Model reformulations for Work and Heat Exchange Network (WHEN) synthesis problem

Haoshui Yu[1], Matias Vikse[1], Rahul Anantharaman[2], Truls Gundersen[1*]

[1]Department of Energy and Process Engineering, Norwegian University of Science and Technology, Kolbjoern Hejes v. 1A, NO-7491 Trondheim, Norway

[2]SINTEF Energy Research, Kolbjoern Hejes v. 1A, NO-7491 Trondheim, Norway

truls.gundersen@ntnu.no

Abstract: The Duran-Grossmann model can deal with heat integration problems with variable process streams. Work and Heat Exchange Networks (WHENs) represent an extension of Heat Exchange Networks. In WHEN problems, the identities of streams (hot/cold) are regarded as variables. The original Duran-Grossmann model has been extended and applied to WHENs without knowing the identity of streams a priori. In the original Duran-Grossmann model, the max operator is a challenge for solving the model. This paper analyzes four ways to reformulate the Duran-Grossmann model. Smooth Approximation, Explicit Disjunctions, Direct Disjunctions and Intermediate Temperature strategy are reviewed and compared. The Extended Duran-Grossmann model for WHEN problems consists of both binary variables and non-smooth functions. The Extended Duran-Grossmann model can be reformulated in similar ways. In this study, the performance of different reformulations of the Extended Duran-Grossmann model for WHEN problems is compared based on a small case study in this paper.

Key words: Work and Heat Exchange Networks, Duran-Grossmann Model, Reformulations, Disjunctive Programming, MINLP

1. Introduction

Heat integration has been widely used to save hot/cold utilities because thermal energy contributes significantly to the total cost of a process (Huang & Karimi, 2013). The classical

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heat integration techniques, such as pinch technology (Klemeš & Kravanja, 2013), can only deal with the heat integration problem with known stream data. If heat integration and process optimization are performed simultaneously, i.e. heat integration considering variable process streams, more benefits can be achieved. Duran and Grossmann proposed a mathematical model for simultaneous process optimization and heat integration (Duran & Grossmann, 1986). The Duran-Grossmann model is a powerful tool to solve the heat integration problem with variable process streams. This paper has been cited more than 350 times by the end of 2018. Their model has been successfully applied to organic Rankine cycle systems recovering low-temperature waste heat (Yu et al., 2017a), processes for liquefaction of natural gas (Wechsung et al., 2011), optimal reactor network synthesis (Lakshmanan & Biegler, 1996), and fuel cell systems (Marechal et al., 2005). To improve the performance of the model, several reformulations are proposed in previous studies, which will be reviewed and compared in this study.

The new topic referred to as Work and Heat Exchange Networks (WHENs) arise if pressure manipulations are considered while designing Heat Exchanger Networks (HENs). There are many potential applications of WHENs theory, such as a novel process for offshore liquefaction of natural gas (Aspelund & Gundersen, 2009), effluent gas recovery (Liao et al., 2017), process integration in carbon capture processes (Fu & Gundersen, 2016), and optimal distillation column integration (Nair et al., 2018). More applications can be found in the literature (Yu et al., 2018a). More generally speaking, not only the temperature but also the pressure have to meet some specifications in a system. Pressure specifications for process streams make the problem more challenging compared with conventional HENs. Holiastos and Manousiouthakis (2002) proposed a mathematical model minimizing hot/cold/work utility cost for HENs. Here "work utility" refers to the generation or consumption of work. Aspelund et al. (2007) proposed a manual methodology referred to as Extended Pinch Analysis and Design

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(ExPAnD), where traditional Pinch Analysis is extended with pressure considerations and Exergy Analysis. Marmolejo-Correa and Gundersen (2012) proposed a methodology combining Exergy and Pinch Analyses to design a Reverse Brayton cycle for the liquefaction of natural gas. Based on this study, Marmolejo-Correa and Gundersen (2013) developed a novel diagram for exergy and energy targeting for a heat recovery system subject to changes in both temperature and pressure. This method is particularly suitable for low temperature systems such as LNG processes. Fu and Gundersen (2015a) presented a systematic graphical design procedure for the integration of compressors in HENs above ambient temperature. Similarly, Fu and Gundersen (2015b) integrated compressors into heat exchanger networks below ambient temperature. Four theorems were proposed and used as the basis for the design methodology. Fu and Gundersen also integrated expanders into heat exchanger networks above (Fu & Gundersen, 2015c) and below (Fu & Gundersen, 2015d) ambient temperature. Wechsung et al. (2011) combined Pinch Analysis, Exergy Analysis, and Mathematical Programming to synthesize HENs below ambient temperature with compression and expansion of process streams.

The WHENs problem involves both heat integration and work integration. The Duran-Grossmann model can be extended to solve WHEN problems. Since the thermodynamic path and the identity (hot/cold) of process streams are unknown in WHENs, classical heat integration methods cannot be applied. In addition, the identity of streams can also temporarily change in WHENs. This paper extends the Duran-Grossmann model to WHEN problems, where the identities of streams are unknown a priori. The various reformulations of the original Duran-Grossmann model are applied to the Extended Duran-Grossmann model for WHEN synthesis problems. There are four different reformulations for the Extended Duran-Grossmann model presented in the literature. This study investigates the different reformulations and their computational expenses.

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2. Original Duran-Grossmann Model and Reformulations

