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On the use of risk-based Shapley values for cost sharing in interplant heat integration programs

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HIGHLIGHTS

- The cost-sharing plan of a multi-plant HEN is modelled as a cooperative game.
- Core and risk-based Shapley values of all plants are computed systematically.
- Cost burden of a plant is determined from its contribution and potential fallouts.
- A simple example is provided to illustrate the proposed methodology.

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ABSTRACT

The heat exchanger network (HEN) is traditionally used for optimal heat recovery in a single chemical plant, while the multi-plant counterparts have been studied in recent years primarily for the purpose of reaping additional overall energy savings. Since all these works focused primarily upon minimization of the total energy cost, the resulting interplant heat integration arrangements were often infeasible due to the fact that the individual savings are not always acceptable to all participating parties. Although a few studies addressed this cost-sharing issue, the existing methodologies are still not mature enough for realistic applications. The present paper outlines a rigorous model-based two-stage procedure to handle this practical problem in the spirit of a cooperative game. The minimum total annual cost (TAC) of each and every potential coalition was first determined with a conventional MINLP model, while the core and the risk-based Shapley values of all players were then computed with explicit formulas derived in this work to settle the benefit allocation issues. A simple example is presented at the end of this paper to demonstrate the feasibility of the proposed approach.

1. Introduction

Operating a typical chemical process usually calls for high consumption levels of hot and cold utilities, while the heat exchanger network (HEN) is indispensable in such a plant for the purpose of maximum heat recovery. Traditionally, a single-plant HEN design was generated with either a simultaneous optimization strategy [1] or a stepwise synthesis procedure [2,3]. The former usually yields a better trade-off between utility and capital costs, but the computational effort required for solving the corresponding mixed-integer nonlinear programming (MINLP) model can be quite demanding. On the other hand, although implementing a stepwise method is clearly easier, the sub-optimal solutions may often be obtained.

On the other hand, a number of recent studies have also been carried out for developing the multi-plant HEN designs on an industrial park, e.g., see Bagajewicz and Rodera [4] and Kralj [5] and Liew et al. [6]. The available synthesis methods for total-site heat integration (TSHI) can be roughly classified into three types: the insight-based pinch methods [7], the model-based methods [8] and the hybrid methods [6]. The corresponding interplant energy flows may be either realized with direct heat exchanges between process streams or facilitated indirectly with one or more extraneous fluid [9]. A comprehensive survey on the synthesis tools can also be found in Kastner et al. [10]

The main advantages of the first approach mentioned above are due to its target-setting strategy and flexible design steps based on engineering insights. Matsuda et al. [11] applied the R-curve analysis and site-source-sink-profile analysis for TSHI of the Kashima industrial park.

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Nomenclature

Indices

i hot process stream
j cold process stream
m hot utility
n cold utility
k index of the stages $(1,\cdots,NOK)$ and the temperature locations $(1,\cdots,NOK+1)$

Sets

H $=\{i|i$ is a hot process stream in coallition$\}$
C $=\{j|j$ is a cold process stream in coallition$\}$
HU $=\{m|m$ is a hot utility in coallition$\}$
CU $=\{n|n$ is a cold utility in coallition$\}$
ST $=\{k|k$ is a stage in the super structure$\}$

Parameters

TIN_i,TIN_j inlet temperature of hot process stream i or cold process stream j
$TOUT_i,TOUT_j$ outlet temperature of hot process stream i or cold process stream j
F_i,F_j heat capacity flowrate of hot process stream i or cold process stream j
TI_m,TI_n inlet temperature of hot utility m or cold utility n
$TT_{i,n}$ outlet temperature of cold utility n, when it exchanged heat with hot process stream i
$TT_{j,m}$ outlet temperature of hot utility m, when it exchanged heat with cold process stream j
$U_{i,j}$ overall heat transfer coefficient between hot process stream i and cold process stream j
$U_{i,n}$ overall heat transfer coefficient between hot process stream i and cold utility n
$U_{j,m}$ overall heat transfer coefficient between cold process stream j and hot utility m
$CQ_{i,n}$ per unit cost for cold utility n, when it exchange heat with hot process stream i
$CQ_{j,m}$ per unit cost for hot utility m, when it exchange heat with cold process stream j
$CF_{i,j}$ fixed charge for exchanger, when hot process stream i exchanged heat with cold process stream j
$CF_{i,n}$ fixed charge for exchanger, when hot process stream i exchanged heat with cold utility n
$CF_{j,m}$ fixed charge for exchanger, when cold process stream j exchanged heat with hot utility m
$CA_{i,j}$ area cost coefficient, when hot process stream i exchanged heat with cold process stream j
$CA_{i,n}$ area cost coefficient, when hot process stream i exchanged heat with cold utility n
$CA_{j,m}$ area cost coefficient, when cold process stream j exchanged heat with hot utility m
β exponent for area cost
NOK total number of stages
NST upper bound of split streams in each stage
ΔT_{min} minimum approach temperature difference
$\Omega_{i,j}$ an upper bound for heat exchange of match (i,j)
$\Omega_{i,n}$ an upper bound for heat exchange of match (i,n)
$\Omega_{j,m}$ an upper bound for heat exchange of match (j,m)
$\Gamma_{i,j}$ an upper bound for temperature difference of match (i,j)
$\Gamma_{i,n}$ an upper bound for temperature difference of match (i,n)
$\Gamma_{j,m}$ an upper bound for temperature difference of match (j,m)

Variables

$t_{i,k}$ temperature of hot process stream i at start of stage k
$t_{j,k}$ temperature of cold process stream j at start of stage k
$q_{i,j,k}$ heat exchanged between hot process stream i and cold process stream j in stage k
$q_{i,n}$ heat exchanged between hot process stream i and cold utility n
$q_{j,m}$ heat exchanged between cold process stream j and hot utility m
$z_{i,j,k}$ binary variable to denote existence of match (i,j) in stage k
$z_{i,n}$ binary variable to denote existence of match (i,n)
$z_{j,m}$ binary variable to denote existence of match (j,m)
$dt_{i,j,k}$ temperature approach for match (i,j) at temperature location k
$dtin_{i,n}$ temperature approach for match (i,n) (hot process stream i flow into utility exchanger)
$dtout_{i,n}$ temperature approach for match (i,n) (hot process stream i flow out utility exchanger)
$dtin_{j,m}$ temperature approach for match (j,m) (cold process stream j flow into utility exchanger)
$dtout_{j,m}$ temperature approach for match (j,m) (cold process stream j flow out utility exchanger)

Symbols of cooperative game

$N=\{1,2,\cdots,n\}$ set of players
n total of players (positive integer)
i player i
$v(\cdot)$ characteristic function
S subset of N
S_{+i} subset of N, which included the player i
$x_{S,i}$ the imputation of $v(S)$,which the player i who was from the coalition S could get
$\mathbf{x}_S$ imputation vector which was consisted by $x_{S,i}$
$C(v)$ The core which was defined by the characteristic function $v(\cdot)$
$\boldsymbol{\pi}_\sigma$ the σ th permutation from the n ! permutations of N
$\mathbf{m}^\sigma(v)$ marginal cost contribution vector which was defined by the characteristic function $v(\cdot)$ and the permutation $\boldsymbol{\pi}_\sigma$
$\mathbf{o}^\sigma(v)$ sorted marginal cost vector of $\mathbf{m}^\sigma(v)$
$\boldsymbol{\varphi}_N(v)$ Shapley Value vector of coalition N
$\varphi_{N,i}$ Shapley Value of the player i in grand coalition N
$\varphi_{S,i}$ Shapley Value of the player i in coalition S
L subset of S
L_{+i} subset of S, which included the player i
L^S broken sub-coalition which was collapsed from the specific coalition S
P subset of L
$w(L{:}\ L^S)$ total cost of coalition L in the case of L^S
$w(i{:}\ L^S)$ cost of player i in the case of L^S
$w(i{:}\ i^S)$ cost of player i, when the L^S collapsed into player i work alone
α_i drop out probability of player i
$p(L|S)$ occurrence probability of broken sub-coalition L^S
$r(i{:}\ L^S)$ risk loss of player i in the case of L^S
$\mathrm{E}[r(i{:}\ L^S)]$ expected loss of player i due to random plant shutdowns
$\mathbf{h}^\sigma(v)$ expected risk marginal cost vector which was defined by the characteristic function $v(\cdot)$ and the permutation $\boldsymbol{\pi}_\sigma$
$\boldsymbol{\theta}^\sigma(v)$ sorted expectation risk marginal cost vector of $\mathbf{h}^\sigma(v)$
$\boldsymbol{\Psi}_S(v)$ allocation coefficient of risk based Shapley Value of coalition N
$\hat{\boldsymbol{\varphi}}_S(v)$ risk based Shapley Value vector of coalition N
$\hat{\varphi}_{S,i}$ risk based Shapley Value of player i of coalition N

For unstable renewable energy supply, Liew et al. [12,13] developed the time-slice based targeting procedures to handle the energy supply/demand variability in TSHI. Liew et al. [14] also proposed a pinch-based TSHI concept that integrates not only heat and power, but also cooling. Furthermore, they constructed a retrofit framework [15] and showed that energy retrofit projects should always be approached from the total-site context first. Finally, the same research group [15] developed a modified TSHI method to address the non-isothermal utility targeting issues.

