HEN synthesis as the identity and inlet/outlet temperatures of some streams are unknown.

3.2 Work Exchange Network (WEN)

Consider a stream s ∈ PCG. In a WEN stage, there are 6 possibilities for each stream. It can enter utility turbine or compressor, SSTC turbine or compressor or valve or bypass the stage. We define binary for each equipment to indicate whether the substream enters that equipment.

$$ut_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ uses an utility turbine in stage } k \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2a}$$

$$uc_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ uses an utility compressor in stage } k \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2b}$$

$$c_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ uses a SSTC compressor in stage } k \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2c}$$

$$t_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ uses a SSTC turbine in stage } k \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2d}$$

$$v_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ uses a valve in stage } k \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2e}$$

$$y_{sk} = \{ \begin{matrix} 1 & \text{if } s \text{ bypasses WEN stage } k \text{ fully} \\ 0 & \text{otherwise} \end{matrix} \qquad s \in PCG;\ 1 \le k \le K_s \tag{2f}$$

For installing a generator or a helper motor on the SSTC, we define the following binary variables

$$g = \{ \begin{matrix} 1 & \text{if SSTC requires a generator} \\ 0 & \text{otherwise} \end{matrix} \tag{3a}$$

$$h = \{ \begin{matrix} 1 & \text{if SSTC requires a helper motor} \\ 0 & \text{otherwise} \end{matrix} \tag{3b}$$

Parallel work exchange units are not considered. Hence, each stage will have only one equipment. Also, the generator (helper motor) can exist only if the SSTC has at least one turbine (compressor). Let P_{sk} be the pressure of $s \in PC$ leaving its stage *k* in WEN, with $P_{s0} = PIN_s$, $P_{sK_s} = POUT_s$ and pressure limits (P_s^L, P_s^U) for each stream. These pressure limits can be based on the process limitations, equipment limitations or the properties of a stream. If a stream enters a mover, it should undergo a certain minimum pressure change Also, we ensure that pressure of the stream reduces in an expander and valve and the pressure increases in a compressor. Hence, we write the following equations

$$P_s^L \le P_{sk} \le P_s^U \qquad s \in PCG;\ 1 \le k \le K_s \tag{4a}$$

$$P_{sk} + \Delta P_s^{\min}(ut_{sk} + t_{sk} + v_{sk}) \le P_{s(k-1)} + P_s^U(uc_{sk} + c_{sk}) \qquad s \in PCG;\ 1 \le k \le K_s \tag{4b}$$

$$P_{sk} + P_s^U(ut_{sk} + t_{sk} + v_{sk}) \ge P_{s(k-1)} + \Delta P_s^{\min}(uc_{sk} + c_{sk}) \qquad s \in PCG;\ 1 \le k \le K_s \tag{4c}$$

where, ΔP^{min} = minimum pressure change in a mover or valve

As a gaseous stream is compressed or expanded, its temperature changes. This temperature change will depend upon the stream, change in pressure and efficiency of the process. Let TI_{sk} (TO_{sk}) be the temperature of stream $s \in PCG$ entering (exiting) stage *k* in WEN. Then, its exit temperature TM_{sk} from the adiabatic mover and TV_{sk} from the valve in stage *k* is given by,

$$\eta_{sk} = \eta_s(ut_{sk} + t_{sk}) + \frac{1}{\eta_s}(uc_{sk} + c_{sk}) \qquad s \in PCG;\ 1 \le k \le K_s \tag{5a}$$

$$TM_{sk} = TI_{s(k-1)}\left\{1 + \eta_{sk}\left[\left(\frac{P_{sk}}{P_{s(k-1)}}\right)^{(r_s-1)/r_s} - 1\right]\right\} \qquad s \in PCG;\ 1 \le k \le K_s \tag{5b}$$

$$TV_{sk} = TI_{s(k-1)} + \mu_{sk}\left(P_{sk} - P_{s(k-1)}\right) \qquad s \in PCG;\ 1 \le k \le K_s \tag{5c}$$

where, η_s = efficiency of the mover for *s*

r_s = heat capacity ratio (C_{ps}/C_{vs}) of *s*

μ_s =average Joule-Thomson coefficient of *s*.