The original Duran-Grossmann model can take into account the utility cost and other economic indicators simultaneously, and it can be written in a compact way as follows:

$$\min obj = F\left(\omega, x\right) + C_{hu}Q_{hu} + C_{cu}Q_{cu}$$

$$s.t.\ \text{(DG.1)}\ h\left(\omega, x\right) = 0$$

$$\text{(DG.2)}\ g\left(\omega, x\right) \le 0$$

$$\text{(DG.3)}\ T_i^p = T_i^{in} \quad \forall i \in H$$

$$\text{(DG.4)}\ T_j^p = T_j^{in} + HRAT \quad \forall\ j \in C$$

$$\text{(DG.5)}\ QSOA(x)^p = \sum_{i \in H} FCp_i \left[\max\left\{0, T_i^{in} - T^p\right\} - \max\left\{0, T_i^{out} - T^p\right\} \right] \quad \forall p \in PC$$

$$\text{(DG.6)}\ QSIA(x)^p = \sum_{j \in C} FCp_j \left[\max\left\{0, T_j^{out} - (T^p - HRAT)\right\} - \max\left\{0, T_j^{in} - (T^p - HRAT)\right\} \right] \quad \forall p \in PC$$

$$\text{(DG.7)}\ Z_{def}^p(x) = QSIA(x)^p - QSOA(x)^p$$

$$\text{(DG.8)}\ Z_{def}^p(x) \le Q_{hu}$$

$$\text{(DG.9)}\ \Omega(x) + Q_{hu} - Q_{cu} = 0$$

$$\text{(DG.10)}\ \Omega(x) = \sum_{i \in H} FCp_i (T_i^{in} - T_i^{out}) - \sum_{j \in C} FCp_j (T_j^{out} - T_j^{in})$$

$$\text{(DG.11)}\ Q_{hu} \ge 0, Q_{cu} \ge 0$$

DG.1 and DG.2 are the equality and inequality constraints for the industrial process. The vector ω denotes process parameters such as pressure, temperature, or parameters in cost correlations. DG.3 and DG.4 are used to assign the inlet temperature of each stream to potential pinch candidates. It should be noticed that only cold stream inlet temperatures are modified to take into account the effect of the Heat Recovery Approach Temperature (HRAT). DG.5 and DG.6 denote the total hot stream heat load and total cold stream heat load above each pinch candidate temperature. DG.7 and DG.8 aim at identifying the correct pinch point, which features the maximum heat deficit among all the pinch candidates. DG.9 and DG.10 are energy balances for the system.

The Duran-Grossmann model incorporates max operators, which result in non-differentiabilities at T^p. Max operators are challenging for deterministic solvers and have to be removed before solving the model. The original Duran-Grossmann model has proven to be powerful in process design. Thus, interest has increased in the Process System Engineering

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(PSE) field to find ways to reformulate the model. Four different reformulations have been found in the literature, and these are presented and used in the Extended Duran-Grossmann model for WHEN synthesis. The four reformulations are the following: (1) Smooth Approximation, (2) Explicit Disjunction, (3) Direct Disjunction, and (4) an Intermediate Temperature strategy.

2.1 Smooth Approximation for the Heat Integration Model

The max operator in the Duran-Grossmann model was reformulated by using smooth approximations proposed by Balakrishna and Biegler (1992). This reformulation has been applied to heat integration problems considering organic Rankine cycles (Yu et al., 2017b) and carbon capture processes considering waste heat recovery (Yu et al., 2018b). The max operator in the original Duran-Grossmann model can be reformulated by using the equation shown in Eq. (1) to modify DG.5 and DG.6.

$$\max\{0, x\} \cong \frac{1}{2}(x + \sqrt{x^2 + \varepsilon}) \quad (1)$$

Here, ε is a small constant, typically between 10^{-3} and 10^{-6}.

However, this reformulation may encounter problems when dealing with isothermal streams. In addition, the performance of the approximation depends on the value of the small constant, which may cause numerical conditioning problem if chosen improperly (Grossmann et al., 1988). The small parameter is close to zero, and the Smooth Approximation can sometimes be ill-conditioned.

2.2 Explicit Disjunction for the Heat Integration Model

To remove the max operator in the original Duran-Grossmann model, Grossmann et al. (1998) proposed a disjunctive reformulation. This reformulation can even handle isothermal streams in a system. The key idea of the disjunctive formulation is the explicit treatment of three

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possibilities for process stream temperatures: a process stream is totally above, totally below or across the pinch candidate temperature, as shown in Figure 1. When a stream is totally above the pinch candidate temperature, both the inlet and outlet temperatures are greater than the pinch candidate temperature. When a stream is totally below the pinch candidate temperature, both the inlet and outlet temperatures are below the pinch candidate temperature. These two statements are valid regardless of the streams being hot or cold. However, if the stream is across a pinch candidate temperature, the constraints are different for hot and cold streams. For hot streams, the inlet temperature is greater than the pinch candidate temperature, and the outlet temperature is less than the pinch candidate temperature. In contrast, different constraints apply to cold streams. To avoid the use of max operators, intermediate variables are introduced to calculate the correct heat load of hot and cold streams respectively, as shown in the Eq. (2).

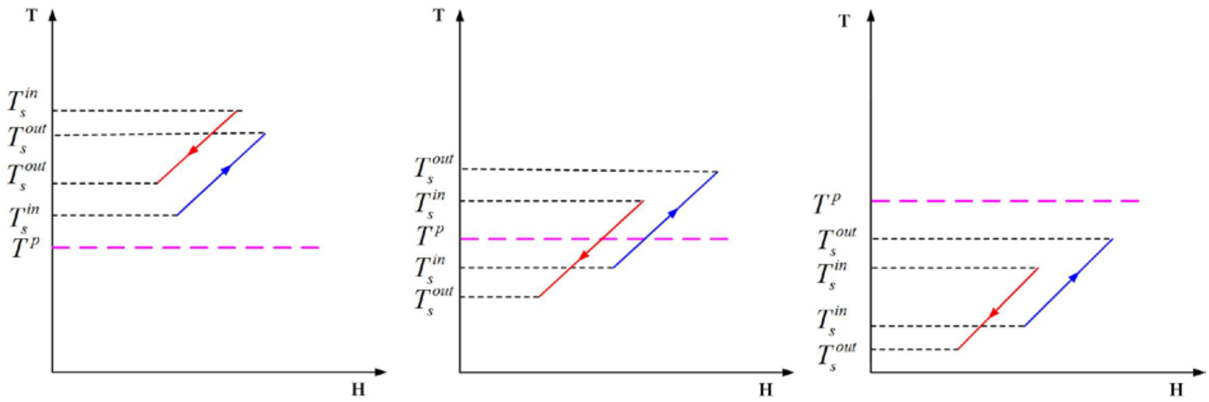

Fig. 1 Relationship between pinch candidate temperature and process streams (Yu et al., 2018c).