The model-based methods are clearly more rigorous and better equipped for locating the true optimum. Zhang et al. [16] proposed a superstructure for building a MINLP model to synthesize multi-plant HEN designs. Chang et al. [8] presented a simultaneous optimization methodology for interplant heat integration using the intermediate fluid circle(s). Finally, Wang et al. [9] adopted a hybrid approach for the same problems. The pros and cons of interplant heat integrations using direct, indirect and combined methods were analyzed and compared on the basis of composite curves, while the mathematical programming models were adopted to determine the optimal solutions.

According to Cheng et al. [17], the TSHI arrangements obtained with the aforementioned approaches may not always be implementable. This is because of the facts that these conventional HEN design strategies only focused upon minimization of the overall energy cost and, as a result, the benefit distribution plan can be unacceptable to one or more participating party. Thus, the key to a successful TSHI project should be to develop, in addition to an energy-efficient multi-plant HEN design, a "fair" cost sharing scheme under uncertainties [18]. Hiete et al. [19] first treated this benefit distribution issue as a cooperative game, but their approach is not rigorous due to the requirements of heuristic judgments. On the other hand, Cheng et al. [17] formulated a series of mathematical programming models by depicting the cost-saving allocation problem as a non-cooperative game and then solved these models with the conventional sequential optimization strategy. The TSHI schemes were generated in a later study [20] with the same approach, but the interplant heat flows were limited to those facilitated by intermediate fluids or utilities. There are two obvious weaknesses of the existing model-based methods. First of all, the HEN design produced with the sequential optimization method cannot always reach a true optimum. More importantly, for total-site heat integration, the assumption of non-cooperative game may not be valid.

The research objective of present study is thus to develop a rigorous synthesis procedure for producing a fair cost sharing plan in the spirit of a cooperative game so as to facilitate realization of the multi-plant HEN design obtained with the simultaneous optimization strategy [1]. The proposed approach is implemented basically in two stages. The minimum total annual cost (TAC) of each and every potential coalition was first determined with a modified version of the conventional MINLP model [1]. An important implication of this model is that, in the resulting multi-plant HEN, the interplant heat flows are primarily facilitated with direct matches between hot and cold process streams. On the other hand, the benefit allocation issue is addressed in the second stage on the basis of the risk-based Shapley values. An effective cost sharing scheme is constructed in this stage according to the core solution of a cooperative game [21] and the risk-based Shapley values of all players [22,23]. The former ensures solution feasibility, while the latter yields a reasonable cost distribution plan. The justifications for adopting the aforementioned two-stage implementation strategy are twofold, i.e., (1) the simultaneous HEN synthesis method usually yields a better trade-off than the sequential counterpart and (2) the Shapley value of any given coalition can be computed in a straightforward fashion in the second stage with only a single aggregated index, i.e., the minimum TACs obtained in the first stage.

Finally, it should be noted that, although the applications of Shapley values in interplant heat integration cannot be found in literature, various studies have been carried out to regulate the electricity market [24,25] and to optimize the distributed hybrid energy networks [26,27]. In addition, several novel solution methods of the cooperative games have also been proposed on the basis of new viewpoints which have not been brought up before. For examples, Maali [28] developed a computation method to determine the Shapley values by optimizing the individual weights in a game, and this method was applied to process integration concerning palm-based biomass processing complex and sago-based bio-refinery [29]. Therefore, in order to achieve the aforementioned research objective, all required formulas have been derived and the corresponding computation methods developed in this work and they are presented in detail in the sequel.

2. Optimal HEN structures across plant boundaries

As mentioned before, the heat exchanger network in a single plant can be designed with either a sequential synthesis procedure [2,3] or a simultaneous optimization strategy [1]. Although the former approach is simpler, the total annual cost of the final solution may not be truly minimized in every application. Since the interplant heat integration scheme is viewed in the present study as a coalition in cooperative game, the latter strategy is adopted in the present study for synthesizing the HEN structure across the plant boundaries so as to achieve an optimal trade-off between utility and capital costs. To this end, the conventional MINLP model has to be reformulated to facilitate proper utilization of the various utilities available in different plants. This modified version is presented in Appendix for the sake of completeness.

3. Core and Shapley values in a cooperative game

Let us consider the grass-root designs of a common heat-exchanger network (HEN) used by multiple chemical plants on an industrial park. If these plants are owned by different companies, the practical issues of fair cost allocation for building and operating such a shared system should be addressed thoroughly so as to reap the potential benefits of interplant heat integration. If this problem is viewed as a cooperative game, it is imperative to identify the most suitable subset of all possible players to form a so-called "coalition." Typically, the core and Shapley values are used to characterize the reasonable and fair solution(s) for distributing the financial burdens within the coalition. Although extensive discussions on their evaluation procedures have already been published, e.g., see Branzei et al. [30], a brief summary is still given in the sequel for the sake of illustration clarity.

3.1. Core

"Core" is in essence the solution set of a cooperative game. Each solution in the set depicts a feasible plan for every member of the coalition to shoulder the cost for building the multi-plant HEN. To facilitate accurate illustration, let us use $N = \{1,2,\cdots,n\}$ to represent the set of all players in a game and $S \subseteq N$ denotes a coalition. Then all possible coalitions should form the power set of N (denoted as 2^N) and a characteristic function $v(\cdot)$ can be defined accordingly as the mapping v: $2^N \to R$. The function value $v(S)$, where $S \in 2^N$, is the total annual cost (TAC) incurred to the coalition as a whole. To ensure function consistency, it is also required that $v(\emptyset) = 0$. To be more specific, let us consider a fictitious example in which $N = \{1,2,3\}$. The corresponding characteristic functions can be written as: $v(\{1,2,3\})$, $v(\{1,2\})$, $v(\{2,3\})$, $v(\{3,1\})$, $v(\{1\})$, $v(\{2\})$ and $v(\{3\})$. For simplicity, it should be noted that the braces in these functions can be removed without causing confusion.

Let us further denote the annual cost allocated to plant $i \in N$ in coalition $S \subseteq N$ as $x_{S,i}$. Thus, $v(S) = \sum_{i \in S} x_{S,i}$ and $\mathbf{x}_S = [x_{S,1}, x_{S,2}, \cdots, x_{S,n}]$ is referred to as the *pre-imputation* vector of coalition S. The pre-imputation vector of grand coalition N, i.e., $\mathbf{x}_N$, in the core $C(v)$ should possess the following properties

1. Individual rationality

$$x_{N,i} \leqslant v(i) ,\forall\ i \in N; \tag{1}$$

2. Group rationality

$$\sum_{i \in N} x_{N,i} = v(N); \tag{2}$$

3. Coalition rationality

$$\sum_{i \in S} x_{N,i} \leqslant v(S) ,\forall\ S \subseteq N; \tag{3}$$

4. No cross subsidization

$$x_{N,i} \geqslant v(N) - v(N\backslash i) ,\forall\ i \in N. \tag{4}$$

Notice that $v(N\backslash i)$ denotes the cost incurred to the sub-coalition formed by excluding player i from the grand coalition N. In other words, Eq. (4) implies that the cost burden of player i for joining coalition N should be larger than or equal to its marginal cost contribution. Notice also that, although $C(v)$ represents a feasible region, a definite one-point solution is still lacking.

3.2. Shapley values

A one-point solution can be produced on the basis of the well-recognized Shapley-value vector, which happens to be located at the centroid of a nonempty convex $C(v)$. More specifically, this solution approach calls for dividing and distributing the TAC of a coalition according to the average cost contribution level of each participating member. In evaluating such contribution levels, it is clearly necessary to consider the cost burdens of all possible sub-coalitions $S \subseteq N$ so as to produce a fair distribution plan. To enumerate all scenarios exhaustively, let us first consider the $n!$ permutations of the n players in N and collect the corresponding sequences in set $\boldsymbol{\pi}(N)$. Let us also denote an element in $\boldsymbol{\pi}(N)$ as $\boldsymbol{\pi}_\sigma$ (where, $\sigma = 1,2,\cdots,n!$), i.e., $\boldsymbol{\pi}(N) = \{\boldsymbol{\pi}_1,\boldsymbol{\pi}_2,\cdots,\boldsymbol{\pi}_{n!}\}$, while a particular sequence σ' in $\boldsymbol{\pi}(N)$ may be expressed explicitly as $\boldsymbol{\pi}_{\sigma'} = (\pi_{\sigma'}(1),\pi_{\sigma'}(2),\cdots,\pi_{\sigma'}(n))$. A set of marginal cost contributions (denoted as $\mathbf{m}^\sigma$) can then be computed for every sequence $\boldsymbol{\pi}_\sigma$ in $\boldsymbol{\pi}(N)$, i.e.

$$\mathbf{m}^\sigma(v) = \{m^\sigma_{\pi_\sigma(1)}(v),m^\sigma_{\pi_\sigma(2)}(v),\cdots,m^\sigma_{\pi_\sigma(k)}(v),\cdots,m^\sigma_{\pi_\sigma(n)}(v)\} \tag{5}$$

where

$$m^\sigma_{\pi_\sigma(1)}(v) = v(\pi_\sigma(1)) - v(\varnothing) \tag{6}$$

$$m^\sigma_{\pi_\sigma(k)}(v) = v(\pi_\sigma(1),\cdots,\pi_\sigma(k)) - v(\pi_\sigma(1),\cdots,\pi_\sigma(k-1)) \tag{7}$$

$k = 2,3,\cdots,n$. Note that the precedence order of the elements in set $\mathbf{m}^\sigma(v)$ corresponds to that in $\boldsymbol{\pi}_\sigma$. These elements can be rearranged according the original precedence order in N and then placed in a column vector $\mathbf{o}^\sigma(v)$. For example, if N= {1,2,3,4}, $\boldsymbol{\pi}_\sigma = (4,3,1,2)$ and $\mathbf{m}^\sigma(v) = \{19,25,11,50\}$, then $\mathbf{o}^\sigma(v) = [11,50,25,19]^T$.