The heat balance for a stream $s \in PC$ leaving WEN at stage k is given by Eq(6a). The upper and lower temperature limits (T_s^U and T_s^L) are defined for the temperatures of substreams.

$$TO_{sk} = y_{sk}TI_{s(k-1)} + TM_{sk}(ut_{sk} + t_{sk} + uc_{sk} + c_{sk}) + TV_{sk}v_{sk} \qquad s \in PCG;\ 1 \le k \le K_s \tag{6a}$$

$$T_s^L \le TI_{sk},\ TO_{sk},\ TM_{sk}, TV_{sk} \le T_s^U \qquad s \in PCG;\ 1 \le k \le K_s \tag{6b}$$

Consider a stream $s \in PCL$. It enters at temperature TIN_s and pressure PIN_s with exit temperature $TOUT_s$ and pressure $POUT_s$. An equation or piecewise function relating specific heat capacity, pressure and temperature should be provided for such streams. Like an adiabatic mover, the temperature will change in pump though it is not as substantial as in a compressor or turbine. This temperature change can be calculated based upon the properties of stream and efficiency of the pump.

3.3 Heat Exchanger Network (HEN)

For simplicity, the authors assume isothermal mixing in the stagewise superstructure of Huang et al. (2012) and use the resulting model to synthesize our HEN. However, this HENS is different since identity, initial and final temperatures of some streams are unknown. Let $THIN_{sk}$ ($THOUT_{sk}$) denote the temperature of a hot stream entering (exiting) HEN, and F_s be its known total flow. Similarly, $TCIN_{sk}$ ($TCOUT_{sk}$) denote the temperature of a cold stream entering (exiting) HEN, and F_s be its known total flow.

There are three types of streams in HEN. One is $s \in NPC$ which enters HEN at the known temperature TIN_s and leaves at $TOUT_s$. The second is $s \in PCG$ that enters HEN in stage *k* of WHENS at temperature TO_{sk} and leaves at TI_{sk}. And the third is $s \in$ PCL that enters at the temperature TP_{sm} and leaves at $TP_{s(m+1)}$. For $s \in PCG$, it can act as hot stream in some stages and cold stream in some stages. Hence, we split these streams into two parts, one as a hot stream and one as cold stream.

$$TO_{sk} = THIN_{sk} = TCIN_{sk} \qquad s \in PCG;\ 1 \le k \le K_s \tag{7a}$$

$$TI_{sk} + TO_{sk} = THOUT_{sk} + TCOUT_{sk} \qquad s \in PCG;\ 1 \le k \le K_s \tag{7b}$$

Thermodynamic insights can be used to fix the identity of the streams as hot or cold streams. For example, if a stream has been compressed in *k* stage of WEN, then its exit stream temperature will be high and it will be considered as a hot stream in HEN. In this case, we force the exit temperature of the cold substream to be same as its entry temperature. Hence, $TCOUT_{sk} = TO_{sk} = TCIN_{sk}$. Similarly, for an expanded stream, its exit temperature will be low and it will be considered as a cold stream. Hence, we force the entry and exit temperatures of hot substream to be the same. $THOUT_{sk} = TO_{sk} = THIN_{sk}$. Also, the exit temperature of a hot (cold) stream in HEN should be lower (higher) than the entry temperature. Hence, we write the following equations to enforce these temperatures.

$$THOUT_{sk} \le TO_{sk} \qquad s \in PCG;\ 1 \le k \le K_s \tag{8a}$$

$$THOUT_{sk} \ge TO_{sk} - \left(T_s^L - T_s^U\right)\left(uc_{sk} + c_{sk}\right) \qquad s \in PCG;\ 1 \le k \le K_s \tag{8b}$$

$$TCOUT_{sk} \le TO_{sk} + \left(T_s^L - T_s^U\right)\left(ut_{sk} + t_{sk} + v_{sk}\right) \qquad s \in PCG;\ 1 \le k \le K_s \tag{9a}$$

$$TCOUT_{sk} \ge TO_{sk} \qquad s \in PCG;\ 1 \le k \le K_s \tag{9b}$$

The area and cost can be calculated by standard equations for HENS with isothermal mixing (Huang et al., 2012). A final heater or cooler is provided for final adjustment of temperature of streams with specified target temperatures.