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$$
\begin{bmatrix} Y1_i^p \\ T_i^{in} \ge T^p \\ T_i^{out} \ge T^p \\ T_i^{in,p} = T_i^{in} - T^p \\ T_i^{out,p} = T_i^{out} - T^p \end{bmatrix} \vee \begin{bmatrix} Y2_i^p \\ T_i^{in} \ge T^p \\ T_i^{out} \le T^p \\ T_i^{in,p} = T_i^{in} - T^p \\ T_i^{out,p} = 0 \end{bmatrix} \vee \begin{bmatrix} Y3_i^p \\ T_s^{in} \le T^p \\ T_s^{out} \le T^p \\ T_s^{in,p} = 0 \\ T_s^{out,p} = 0 \end{bmatrix}
$$

$$
\begin{bmatrix} Y1_j^p \\ T_j^{in} \ge T^p \\ T_j^{out} \ge T^p \\ T_j^{in,p} = T_j^{in} - T^p \\ T_j^{out,p} = T_j^{out} - T^p \end{bmatrix} \vee \begin{bmatrix} Y2_j^p \\ T_j^{in} \le T^p \\ T_j^{out} \ge T^p \\ T_j^{in,p} = 0 \\ T_j^{out,p} = T_j^{out} - T^p \end{bmatrix} \vee \begin{bmatrix} Y3_j^p \\ T_j^{in} \le T^p \\ T_j^{out} \le T^p \\ T_j^{in,p} = 0 \\ T_j^{out,p} = 0 \end{bmatrix} \quad (2)
$$

$$
QSOA(x)^p = \sum_{i \in H} FCp_s (T_i^{in,p} - T_i^{out,p})
$$

$$
QSIA(x)^p = \sum_{j \in C} -FCp_j (T_j^{in,p} - T_j^{out,p})
$$

Then the max operators in the original Duran-Grossmann model can be replaced by the disjunctions shown in Eq. (2). In our study, we refer to this disjunctive reformulation as Explicit Disjunction.

2.3 Direct Disjunction for the Heat Integration Model

Recently, Quirante et al. (2017) proposed another novel and robust disjunctive reformulation. This method reformulates the max operator from a pure mathematical point of view without any physical insight regarding the heat integration background. We refer to this reformulation as Direct Disjunction in this study. This reformulation has fewer Boolean variables compared with the Explicit Disjunction (Grossmann et al., 1998), thus shows better relaxation gaps and reduced number of equations.

The max operator is expressed as follows:

$$
\phi = \max(0, c^T x) \quad (3)
$$

Based on mathematical analysis, the max operator can be either 0 or a positive number. Therefore, a direct disjunction is proposed as shown in Eq. (4).

$$
\begin{array}{cc} Y & \neg Y \\ \begin{bmatrix} c^T x \geq 0 \\ \phi = c^T x \end{bmatrix} \vee & \begin{bmatrix} c^T x \leq 0 \\ \phi = 0 \end{bmatrix} \end{array}
$$
$$
Y \in \{True, False\} \tag{4}
$$

Using this formulation, the max operator in Eqs. DG.4 and DG.5 can be replaced by the disjunctions as shown in Eq. (5).

$$
\begin{gathered}
\begin{bmatrix} Y_i^{in} \\ T_i^{in} - T^p \geq 0 \\ \phi_i^{in} = T_i^{in} - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_i^{in} \\ T_i^{in} - T^p \leq 0 \\ \phi_i^{in} = 0 \end{bmatrix} \\
\begin{bmatrix} Y_i^{out} \\ T_i^{out} - T^p \geq 0 \\ \phi_i^{out} = T_i^{out} - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_i^{out} \\ T_i^{out} - T^p \leq 0 \\ \phi_i^{out} = 0 \end{bmatrix} \\
\begin{bmatrix} Y_j^{in} \\ T_j^{in} + HRAT - T^p \geq 0 \\ \phi_j^{in} = T_j^{in} + HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_j^{in} \\ T_j^{in} + HRAT - T^p \leq 0 \\ \phi_j^{in} = 0 \end{bmatrix} \\
\begin{bmatrix} Y_j^{out} \\ T_j^{out} + HRAT - T^p \geq 0 \\ \phi_j^{out} = T_j^{out} + HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_j^{out} \\ T_j^{out} + HRAT - T^p \leq 0 \\ \phi_j^{out} = 0 \end{bmatrix} \\
QSOA(x)^p = \sum_{i \in H} FCp_i (\phi_i^{in} - \phi_i^{out}) \\
QSIA(x)^p = \sum_{j \in C} -FCp_j (\phi_j^{in} - \phi_j^{out})
\end{gathered} \tag{5}
$$

2.4 Intermediate Temperature Strategy for the Heat Integration Model

Anantharaman et al. (2014) revisited the Duran-Grossmann model to improve the solution of the formulation. They pointed out that the Explicit Disjunction reformulation has the drawback of introducing a large number of binary variables. The novel idea in this study is to introduce a new variable named intermediate temperature, to represent the pinch candidate temperature and avoid using max operators. We refer to this reformulation as the Intermediate Temperature (IT) strategy in this study. The key idea of the three reformulations discussed in Sections 2.1-2.3 is how to reformulate the max operators in the Duran-Grossmann model. The Intermediate Temperature strategy, however, is different from the three previous reformulations. Eqs. DG.5-

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DG.8 in the original Duran-Grossmann model can be written in one single compact equation as shown in Eq. (6).

$$Q_{hu} \geq \sum_{j \in C} (T_j^{out} - t_{j,p}^M) FCp_j - \sum_{i \in H} (T_i^{in} - t_{i,p}^M) FCp_i \tag{6}$$