After obtaining the vector $\mathbf{o}^\sigma(v)$ that stores the rearranged marginal contributions for every sequence $\boldsymbol{\pi}_\sigma$ in $\boldsymbol{\pi}(N)$, one can then compute the Shapley-value vector $\boldsymbol{\varphi}_N(v)$ with the following formula

$$\boldsymbol{\varphi}_N(v) = \frac{1}{n!} \sum_{\boldsymbol{\pi}_\sigma \in \boldsymbol{\pi}(N)} \mathbf{o}^\sigma(v) \tag{8}$$

where $\boldsymbol{\varphi}_N(v) = [\varphi_{N,1},\varphi_{N,2},\cdots,\varphi_{N,n}]^T$ and $\varphi_{N,i}$ (where, $i = 1,2,\cdots,n$) denotes the average cost shared by player i for joining coalition N. It should be noted that the above notation on the Shapley values can be extended to any subset of the grand coalition, i.e., $S \subseteq N$. If the players in S form a coalition, then the Shapley value of player i ($\forall\ i \in S$) can be written as $\varphi_{S,i}$.

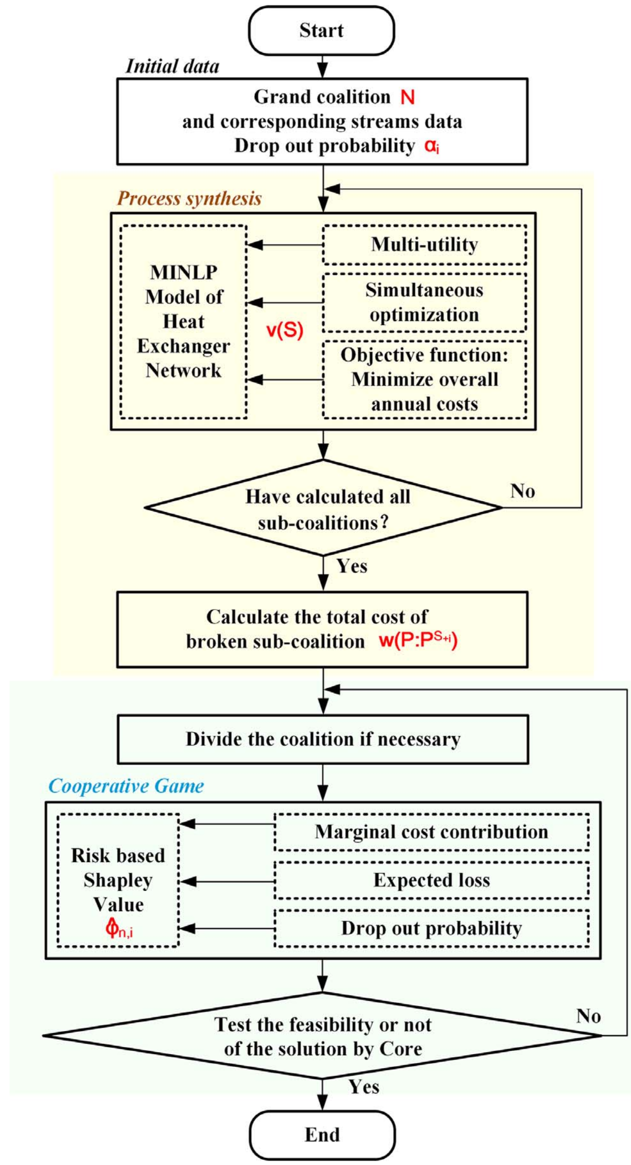

Fig. 1. Risk-based evaluation procedure for cost allocation in a coalition.

Table 1
Stream data.

Plant	Stream	*TIN* (°C)	*TOUT* (°C)	*F* (kW/°C)
P1	H1	150	40	7.0
P1	C1	60	140	9.0
P1	C2	110	190	8.0
P2	H1	200	70	5.5
P2	C1	30	110	3.5
P2	C2	140	190	7.5
P3	H1	370	150	3.0
P3	H2	200	40	5.5
P3	C1	110	360	4.5

4. Potential fallouts of interplant heat integration

In computing the aforementioned Shapley values, the marginal cost contributions of each player in all possible scenarios (i.e., all precedence orders in forming the coalitions) are averaged so as to ensure that the TAC of the coalition is distributed fairly. However, this computation procedure still ignores the potential risk of coalition breakdowns.

Table 2
Utility data.

Plant	Utility	*TI* (°C)	*CQ* ("$"/kW·yr)
P1	Cooling water	25	100
P1	HP steam	200	800
P1	Hot oil	500	1200
P2	Cooling water	25	150
P2	HP steam	200	900
P2	Hot oil	500	1300
P3	Cooling water	25	80
P3	HP steam	200	850
P3	Hot oil	500	1100

Table 3
Minimum TACs of HEN Designs in All Possible Coalitions ("$"/yr).

$v(1) = 725{,}433.4$	$v(2) = 168{,}593.8$	$v(3) = 404{,}900.8$	$v(1,2) = 696{,}886.1$
$v(1,3) = 880{,}416.7$	$v(2,3) = 463{,}990.1$	$v(1,2,3) = 887{,}932.4$	$v(\varnothing) = 0$

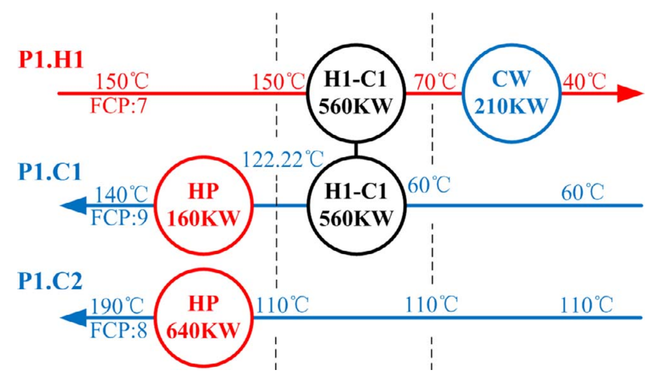

Fig. 2. Optimal HEN design of {P1}.

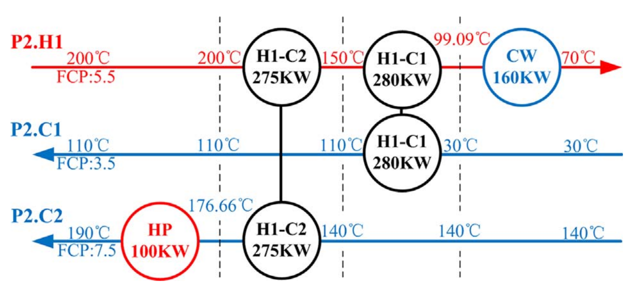

Fig. 3. Optimal HEN design of {P2}.

As a general rule, the reliability of an interconnected engineering system should be treated as an important design issue. If the interplant heat integration scheme is viewed as a coalition in cooperative game, then the potential risk of its collapse must be considered seriously. An unplanned plant shutdown, which may be due to a wide variety of equipment failures and/or human errors, obviously disables some of the hot and cold streams in the multi-plant HEN and forces the other functional plants in coalition take emergency measures. Thus, it is necessary to adjust the aforementioned conventional Shapley values by assessing penalties for the potential fallouts of interplant heat integration. Since the characteristic function $v(S)$ yields the minimum TAC of a *functional* HEN for coalition $S \subseteq N$, the shutdown risk of plant $i \in S$ can be expressed with its time-averaged unreliability over a year (denoted as α_i). Note that the failure rate of a hardware item may be extracted from the historical maintenance data, e.g., see Hoyland and Rausand [31], which should be viewed as an intrinsic parameter of the given plant. On the other hand, the financial penalties of other plants in coalition S in this scenario can only be estimated on a case-by-case basis. For illustration convenience and computation simplicity, their lower limits are adopted in all case studies presented in this paper. More specifically, it is assumed that every interplant heat exchange that involves the process stream in the disabled plant can always be facilitated with a utility supplied by its counterpart.

5. Individual costs in a defective coalition

As mentioned before, the characteristic function $v(S)$ determines the minimum TAC of coalition $S \subseteq N$. If for some reason player $s \in S$ drops out of the coalition, the cost burden of defective coalition $S\backslash s$ clearly should be higher than $v(S\backslash s)$ because of the extra penalty incurred by coalition break-up. To facilitate precise explanation, let us use S_{+i} and L_{+i} to represent two subsets of the grand coalition that both contain player i. The former subset $S_{+i} \subseteq N$ denotes the original coalition, while the latter $L_{+i} \subseteq S_{+i}$ represents the defective coalition formed by excluding all members in $S_{+i}\backslash L_{+i}$.