3.4 Objective function

There are turbines, compressors, generator or motor on the SSTC which will either generate or consume electricity. As the total power produced in an SSTC must be equal to the total power consumed by the SSTC, the power balance on the SSTC gives,

$$\sum_{s \in PCG} \sum_{k=1}^{K_s} F_s t_{sk} \left(TI_{s(k-1)} - TM_{sk}\right) + WH = \sum_{s \in PCG} \sum_{k=1}^{K_s} F_s c_{sk} \left(TM_{sk} - TI_{s(k-1)}\right) + WG \tag{10}$$

where, *WG (WH)* is the capacity of the generator (motor).

The objective of WHENS can be either energy minimization or total annualized costs.

In case of minimization of energy, our objective is to reduce the energy consumption by maximizing the heat and work exchange among the available streams. Different weighing factors can be assigned to heat and work depending on their relative energy cost.

For calculating the total annualized costs, the capital expenses *CAPEX* ($), operating expenses per year *OPEX* ($/y) and the revenue earnings per year *REV* ($/y) should be known. *CAPEX* includes the costs of generator, motor, SSTC turbines and compressors, utility turbines and compressors, final heater/cooler, valves, pumps, and heat exchangers. The cost for mixers and splitters are ignored. The cost factors for each equipment will include both the fixed as well as the variable component. *OPEX* includes the costs of running the helper motor and utility compressors, pumps, and the utility costs in heat exchange network. The revenue comes from selling the generated electricity.

The objective function of minimization of TAC is given by

$$\text{Minimize } TAC = f.CAPEX + \left(OPEX - REV\right) \tag{11}$$

where, f = annualized factor for the capital cost.

4. Case study

Wechsung et al. (2011) introduced the optimization of offshore liquefaction process for liquid energy chain. It uses three streams; natural gas NG, liquid carbon dioxide LCO_2 and liquid nitrogen LIN. NG is liquefied using the other two streams. Wechsung et al. (2011) considered variable heat capacity values for different regions of the streams and used multi-stream exchangers. The final network given by Wechsung et al. (2011) for minimization of external wok showed that the same stream underwent compression and expansion. We consider a simplistic case of constant heat capacities and exclude pumps and flash valve for NG. The stream data as adopted from Huang and Karimi (2016) is listed in Table 1. Since it is an offshore process, we assume that hot or cold utility is not available for liquefaction of NG and only LIN and LCO_2 are available. Hence, we set hot and cold utility duty to be zero. As a result, all compressions and expansions are performed on SSTC or valves without any utility turbines and compressors.

We solve the model for minimization of total annualized cost with the cost parameters from Huang and Karimi (2016). Here, we provide flexibility for the stream to either be heated or cooled in the first WEN stage. With no external utility, the total annual cost computed is lower ($ 111,930). Also, incorporation of simplistic assumptions such as no-parallel work units and no utility turbines/compressors increases the solution speed. As specific heat values for these streams varies considerably with pressure and temperature, appropriate properties should be considered to make the model more realistic and accurate. The model can be extended for variable physico-chemical properties.

Table 1: Stream data

Stream	TIN (K)	TOUT (K)	PIN (MPa)	POUT (MPa)	F (kW/K)	h (kW/m^2-K)
PCG1 (LIN)	103.45	-	10	0.1	2.47	0.1
PCG2 (NG)	288.15	104.75	7	10	4.10	0.1
NPC1 (LCO_2)	221.12	-	-	-	5.70	0.1

5. Conclusions

We have developed an MINLP formulation for work and heat exchange network synthesis (WHENS) where the pressure changing streams are not pre-classified as low-pressure or high-pressure streams and hot or cold streams. This formulation is particularly useful for designing a network in cases where some of the process streams must undergo both compression and expansion due to utility constraints. For a simplistic case study of an offshore natural gas liquefaction process, we synthesized a network with lower total annualized cost with no external utility. Also, the incorporation of variable physico-chemical properties in the model can lead to more accurate results.

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