In Eq. (6), intermediate temperatures ($t_{i,p}^M$ and $t_{j,p}^M$) are introduced. Hot utility consumption is determined by the heat deficit between hot and cold streams above each potential pinch temperature. To determine the correct intermediate temperature corresponding to the correct pinch temperature, more constraints are incorporated in the model. More detailed and updated information about this model can be found in the updated notes (Anantharaman, 2018). In this reformulation, max operators are avoided but binary variables are introduced. The reformulated Duran-Grossmann model with the IT strategy is as follows:

$$\begin{aligned}
&\min obj = F(\omega, x) + C_{hu}Q_{hu} + C_{cu}Q_{cu} \\
&s.t.\ \text{(IT.1)}\ h(\omega, x) = 0 \\
&\quad \text{(IT.2)}\ g(\omega, x) \leq 0 \\
&\quad \text{(IT.3)}\ T_i^p = T_i^{in} \qquad \forall i \in H \\
&\quad \text{(IT.4)}\ T_j^p = T_j^{in} + HRAT \qquad \forall j \in C \\
&\quad \text{(IT.5)}\ Q_{hu} \geq \sum_{j \in C} FCp_j \left(T_j^{out} - T_{j,p}^M\right) - \sum_{i \in H} FCp_i \left(T_i^{in} - T_{i,p}^M\right) \qquad \forall p \in PC \\
&\quad \text{(IT.6)}\ T_{i,p}^M \geq T_i^{out} \qquad \forall i \in H, p \in PC \\
&\quad \text{(IT.7)}\ T_{i,p}^M \geq T^p - M_{i,p} \cdot y_{i,p} \qquad \forall i \in H, p \in PC \\
&\quad \text{(IT.8)}\ T_{i,p}^M \geq T^p - U_{i,p} \cdot \left(1 - y_{i,p}\right) \qquad \forall i \in H, p \in PC \\
&\quad \text{(IT.9)}\ T_{j,p}^M \leq T_i^{out} \qquad \forall j \in C, p \in PC \\
&\quad \text{(IT.10)}\ T_{j,p}^M \leq T^p + M_{j,p} \cdot \left(1 - y_{j,p}\right) \qquad \forall j \in C, p \in PC \\
&\quad \text{(IT.11)}\ T_{j,p}^M \leq T_j^{in} + U_{j,p} \cdot y_{j,p} \qquad \forall j \in C, p \in PC \\
&\quad \text{(IT.12)}\ \Omega(x) + Q_{hu} - Q_{cu} = 0 \\
&\quad \text{(IT.13)}\ \Omega(x) = \sum_{i \in H} FCp_i (T_i^{in} - T_i^{out}) - \sum_{j \in C} FCp_j (T_j^{out} - T_j^{in}) \\
&\quad \text{(IT.14)}\ Q_{hu} \geq 0, Q_{cu} \geq 0
\end{aligned}$$

Here, $y_{i,p}$ and $y_{j,p}$ are binary variables indicating whether a stream is above or below a pinch candidate. The case where a stream is across the pinch candidate temperature is not treated

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separately. For hot streams, $y_{i,p} = 1$ corresponds to the case where stream *i* is below the pinch candidate temperature and $y_{i,p} = 0$ corresponds to the case where stream *i* is above or across the pinch candidate temperature. For cold streams, $y_{j,p} = 1$ corresponds to the case where stream *j* is across or below the pinch candidate temperature and $y_{j,p} = 0$ corresponds to the case where stream *j* is above the pinch candidate temperature. *M* and *U* are valid upper bounds associated with binary variables $y_{i,p}$ and $y_{j,p}$.

2.5 Model Complexity

The four reformulations are proposed in the following chronological order: Smooth Approximation (Balakrishna & Biegler, 1992), Explicit Disjunction (Grossmann et al., 1998), Intermediate Temperature strategy (Anantharaman et al., 2014) and Direct Disjunction (Quirante et al., 2017). Smooth Approximation has the following advantages: no binary variables are needed and it is computationally efficient. However, the reformulation has difficulty when handling isothermal streams and intermediate utilities. In addition, the Smooth Approximation parameter has to be chosen properly, otherwise numerical issues could arise. To overcome the limitations of Smooth Approximation, Explicit Disjunction, which is capable of handling isothermal streams and multiple utilities, is proposed. However, 3 Boolean variables are introduced for each pair of streams and pinch candidates. The number of binaries are increasing rapidly with the scale of the problem. Therefore, it becomes challenging to solve the model if the problem size is large. Motivated by this challenge, Direct Disjunction, which only needs 2 Boolean variables for each pair of streams and pinch candidates, provides a better reformulation of the original Duran-Grossmann model. Direct Disjunction should perform much better than Explicit Disjunction, especially for medium or large-scale problems. The Intermediate Temperature strategy introduces a new continuous variable to avoid using max operators. One binary variable to activate/deactivate the corresponding constraints has to be

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introduced. The different reformulations are subject to the trade-off between continuous variables and binary variables.

3. Extended Duran-Grossmann model for Work and Heat Integration

In this study, we mainly focus on the application of the Duran-Grossmann model for Work and Heat Exchange Networks (WHENs). The Duran-Grossmann model has been successfully extended to WHEN problems (Yu et al., 2018c). A brief introduction to the WHENs problem is presented here. The WHENs problem can be stated as follows: Given a set of process streams with supply and target state (temperature, pressure), as well as hot, cold and power utilities; the objective is to design a network consisting of heat transfer equipment such as heat exchangers, heaters and coolers, and pressure manipulation equipment such as expanders, compressors, pumps and valves with minimum Exergy Consumption or minimum Total Annualized Cost.

In the WHENs problem, a process stream whose target pressure is greater than the supply pressure is called a work sink stream (WSK). Opposite, a work source stream (WSR) can be defined as a process stream whose target pressure is less than the supply pressure. Any process stream can be heated, cooled or simply not changed before pressure manipulation. Figure 2 illustrates the superstructure of a stream in the category of WSK. Detailed information about the superstructure is available in Yu et al., 2018c.