Let us next denote the total cost of defective coalition L_{+i} as $w(L_{+i}\colon L_{+i}^{S_{+i}})$ and the corresponding individual cost of player $i \in L_{+i}$ as $w(i\colon L_{+i}^{S_{+i}})$. It must be first noted that the latter is not equivalent to player i working alone, i.e., $w(i\colon L_{+i}^{S_{+i}}) \neq w(i\colon i^{S_{+i}})$. In this study, the computation procedure of $w(i\colon L_{+i}^{S_{+i}})$ is essentially the same as that for the conventional Shapley values. First of all, the group rationality must be satisfied, i.e.

$$\sum_{j \in L_{+i}} w(j\colon L_{+i}^{S_{+i}}) = w(L_{+i}\colon L_{+i}^{S_{+i}}) \tag{9}$$

If the defective coalition L_{+i} further collapses into $P \subseteq L_{+i}$, the corresponding total cost of sub-coalition P is denoted in this paper as

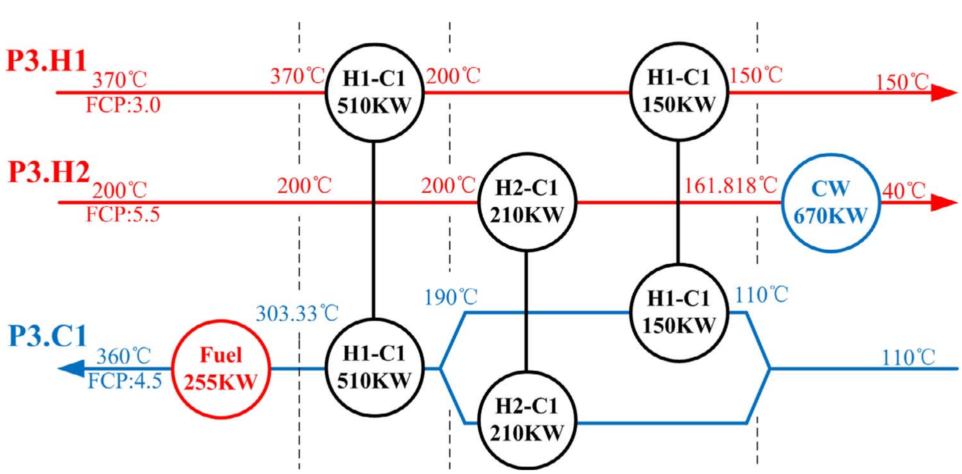

Fig. 4. Optimal HEN design of {P3}.

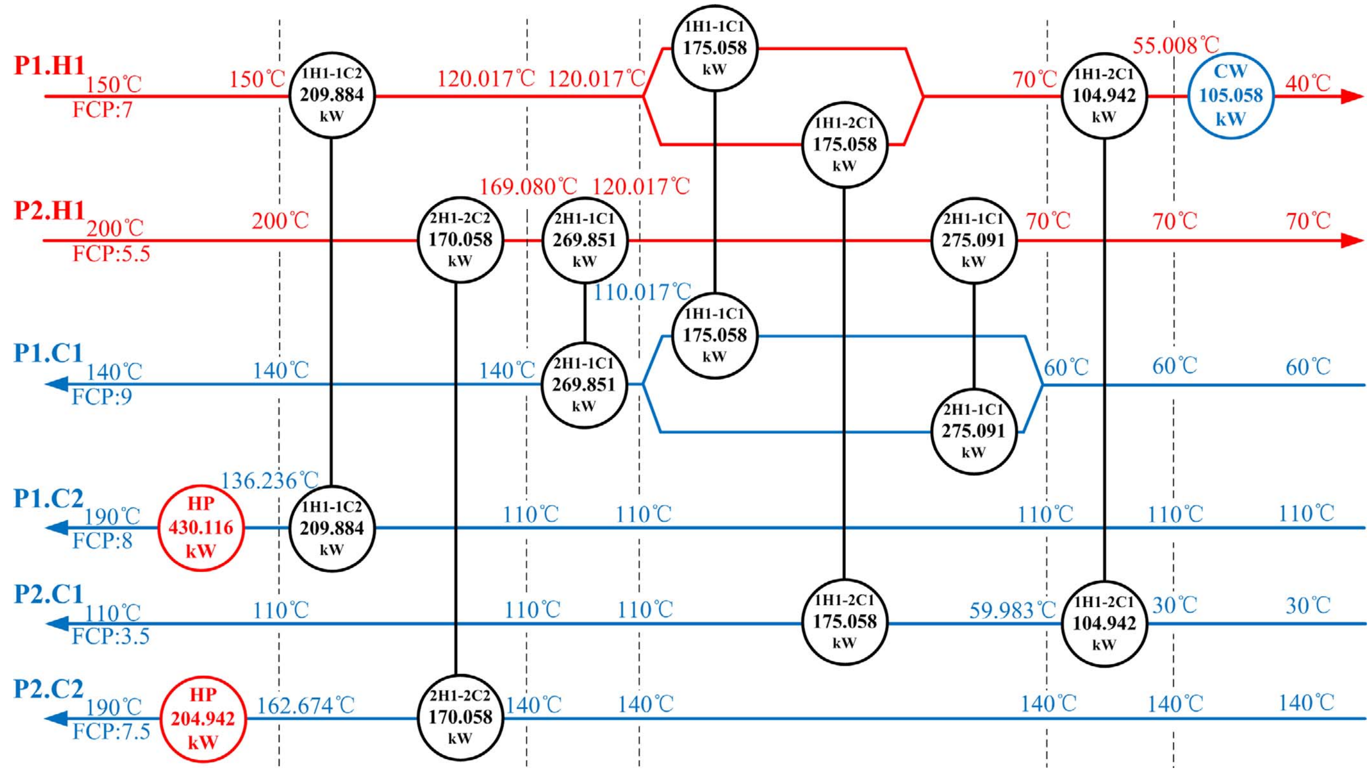

Fig. 5. Optimal HEN design of {P1,P2}.

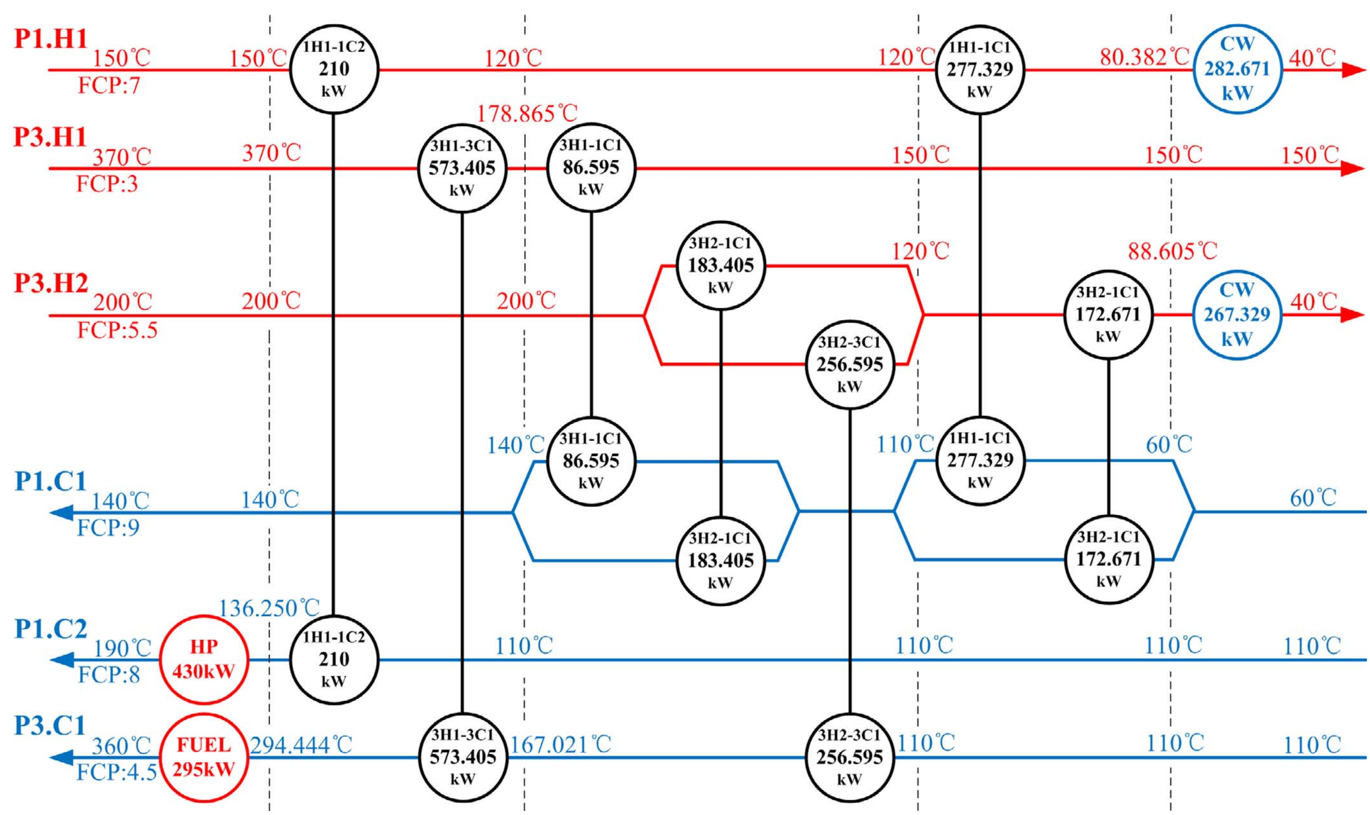

Fig. 6. Optimal HEN design of {P1,P3}.