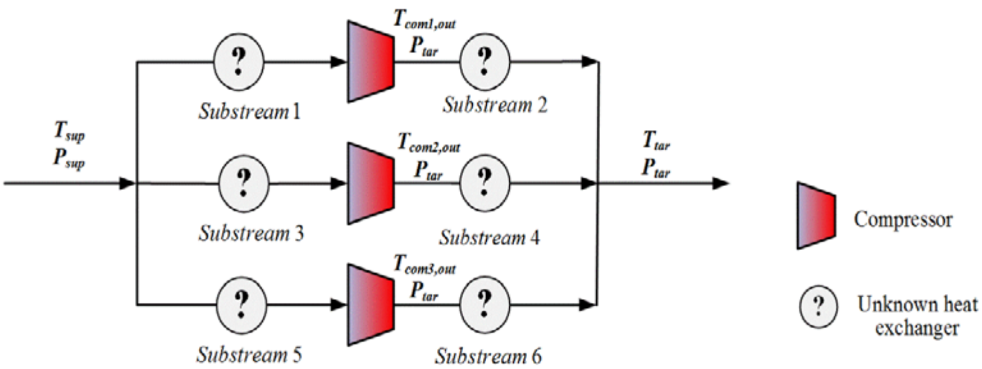

Fig. 2 Superstructure for streams belonging to WSK (Yu et al., 2018c)

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Since the identity of streams in the WHEN is unknown a priori, the Duran-Grossmann model cannot be applied directly and has to be extended to a new model using binary variables to denote the identity of streams. In the Extended Duran-Grossmann (EDG) model, separate sets of hot and cold streams do no longer exist. Binary variables are used to automatically distinguish the hot and cold streams in the model. The Extended Duran-Grossmann model can be formulated as follows:

$$
\begin{aligned}
&\text{Min } obj = Exergy\ Consumption \\
&s.t.\ (\text{EDG.1})\ h(\omega, x) = 0 \\
&(\text{EDG.2})\ g(\omega, x) \le 0 \\
&(\text{EDG.3})\ T_s^p = T_s^{in} + y_s \cdot HRAT \qquad \forall s \in S \\
&(\text{EDG.4})\ QSOA(x)^p = \sum_{s \in S} (1 - y_s) FCp_s \left[\max\left\{0, T_s^{in} + y_s \cdot HRAT - T^p\right\} - \max\left\{0, T_s^{out} + y_s \cdot HRAT - T^p\right\} \right] \quad \forall p \in PC \\
&(\text{EDG.5})\ QSIA(x)^p = \sum_{s \in S} y_s \cdot FCp_s \left[\max\left\{0, T_s^{out} + y_s \cdot HRAT - T^p\right\} - \max\left\{0, T_s^{in} + y_s \cdot HRAT - T^p\right\} \right] \quad \forall p \in PC \\
&(\text{EDG.6})\ Z_{def}^p(x) = QSIA(x)^p - QSOA(x)^p \quad \forall p \in PC \\
&(\text{EDG.7})\ Z_{def}^p(x) \le Q_{hu} \qquad \forall p \in PC \\
&(\text{EDG.8})\ \Omega(x) + Q_{hu} - Q_{cu} = 0 \\
&(\text{EDG.9})\ \Omega(x) = \sum_{s \in S} (1 - y_s) FCp_s (T_s^{in} - T_s^{out}) - \sum_{s \in S} y_s \cdot FCp_s (T_s^{out} - T_s^{in}) \\
&(\text{EDG.10})\ Q_{hu} \ge 0, Q_{cu} \ge 0
\end{aligned}
$$

Here, x represents the flow rates and temperatures of the streams involved in heat integration. ω represents all the other process variables. Eqs. EDG.1 and EDG.2 denote the process equality and inequality constraints as those in the original Duran-Grossmann model. y_s is a binary variable to denote the identity of a process stream. In this study, $y_s = 1$ means stream s is a cold stream. *QSOA* and *QSIA* denote the total heat load of hot and cold streams above each pinch candidate $p \in PC$. $Z_{def}^p(x)$ is heat deficit above each pinch candidate. $\Omega(x)$ is the heat load difference between hot and cold streams. *HRAT* denotes the heat recovery approach temperature. The objective function is minimizing the exergy consumption of the system, which is related to the use of thermal utilities and shaft work consumed in the system. In the

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next sections, the previously reviewed reformulations for the original Duran-Grossmann model are applied to the Extended Duran-Grossmann model. Since the identity of the streams are unknown a priori, these reformulations have to be revised accordingly. The reformulations for the extended Duran-Grossmann model are presented as follows.

3.1 Smooth Approximation for the Work and Heat Integration Model

For the Extended Duran-Grossmann model, the max operators can be replaced by Smooth Approximations as well. It is similar to the reformulation for the original Duran-Grossmann model as discussed in Section 2.1. However, binary variables are involved in the Smooth Approximation reformulation in this case. The detailed model is omitted in this section since it is straightforward.

3.2 Explicit Disjunction for the Work and Heat Integration Model

For the explicit disjunction reformulation, it is not necessary to distinguish between hot and cold streams in the Extended Duran-Grossmann model. In contrast to the reformulation in Section 2.2, only three disjunctions are needed in the Extended Duran-Grossmann model. However, more constraints are needed to take the identity of streams into account in the disjunction. Especially for the case where a stream operates across the pinch candidate temperature, the constraints are different for hot and cold streams. Therefore, there are 3 more constraints in the second disjunction as shown in Eq. (7) compared with the Explicit Disjunction reformulation for the original Duran-Grossmann model.

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$$
\begin{bmatrix} Y1_s^p \\ T_s^{in} + y_s \cdot HRAT \geq T^p \\ T_s^{out} + y_s \cdot HRAT \geq T^p \\ T_s^{in,p} = T_s^{in} + y_s \cdot HRAT - T^p \\ T_s^{out,p} = T_s^{out} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} Y2_s^p \\ T_s^{in} + y_s \cdot HRAT \geq T^p - y_s \cdot R \\ T_s^{out} + y_s \cdot HRAT \geq T^p - (1-y_s) \cdot R \\ T_s^{in} + y_s \cdot HRAT \leq T^p + (1-y_s) \cdot R \\ T_s^{out} + y_s \cdot HRAT \leq T^p + y_s \cdot R \\ T_s^{in,p} = (1-y_s)T_s^{in} - (1-y_s)T^p \\ T_s^{out,p} = y_s \cdot T_s^{out} + y_s \cdot HRAT - y_s \cdot T^p \end{bmatrix} \vee \begin{bmatrix} Y3_s^p \\ T_s^{in} + y_s \cdot HRAT \leq T^p \\ T_s^{out} + y_s \cdot HRAT \leq T^p \\ T_s^{in,p} = 0 \\ T_s^{out,p} = 0 \end{bmatrix} \tag{7}
$$

$$
QSOA(x)^p = \sum_{s \in S} (1-y_s) FCp_s (T_s^{in,p} - T_s^{out,p})
$$

$$
QSIA(x)^p = \sum_{s \in S} -y_s \cdot FCp_s (T_s^{in,p} - T_s^{out,p})
$$

Here, R is a valid upper bound to relax the constraints for the binary variables denoting stream identities. The value of R can be estimated based on temperatures of the process streams.

After the reformulation, the Extended Duran-Grossmann model becomes a disjunctive model, which can be transformed into a Mixed Integer Non-Linear Programming (MINLP) problem by the Big-M method or the convex hull method (Türkay & Grossmann, 1996). In this study, LogMIP (Vecchietti & Grossmann, 2004), a specially designed program for disjunctive programming, is adopted as the solver. Users can freely choose the Big-M method or convex hull method in the GAMS environment, which facilities the modeling and solution substantially.

3.3 Direct Disjunction for the Work and Heat Integration Model

Recently, Quirante et al. (2018) proposed a disjunctive model considering unclassified streams and area estimation. In their study, the stream identity is expressed as a disjunction. This is in contrast to our study, where the stream identity is denoted by using binary variables. Based on the reformulation presented in Section 2.4, the direct disjunction reformulation can be applied to the Extended Duran-Grossmann model in a similar way. However, only two disjunctions are necessary since the Extended Duran-Grossmann model only has one common set for the process streams, and does not distinguish between hot and cold streams. The direct disjunction can replace the max operator in Eqs. EDG.4 and 5. The resulting disjunctions are shown in Eq. (8). Intermediate variables ϕ_{in} and ϕ_{out} are introduced in the direct disjunction reformulation.

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$$
\begin{bmatrix} Y_{in} \\ T_s^{in} + y_s \cdot HRAT - T^p \geq 0 \\ \phi_{in} = T_s^{in} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_{in} \\ T_s^{in} + y_s \cdot HRAT - T^p \leq 0 \\ \phi_{in} = 0 \end{bmatrix}
$$

$$
\begin{bmatrix} Y_{out} \\ T_s^{out} + y_s \cdot HRAT - T^p \geq 0 \\ \phi_{out} = T_s^{out} + y_s \cdot HRAT - T^p \end{bmatrix} \vee \begin{bmatrix} \neg Y_{out} \\ T_s^{out} + y_s \cdot HRAT - T^p \leq 0 \\ \phi_{out} = 0 \end{bmatrix} \tag{8}
$$

$$
QSOA(x)^p = \sum_{s \in S} (1 - y_s) FCp_s (\phi_{in} - \phi_{out})
$$

$$
QSIA(x)^p = \sum_{s \in S} -y_s \cdot FCp_s (\phi_{in} - \phi_{out})
$$

Compared with Explicit Disjunction, only two Boolean variables are needed for each pair of streams and pinch candidates. With the above disjunctions, the model can easily be implemented in the GAMS environment along with other equations related to the process.

3.4 Intermediate Temperature Strategy for the Work and Heat Integration Model

For the Intermediate Temperature strategy, the reformulation is very different from that for the original Duran-Grossmann model. In the Extended Duran-Grossmann model, there is only one set including both hot and cold streams. Therefore, all the equations are defined based on a single stream set. To activate the corresponding constraints for a stream changing from hot stream to cold stream, a big-M relaxation strategy is adopted. The Intermediate Temperature reformulation for work and heat integration model can be expressed as follows:

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$$
\begin{aligned}
&\min obj = F\left(\omega, x\right) + C_{hu}Q_{hu} + C_{cu}Q_{cu} \\
&s.t. \text{ (EDG-IT.1) } h\left(\omega, x\right) = 0 \\
&\quad \text{(EDG-IT.2) } g\left(\omega, x\right) \le 0 \\
&\quad \text{(EDG-IT.3) } T_s^p = T_s^{in} + y_s \cdot HRAT \qquad \forall s \in S \\
&\quad \text{(EDG-IT.4) } Q_{hu} \ge \sum_{s \in S} y_s \cdot FCp_s\left(T_s^{out} - T_{s,p}^M\right) - \sum_{s \in S}\left(1 - y_s\right) FCp_s\left(T_s^{in} - T_{s,p}^M\right) \quad \forall p \in PC \\
&\quad \text{(EDG-IT.5) } T_{s,p}^M \ge T_s^{out} - M_s \cdot y_s \qquad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.6) } T_{s,p}^M \ge T^p - M_{s,p} \cdot y_{s,p} - M_s \cdot y_s \quad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.7) } T_{s,p}^M \ge T^p - U_{s,p} \cdot \left(1 - y_{s,p}\right) - M_s \cdot y_s \quad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.8) } T_{s,p}^M \le T_s^{out} + M_s \cdot \left(1 - y_s\right) \qquad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.9) } T_{s,p}^M \le T^p + M_{s,p} \cdot \left(1 - y_{s,p}\right) + M_s \cdot \left(1 - y_s\right) \qquad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.10) } T_{s,p}^M \le T_s^{in} + U_{s,p} \cdot y_{s,p} + M_s \cdot \left(1 - y_s\right) \qquad \forall s \in S, p \in PC \\
&\quad \text{(EDG-IT.11) } \Omega(x) + Q_{hu} - Q_{cu} = 0 \\
&\quad \text{(EDG-IT.12) } \Omega(x) = \sum_{i \in H} FCp_i (T_i^{in} - T_i^{out}) - \sum_{j \in C} FCp_j (T_j^{out} - T_j^{in}) \\
&\quad \text{(EDG-IT.13) } Q_{hu} \ge 0, Q_{cu} \ge 0
\end{aligned}
$$

It should be noticed that y_s is a binary variable to denote the stream identity, while $y_{s,p}$ is a binary variable to denote the relationship between the intermediate temperature and the pinch candidate temperature. If the stream identity is a hot stream (i.e. $y_s = 0$), then constraints EDG-IT.5-7 are active and constraints EDG-IT.8-10 are relaxed. If the stream identity is a cold stream (i.e. $y_s = 1$), then constraints EDG-IT.8-10 are active and constraints EDG-IT.5-7 are relaxed. M_s are valid upper bounds for temperatures to relax the constraints related to binary variables y_s . Similarly, $M_{s,p}$ and $U_{s,p}$ are valid upper bounds associated with binary variables $y_{s,p}$. It should be noted that the value of these parameters will affect the computational time of the model.