$w(P{:}\ P^{S_{+i}})$. It should be noted that this cost should be used to replace $v(P)$ in computing the conventional Shapley values. As a result, a fair cost distribution scheme can also be stipulated for the defective coalition L_{+i} by calculating $w(L_{+i}{:}\ L_{+i}^{S_{+i}})$ and all $w(i{:}\ L_{+i}^{S_{+i}})$ that satisfy Eq. (9).

More specifically, this computation procedure can be expressed mathematically as follows

$$w(i{:}\ L_{+i}^{S_{+i}}) = \sum_{i\in P\subseteq L_{+i}} \omega(P)M(P) \tag{10}$$

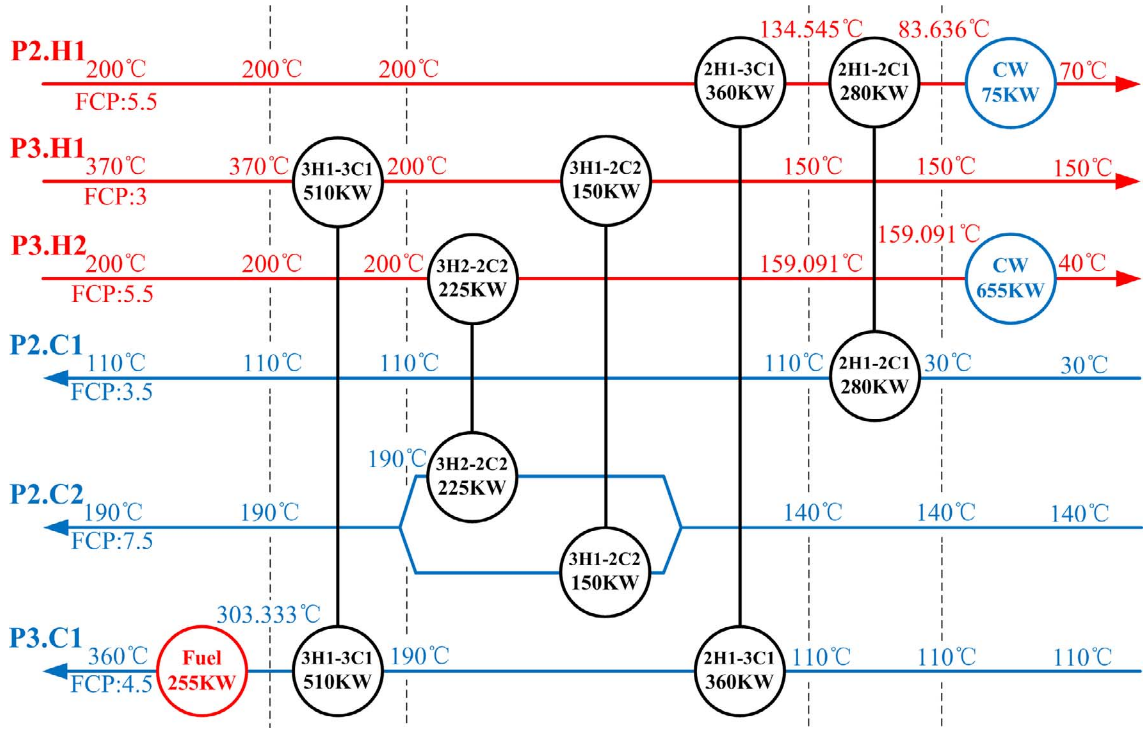

Fig. 7. Optimal HEN design of {P2,P3}.

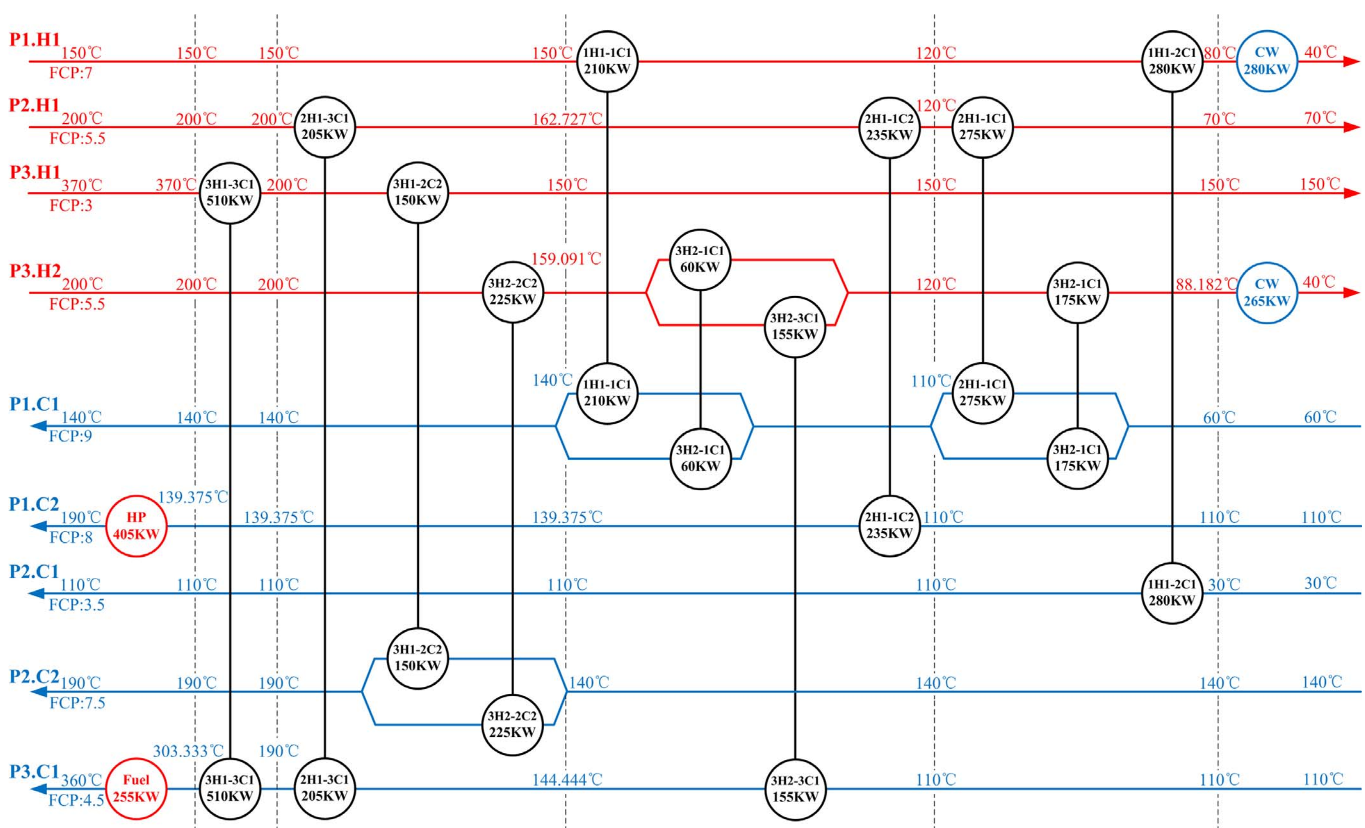

Fig. 8. Optimal HEN design of {P1,P2,P3}..

$$\omega(P) = \frac{(|P|-1)!(|L_{+i}|-|P|)!}{|L_{+i}|!} \tag{11}$$

$$M(P) = w(P\colon P^{S_{+i}}) - w(\{P\backslash i\}\colon \{P\backslash i\}^{S_{+i}}) \tag{12}$$

where $\omega(P)$ is the weighting factor of $P \subseteq L_{+i}$; $M(P)$ is the marginal cost contribution of player i in the defective sub-coalition P; $|P|$ and $|L_{+i}|$ denote the cardinalities of sets P and L_{+i} respectively. The weighted average w(i: $L_{+i}^{S_{+i}}$) clearly represents the contribution of player i in the defective coalition L_{+i}. It should be noted that the above calculations should be carried out without sorting the marginal contributions since

Table 4
Cost allocations: shapley values in different coalitions.

Coalition	Cost shared by P1 ("\$"/yr)	Cost shared by P2 ("\$"/yr)	Cost shared by P3 ("\$"/yr)
{1}	$\varphi_{\{1\},1}$ = 725,433.4	0	0
{2}	0	$\varphi_{\{2\},2}$ = 168,593.8	0
{3}	0	0	$\varphi_{\{3\},3}$ = 404,900.8
{1,2}	$\varphi_{\{1,2\},1}$ = 626,862.8	$\varphi_{\{1,2\},2}$ = 70,023.2	0
{1,3}	$\varphi_{\{1,3\},1}$ = 600,474.7	0	$\varphi_{\{1,3\},3}$ = 279,942.1
{2,3}	0	$\varphi_{\{2,3\},2}$ = 113,841.5	$\varphi_{\{2,3\},3}$ = 350,148.5
{1,2,3}	$\varphi_{\{1,2,3\},1}$ = 550,426.6	$\varphi_{\{1,2,3\},2}$ = 63,793.5	$\varphi_{\{1,2,3\},3}$ = 273,712.3

all possible scenarios are inherently included. Finally, the individual cost of player i in the original non-defective coalition S_{+i} should be identical to its conventional Shapley value, i.e.

$$w(i:\, S_{+i}^{S_{+i}}) = \varphi_{S_{+i},i} \tag{13}$$

As a result, it is clear that

$$w(S_{+i}:\, S_{+i}^{S_{+i}}) = v(S_{+i}) \tag{14}$$

6. Expected loss due to random plant Shutdown(s)

Let us consider plant $i \in N$ in a coalition $S_{+i} \subseteq N$. If all other plants can be assumed to always stay within the coalition, the marginal contribution of plant i joining S_{+i} should be $v(S_{+i})-v(S_{+i}\backslash i)$. However, as mentioned previously, since the average unreliability of plant j, i.e., α_j ($\forall\, j \in S_{+i}$), is not negligible, it is necessary to evaluate the corresponding expected losses. To facilitate accurate analysis, let us again divide S_{+i} into two subsets as before, that is, the defective coalition L_{+i} and also the subset formed by the dropouts ($S_{+i}\backslash L_{+i}$). By assuming that the plants in $S_{+i}\backslash L_{+i}$ break down independently, the conditional probability of this scenario can be expressed as

$$p(L_{+i}|S_{+i}) = \Big(\prod_{j\in\{S_{+i}\backslash L_{+i}\}} \alpha_j\Big)\cdot\Big(\prod_{k\in L_{+i}} \beta_k\Big) \tag{15}$$

where $\beta_k = 1-\alpha_k$. As mentioned before, the corresponding cost should be written as $w(i:\, L_{+i}^{S_{+i}})$ and its value is obviously larger than $\varphi_{S_{+i},i}$. Consequently, the potential "risk" in this case can be expressed as

$$r(i:\, L_{+i}^{S_{+i}}) = p(L_{+i}|S_{+i})\cdot(w(i:\, L_{+i}^{S_{+i}})-\varphi_{L_{+i},i}) = \Big(\prod_{j\in\{S_{+i}\backslash L_{+i}\}} \alpha_j\Big)\cdot\Big(\prod_{k\in L_{+i}} \beta_k\Big)\cdot (w(i:\, L_{+i}^{S_{+i}})-\varphi_{L_{+i},i}) \tag{16}$$

By enumerating all possible defective coalitions in S_{+i}, one can then construct a formula for computing the expected loss due to random plant shutdowns:

$$E[r(i:\, L_{+i}^{S_{+i}})] = \sum_{L_{+i}\subseteq S_{+i}} r(i:\, L_{+i}^{S_{+i}}) = \sum_{L_{+i}\subseteq S_{+i}} \Big\{\Big(\prod_{j\in\{S_{+i}\backslash L_{+i}\}} \alpha_j\Big)\cdot\Big(\prod_{k\in L_{+i}} \beta_k\Big)\cdot(w(i:\, L_{+i}^{S_{+i}})-\varphi_{L_{+i},i})\Big\} \tag{17}$$

7. Risk-based Shapley values

Having obtained the expected losses with Eq. (17), one can then try to allocate the proper cost for *every* plant in a coalition accordingly. Specifically, from the point of view of any plant in a coalition (say $j \in S$), it is reasonable to demand for a cost cut if there are significant risks of other plants breaking down unexpectedly. In other words, other than the marginal contribution levels considered in Eqs. (5-7), the aforementioned expected losses must also be incorporated in the computation procedure of risk-based Shapley values.

Since $v(S)-v(S\backslash j)$ represents the marginal cost contribution of plant j to the TAC of coalition S without considering dropouts, then its demand level for actual allocation should be made higher by considering the corresponding expected loss in Eq. (17). Eqs. (5-8) can be modified according to the above arguments. To be specific, let us assume $S = \{1,2,\cdots,n\}$ and consider sequence σ in $\boldsymbol{\pi}(S)$, i.e., $\boldsymbol{\pi}_\sigma = (\pi_\sigma(1),\pi_\sigma(2),\cdots,\pi_\sigma(n))$. Let us further express the risk-adjusted marginal costs as

$$\mathbf{h}^\sigma(v) = \{h^\sigma_{\pi_\sigma(1)}(v),h^\sigma_{\pi_\sigma(2)}(v),\cdots,h^\sigma_{\pi_\sigma(k)}(v),\cdots,h^\sigma_{\pi_\sigma(n)}(v)\} \tag{18}$$

All elements in this set can be computed as follows:

$$h^\sigma_{\pi_\sigma(1)}(v) = v(\pi_\sigma(1))-v(\varnothing)-E[r(\pi_\sigma(1):\, L_{+\pi_\sigma(1)}^{\{\pi_\sigma(1)\}})] \tag{19}$$

$$h^\sigma_{\pi_\sigma(k)}(v) = v(\pi_\sigma(1),\cdots,\pi_\sigma(k))-v(\pi_\sigma(1),\cdots,\pi_\sigma(k-1)) -E[r(\pi_\sigma(k):\, L_{+\pi_\sigma(k)}^{\{\pi_\sigma(1),\cdots,\pi_\sigma(k)\}})] \tag{20}$$

where $k = 2,3,\cdots,n$. The precedence order of the elements in set $\mathbf{h}^\sigma(v)$ must correspond to that in $\boldsymbol{\pi}_\sigma$, and these elements should be rearranged

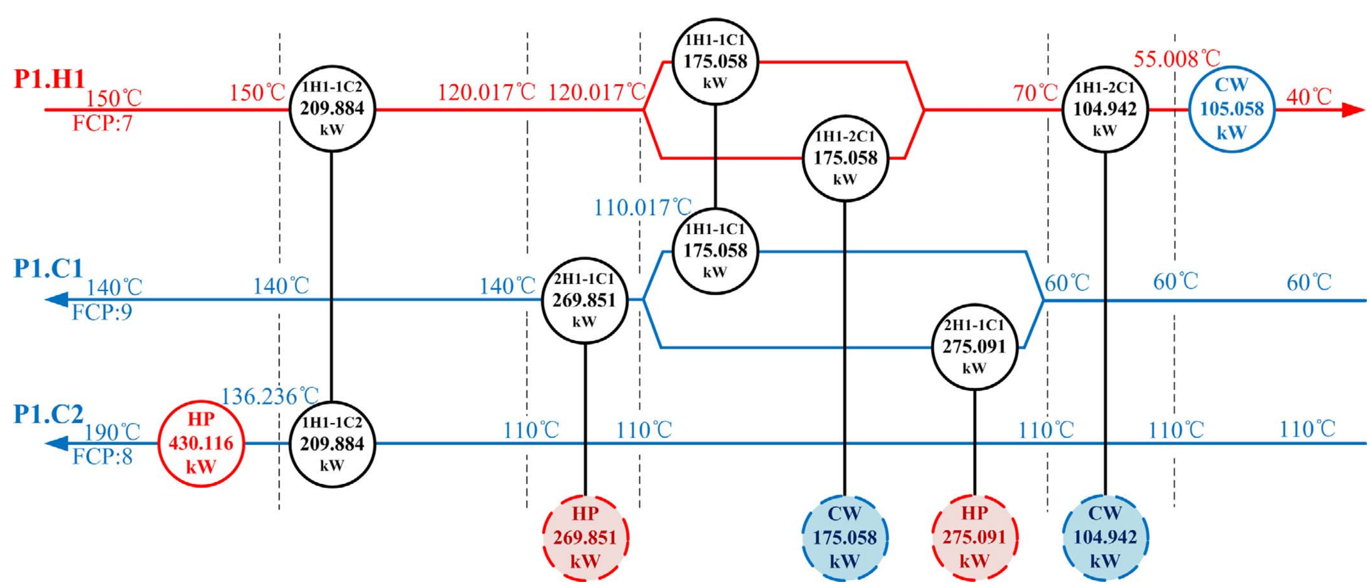

Fig. 9. HEN of {P1} evolved from {P1,P2}..

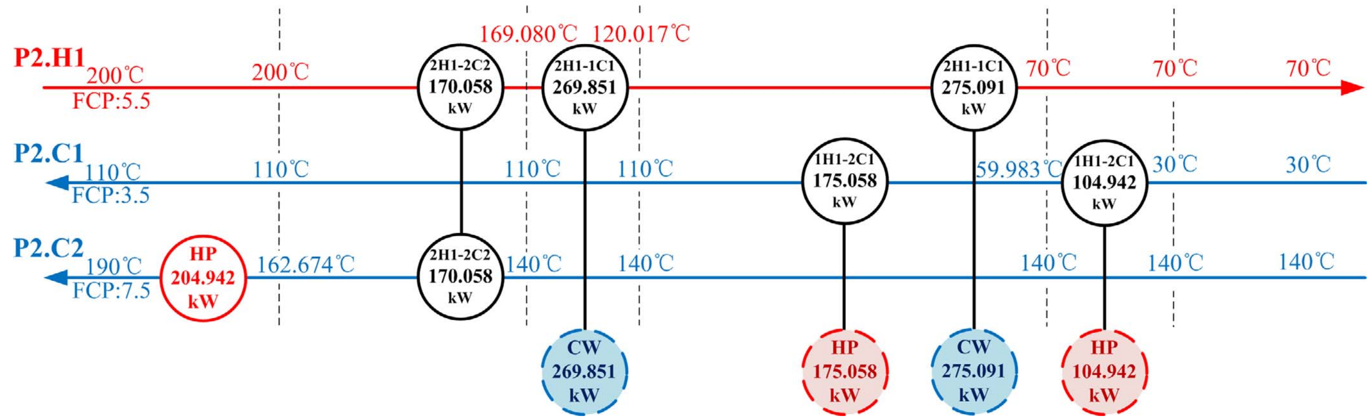

Fig. 10. HEN of {P2} evolved from {P1,P2}.