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4. Case Study

This case study is taken from the study by Fu and Gundersen (2015a). The stream data are listed in Table 1. There are 4 process streams. Stream C1 is subject to pressure change and needs to be compressed from 100 kPa to 300 kPa. The hot and cold utilities are supplied at 400°C and 15°C respectively. The problem is to determine if stream C1 needs to be split into substreams, and to find the optimal inlet temperature(s) for the compressor(s). Since this is a small-scale problem, C1 is split only into two substreams in the superstructure to reduce the model size. The HRAT is set to be 20°C. The ambient temperature is assumed to be 15°C, thus the exergy of cold utility (at 15°C) is zero in this case. The fluids to be compressed are assumed to behave like ideal gas with constant specific heat capacity ratio $\gamma = 1.4$.

Table 1. Stream data for the case study

Stream	T^{sup} (°C)	T^{tar} (°C)	FCp (kW/°C)	ΔH (kW)	P^{sup} (kPa)	P^{tar} (kPa)
H1	300	50	4	1000	-	-
H2	120	40	4	320	-	-
C1	70	380	3	930	100	300
C2	30	180	3	450	-	-
Hot utility	400	400	-	-	-	-
Cold utility	15	15	-	-	-	-

The Extended Duran-Grossmann model can determine the optimal split ratio of stream C2 and the optimal temperature(s) of stream C1 before compression. For this case study, all the reformulations are able to find the global optimum. The detailed results concerning stream C1 are listed in Table 2. Without considering pressure manipulation, the original pinch temperatures are 120/100°C for hot and cold streams respectively. In the optimal configuration, stream C1 is split into two substreams with heat capacity flowrates being 1.47 kW/°C and 1.53 kW/°C respectively. A new pinch is created and located at 300/280°C. It can be seen that part of C1 (substream C1_S1) is heated to the new pinch temperature 280°C before compression.

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The other part is cooled down to ambient temperature before compression. The optimized superstructure of C1 is shown in Figure 3. The results are consistent with the study by Fu and Gundersen (2015a).

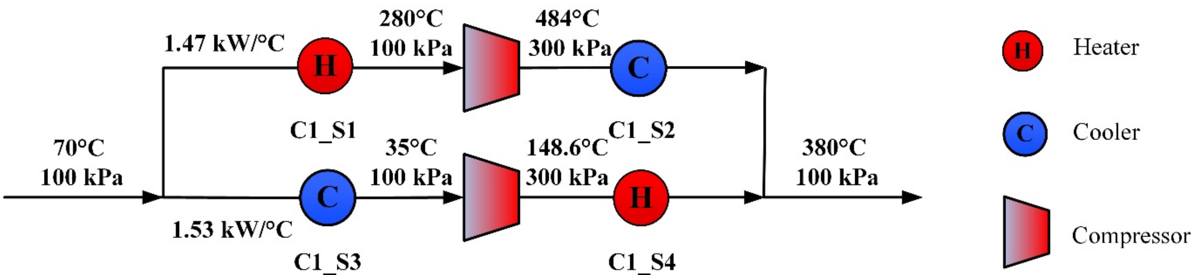

Fig. 3 The optimized superstructure of C1

Table 2. Optimal stream data for C1 for all reformulations

Stream	T^{sup} (°C)	T^{tar} (°C)	FCp(kW/°C)	ΔH(kW)	P^{sup} (kPa)	P^{tar} (kPa)
C1_S1	70	280	1.47	308.7	100	100
C1_S2	484	380	1.47	152.9	300	300
C1_S3	70	35	1.53	53.6	100	100
C1_S4	148.6	380	1.53	354	300	300

The overall system performance under optimal conditions are summarized in Table 3. The Composite Curves and the Grand Composite Curve are shown in Figure 4. The hot utility demand is zero because the compression heat of C1_S2 can be fully utilized to heat cold streams in the system above the pinch. Stream C1 is compressed at the new pinch temperature and at ambient temperature. In contrast, compression at the original pinch temperature or the supply temperature are not good options from the perspective of exergy consumption. The compression of C1_S1 has the similar effect as a heat pump. After compression, the substream C1_S2 becomes a hot stream in the system that will reduce hot utility. The hot and cold Composite Curves are closer to each other and there are two pinch points in the GCC. This demonstrates that an efficient heat exchanger network can be derived with the optimized superstructure for stream C1.

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Table 3. System performance under the optimal configuration

Items	Value
Hot utility (kW)	0
Cold utility (kW)	413.9
Pinch temperature (°C)	290
Compression work (kW)	473.8
Exergy consumption (kW)	473.8
Original Pinch compression flowrate (kW/°C)	0
New Pinch compression flowrate (kW/°C)	1.47
Ambient compression flowrate (kW/°C)	1.53
Compression at T^{sup} flowrate (kW/°C)	0

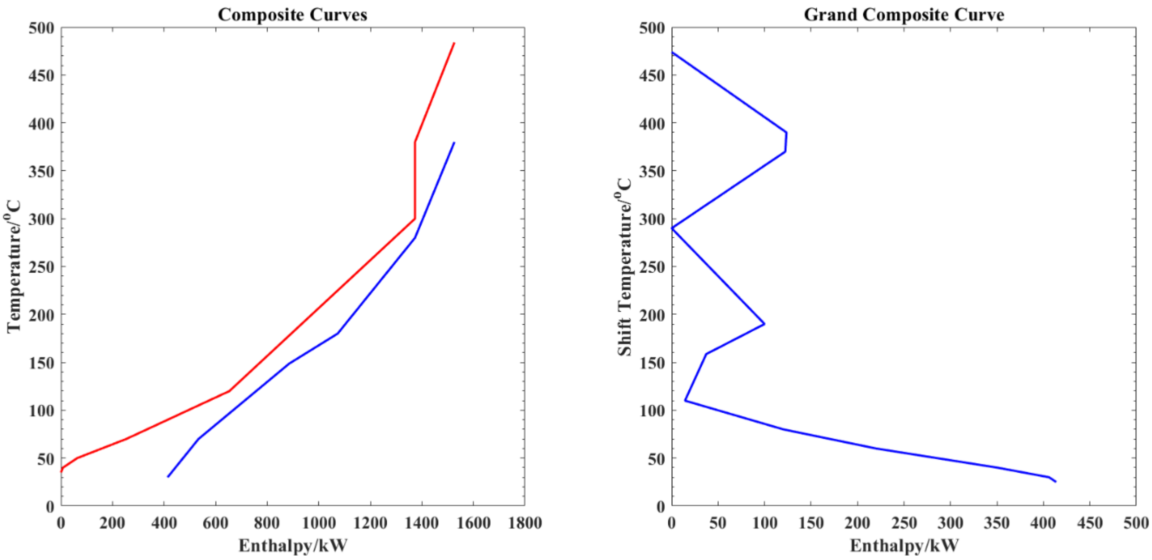

Fig. 4 Composite Curves and Grand Composite Curve under optimal conditions

Even though all the reformulations can reach the same global optimum as discussed above, the computational expense shows big differences for the different reformulations. For the Explicit Disjunction and the Direct Disjunction reformulations, the disjunctive programming models can be reformulated into MINLP models by the Big-M or convex hull methods with LogMIP as the solver. In essence, the LogMIP solver calls other MINLP algorithms to solve the disjunctive model. For this small-sized problem, BARON (Tawarmalani & Sahinidis, 2004) is adopted as the MINLP solver.

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Table 4 shows the computational performance of each reformulation. It is clear that Smooth Approximation performs much better than the other reformulations for this case study. The Smooth Approximation reformulation has fewer continuous variables and significantly fewer binary variables. The computation time is also considerably less than for the other three reformulations. The Direct Disjunction model has more disjunctions and continuous variables but fewer binary variables compared with the Explicit Disjunction model. The advantage of the Direct Disjunction reformulation is that it can easily be extended to cases with isothermal streams and multiple utilities. However, in the WHENs problem, phase change process streams are difficult to handle in a general way. Such streams need special attention in WHEN problems. The convex hull reformulation performs slightly better than the Big-M method for both Explicit and Direct Disjunction. It is clear that the intermediate temperature strategy has much fewer binary variables compared with the other two disjunctive reformulations. However, the performance of intermediate the temperature strategy is not satisfactory. This reformulation can only find an upper bound of the objective function within the CPU time limitation of 4000 s. The optimality gap is still very large when the solver terminates. The Intermediate Temperature strategy shows slow convergence properties. This case study is a simple and small size problem and only non-isothermal streams are considered. For large-scale problems, the intermediate temperature strategy may fail to get the optimal results using global solvers, such as BARON. It has been reported that the Smooth Approximation might cause numerical problems when isothermal streams or multiple utilities are involved. For cases without isothermal streams, Smooth Approximation performs better than other reformulations, as shown in this study. Each reformulation has its own merits and flaws. Which reformulation is better depends on the problem size and the stream properties involved in the system. For large-scale problems, BARON could be unable to reach the global optimum within rational time.

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Decomposition algorithms are likely to improve the computational efficiency of the Extended Duran-Grossmann model.

Table 4. Computational results for the case study

Items	SA	IT strategy	Explicit Disjunction		Direct Disjunction	
			Big-M	Convex hull	Big-M	Convex hull
Disjunctions	-	-	49	49	98	98
Continuous Variables	161	146	411	908	462	994
Binary Variables	4	53	151	151	102	102
Equations	171	339	762	1448	467	663
CPU time (s)	17.5	4000	207.3	196.3	76.6	61.2
Objective function (kW)	473.8	473.8*	473.8	473.8	473.8	473.8

* Upper bound obtained with the maximum computational time being 4000 s.

5. Conclusions

In this paper, the Duran-Grossmann model for heat integration is extended to solve Work and Heat Exchange Network problems. To solve the model efficiently, four reformulations of the original Duran-Grossmann model are reviewed and applied to the WHENs problem. In the Extended Duran-Grossmann model, even stream identities are variables in addition to temperature and heat capacity flowrate for the process streams. The Extended Duran-Grossmann model can get the same results as a manual procedure for WHENs based on Pinch Analysis and Thermodynamics. Each reformulation has its own advantages and disadvantages. For small-scale WHEN problems, all the reformulations can find the global optimum. However, the computational efforts and results of different reformulations have been compared. For the case study, the results show that the Smooth Approximation outperforms the other three reformulations. However, this case study represents a small size problem. Large-scale problems should be tested in future work. Isothermal process streams and multiple utilities should also be considered. The small parameter ε in the Smooth Approximation and the Big-

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M value in the disjunctive programming models have significant influence on the solution of the problems.

In summary, the reformulations of the Extended Duran-Grossmann model can only deal with small to moderate scale problems. Since there is a large number of binary variables in the model, it is quite computationally expensive for large-scale problems with the four reformulations evaluated in this study. In the future, other reformulations or decomposition algorithms should be developed for the Extended Duran-Grossmann model in order to solve more complex WHEN problems in PSE field.

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Nomenclature

CC	Composite Curve
C	Cold Stream Set
cu	Cold Utility
def	Heat deficit
DG	Duran-Grossmann Model
EDG	Extended Duran-Grossmann Model
ExPAnD	Extended Pinch Analysis and Design
FCp	Heat Capacity Flowrate
GAMS	General Algebraic Modeling System
GCC	Grand Composite Curve
H	Enthalpy/Hot Stream Set

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HEN	Heat Exchange Network
HRAT	Heat Recovery Approach Temperature
hu	Hot utility
i	Hot Streams
IT	Intermediate Temperature
j	Cold Streams
LogMIP	Logic-based disjunctive model solver
MINLP	Mixed Integer Non-Linear Programming
NLP	Non-Linear Programming
ORC	Organic Rankine Cycle
P	Pressure
p	Pinch candidate
PC	Pinch candidate set
PSE	Process System Engineering
QSOA	Heat load of hot streams above pinch candidates
QSIA	Heat load of cold streams above pinch candidates
R	A large number used in the explicit disjunction reformulation
S	Entropy/Stream set
SA	Smooth Approximation
sup	Supply state
tar	Target state
T	Temperature
WHEN	Work and Heat Exchange Network
WSK	Work sink stream
WSR	Work source stream
Y	Boolean variables
y	Binary variables

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γ	Specific heat capacity ratio
ω	Process variables

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