Table 5
Cost burdens of individual plants in defective coalitions in all scenarios.

$w(1: 1^{1}) = 725{,}433.4$	$w(3: 3^{\{1,3\}}) = 477{,}863.2$
$w(2: 2^{2}) = 168{,}593.8$	$w(2: 2^{\{2,3\}}) = 479{,}079.9$
$w(3: 3^{3}) = 404{,}900.8$	$w(3: 3^{\{2,3\}}) = 764{,}239.8$
$w(1: \{1,2\}^{\{1,2\}}) = 626{,}862.8$	$w(1: 1^{\{1,2,3\}}) = 1{,}103{,}470.5$
$w(2: \{1,2\}^{\{1,2\}}) = 70{,}023.2$	$w(2: 2^{\{1,2,3\}}) = 797{,}944.4$
$w(1: \{1,3\}^{\{1,3\}}) = 600{,}474.7$	$w(3: 3^{\{1,2,3\}}) = 658{,}271.2$
$w(3: \{1,3\}^{\{1,3\}}) = 279{,}942.1$	$w(\{1,2\}: \{1,2\}^{\{1,2,3\}}) = 1{,}085{,}074.7$
$w(2: \{2,3\}^{\{2,3\}}) = 113{,}841.5$	$w(\{1,3\}: \{1,3\}^{\{1,2,3\}}) = 1{,}528{,}182.4$
$w(3: \{2,3\}^{\{2,3\}}) = 350{,}148.5$	$w(\{2,3\}: \{2,3\}^{\{1,2,3\}}) = 877{,}561.5$
$w(1: \{1,2,3\}^{\{1,2,3\}}) = 550{,}426.6$	$w(1: \{1,2\}^{\{1,2,3\}}) = 695{,}300.3$
$w(2: \{1,2,3\}^{\{1,2,3\}}) = 63{,}793.5$	$w(2: \{1,2\}^{\{1,2,3\}}) = 389{,}774.3$
$w(3: \{1,2,3\}^{\{1,2,3\}}) = 273{,}712.3$	$w(1: \{1,3\}^{\{1,2,3\}}) = 986{,}690.8$
$w(1: 1^{\{1,2\}}) = 949{,}223.0$	$w(3: \{1,3\}^{\{1,2,3\}}) = 541{,}491.6$
$w(2: 2^{\{1,2\}}) = 635{,}617.7$	$w(2: \{2,3\}^{\{1,2,3\}}) = 508{,}617.3$
$w(1: 1^{\{1,3\}}) = 831{,}061.5$	$w(3: \{2,3\}^{\{1,2,3\}}) = 368{,}944.1$

Table 6
Conventional and risk-based shapley values ("$"/yr).

i	1	2	3
$\varphi_{\{1,2,3\},i}$	550,426.6	63,793.5	273,712.3
$\hat{\varphi}_{\{1,2,3\},i}$	578,443.7	23,388.7	286,100.0

according the original precedence order in S and then placed in a column vector $\theta^{\sigma}(v)$. Next, a column vector of the risk-based distribution coefficients can be determined according to the following formula

$$\mathbf{\Psi}_S(v) = \frac{1}{n!}\sum_{\pi_\sigma \in \pi(S)} \theta^{\sigma}(v) \tag{21}$$

Notice that this vector is not yet the finalized allocation plan since the requirement of group rationality is not satisfied. To address this need, $\mathbf{\Psi}_S$ should be normalized so as to produce the risk-based Shapley values as follows

$$\hat{\boldsymbol{\varphi}}_S(v) = \frac{\mathbf{\Psi}_S(v)}{\mathbf{\Psi}_S(v)^T 1_{n\times 1}} v(S) \tag{22}$$

where $\hat{\boldsymbol{\varphi}}_S(v) = [\hat{\varphi}_{S,1},\hat{\varphi}_{S,2},\cdots,\hat{\varphi}_{S,n}]^T$ and $\hat{\varphi}_{S,j}$ $(j = 1,2,\cdots,n)$ denotes the risk-based Shapley value of plant $j \in S$; $1 = [11\cdots1]^T$; $v(S)$ is the total cost of coalition S.

8. Computation flowchart

The proposed two-stage computation procedure can be summarized in the flowchart given below in Fig. 1. Notice that the required inputs are: (1) all n plants in the grand coalition; (2) the stream data (i.e., the heat capacity flow rates of all process streams and their initial and target temperatures) and utility specifications (i.e., the temperature ranges and unit costs of all hot and cold utilities) of each plant; (3) the drop-out probabilities of all plants.

In the first stage, the modified simultaneous optimization strategy [1] is first applied repeatedly to generate optimal HEN designs for 2^n-1 combinations of potential coalitions. The resulting minimum TAC of each coalition is treated as its characteristic value in cooperative game. The actual cost burdens of sub-coalitions in all possible defective coalitions, i.e., $w(P: P^{S_{+i}})$ s, and the corresponding costs of players remained in the defective coalitions, i.e., $w(i: L_{+i}^{S_{+i}})$, can then be computed according to Eqs. (9-14).

The computations in stage 2 address the allocation issues. Eq. (17) determines the expected loss due to random plant shutdowns, while Eqs. (18-22) yield the risk-based Shapley values. Finally, it is necessary to check whether or not the solution at hand is inside the core. If so, then the implementation procedure can be terminated. If not, then the current grand coalition should be partitioned into two non-overlapping sub-coalitions. These two sub-coalitions should be treated as the grand coalition in turn and repeat the aforementioned steps respectively. This iteration process should be continued until the feasibility check is satisfied.

9. An illustrative example

A simple example is presented below to illustrate the aforementioned computation procedure. Let us consider the stream and utility data given in Tables 1 and 2 respectively.

A minimum temperature approach (ΔT_{min}) of 10 °C was assumed in designing heat exchangers. The annualized capital investment of every unit was calculated according to the following formula: $10{,}000 + 670 \times area^{0.83}$ ("$"/yr). All multi-plant HEN designs in this example were generated according to the MINLP model formulation presented in Appendix, while all optimization runs were performed with solver COUENNE in GAMS 24.0.

9.1. Conventional Shapley values

By performing repeated optimization runs to generate the interplant HENs in all possible coalitions, on can determine the corresponding TAC in Table 3 and network structures in Figs. 2–8.

From the above results, the conventional Shapley values can be computed according to Eqs. (5-8) and these values are presented in Table 4. Notice that the individual cost of each plant in coalition {1,2,3} is much lower than that of the standalone counterpart. However, as indicated previously in Section 4, it may not be reasonable to ask the all three participating members to share the costs accordingly since there is

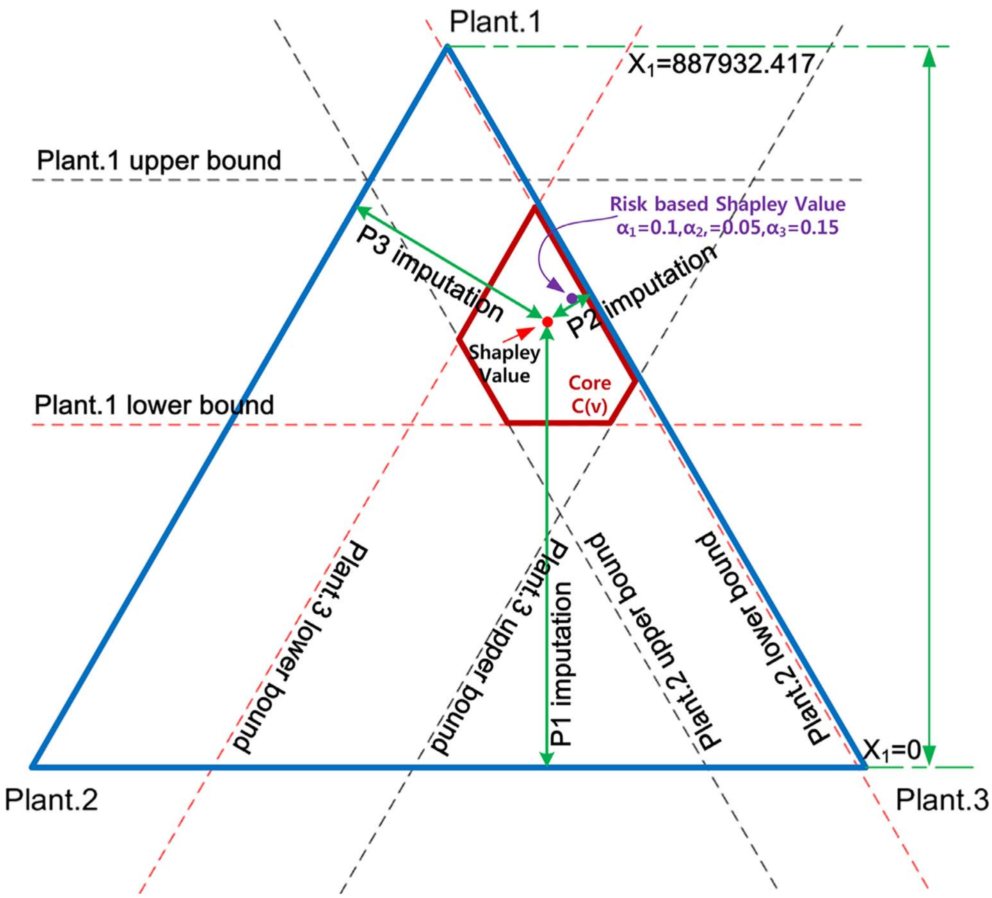

Fig. 11. Representation of Shapley values in triangular coordinate system.

a real chance for unexpected plant shutdown.

9.2. Risk-based Shapley values

As mentioned in Section 4, the average unreliability of each plant could be assumed to be available in advance and, specifically, $\alpha_1 = 0.1$, $\alpha_2 = 0.05$ and $\alpha_3 = 0.15$ were adopted for the present example. To facilitate clear illustration of the computation procedure, let us consider a simple scenario in which only P1 and P2 form a coalition. It is assumed that every interplant heat exchange can be facilitated with the utility supplied by P2 if P1 breaks down, and vice versa if otherwise. More specifically, let us consider the defective coalitions evolved from the original coalition in Fig. 5 (see Figs. 9and 10). The two corresponding scenarios can be described respectively as follows:

- P1 is forced to operate the interplant heat exchangers with high-pressure steam (544.9 kW) and cooling water (280.0 kW) due to P2 outage. The resulting financial burden of P1 should be increased from a Shapley value of $\varphi_{\{1,2\},1} = 626{,}862.8$ to $w(1{:}\ 1^{\{1,2\}}) = 949{,}223.0$ "$"/yr.
- P2 is forced to operate the interplant heat exchangers with high-pressure steam (280.0 kW) and cooling water (544.9 kW) due to P1 outage. The resulting financial burden of P2 should be increased from a Shapley value of $\varphi_{\{1,2\},2} = 70{,}023.2$ to $w(2{:}\ 2^{\{1,2\}}) = 635{,}617.7$ "$"/yr.

To facilitate clearer understanding, let us analyze the second scenario in further detail. It can be observed from the traditional Shapley values listed in Table 3 that the total cost burden of coalition {P1,P2} is $v(1,2) = 696{,}886.1$. According to Table 4, P1 and P2 are required to shoulder 626,862.8 (i.e., $\varphi_{\{1,2\},1}$) and 70,023.2 (i.e., $\varphi_{\{1,2\},2}$) respectively. However, if the risks of plant breakdowns are directly taken into consideration, the corresponding expected expenditures of both plants should obviously be higher. Specifically, the expected costs of P1 and P2 can be determined respectively as follows

$$(1-\alpha_2)\varphi_{\{1,2\},1} + \alpha_2 w(1{:}\ 1^{\{1,2\}}) = 642{,}980.81 \leqslant v(1)$$

$$(1-\alpha_1)\varphi_{\{1,2\},2} + \alpha_1 w(2{:}\ 2^{\{1,2\}}) = 126{,}582.65 \leqslant v(2)$$

Although in this case the expected expenditures of both plants are smaller than those of their standalone counterparts, there are still unsettled subtle allocation issues. Further calculations should reveal that the aforementioned cost increases differ significantly. P1 is financially penalized by only 3%, but the expected expenditure of P2 is raised to 81% higher level. Therefore, instead of computing the expected cost burdens mentioned above, the risk-based Shapley values must be determined to produce a fairer cost allocation scheme.

The cost burdens of every sub-coalition in all possible scenarios can be computed according to Eqs. (10-12) and all results are given in Table 5, while the corresponding risk-based Shapley values can be found in Table 6. Notice that the conventional Shapley values are also presented in Table 6 to facilitate convenient comparison. It can be observed that, due to considerations of potential shutdowns, only plant P2 is allowed to reduce its share of financial burden and the other two plants, P1 and P3, are both required to shoulder larger portions of TAC. This is reasonable since the cost hikes of P2 due to various plant shutdowns in coalition are all relatively large and other member(s) may be willing to shoulder a heavier burden within the core.

9.3. Sensitivity analyses

In realistic applications, the drop-out probability (α_i) of one or more plant in coalition can only be determined approximately. In other words, the estimate of α_i is believed to be present in a finite interval

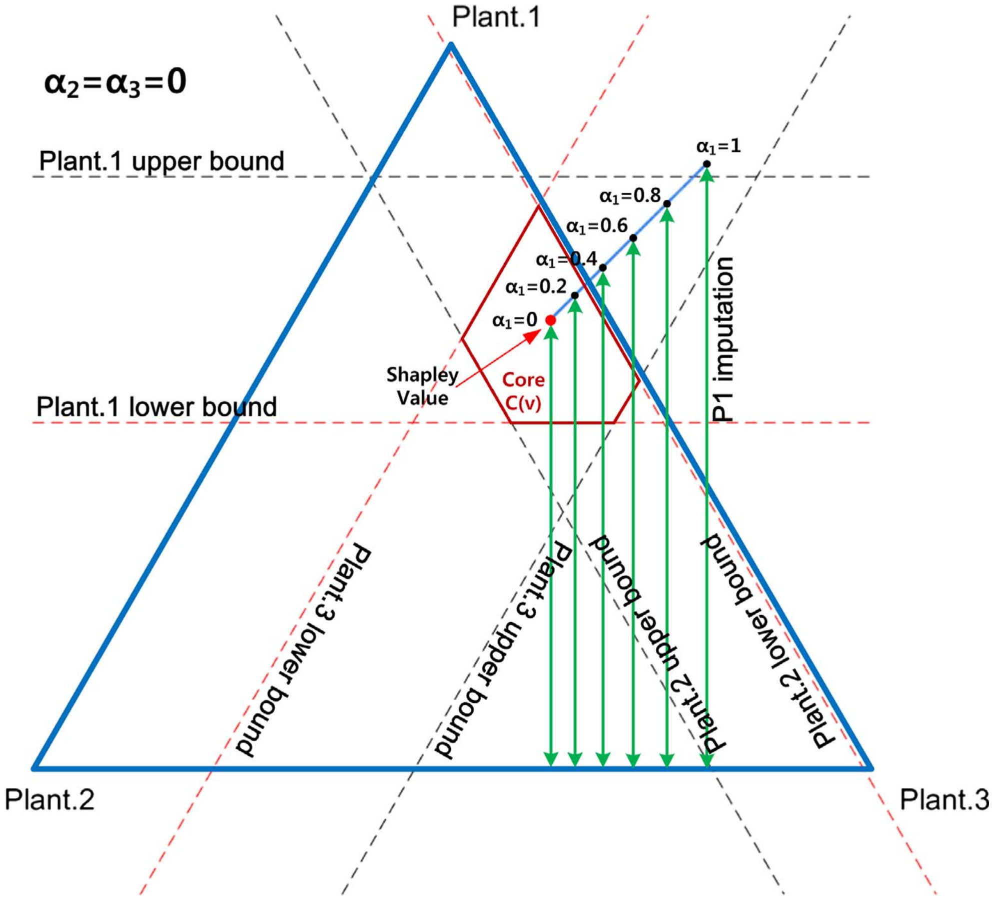

Fig. 12. Cost-allocation trajectory when P1 is at risk.

with a desired degree of confidence. To address this uncertainty issue, the sensitivity analyses presented below may be performed to evaluate the merit of TAC sharing plan for interplant heat integration.

Notice first that the aforementioned risk-based Shapley values can be represented with a point in the triangular coordinate system (see Fig. 11). Since the sum of shortest distances from any point to all three sides of an equilateral triangle is a constant, this total distance can be treated as the TAC of coalition {1,2,3}, i.e., $v(1,2,3) = 887{,}932.4$. Notice that the pentagon inside the triangle is the core determined on the basis of Eqs. (1-4). If a particular solution point, which represents a specific TAC distribution, is located within the core, then the corresponding cost sharing scheme should be acceptable to all three plants. Otherwise, it is considered as an infeasible solution. Notice also that the red[1] and purples dots in Fig. 11 are placed according to the conventional and risk-based Shapley values, respectively, and both are feasible.

In each of the following analyses, the shutdown probabilities of a selected combination of plants are allowed to vary while keeping the remaining ones fixed at zero. Further insights can be gained by tracing the corresponding trajectories.

9.3.1. One plant is at risk

Let us first consider all possible scenarios in which exactly one plant is at risk. Figs. 12–14 show the cost-allocation trajectories corresponding to P1, P2 and P3 respectively. It can be observed that the shared cost of a plant increases with its unreliability level. In addition, after the shutdown probability exceeds a certain threshold value, forming coalition is no longer a desired option (Figs. 12 and 14).

9.3.2. Two plants are at risk

Let us next consider all cases in which exactly one plant always stays in the coalition. The cost-allocation trajectories for P1, P2 and P3 are presented in Figs. 15–17 respectively. Fig. 15 reveals two conflicting trends. Firstly, since P1 is completely reliable in this case, this plant may have to shoulder a larger portion of TAC so as to reap the coalition benefit if the shutdown probabilities of the other two plants are relatively low. Secondly, in cases when these dropout risks are significant, it may be necessary for P1 to ask for an extra compensation fee, that is, to share a cost which is much lower than that committed without serious concerns for plant shutdowns. Note also that only the second phenomenon can be observed from the trajectory in either Figs. 16 or 17. Specifically, the shared cost of the reliable plant can be expected to decrease as the dropout risks of the others go up.

9.3.3. Three plants are at risk

Finally, let us consider the situation in which all plants are at the same risk. From the cost-allocation trajectory in Fig. 18, it can be observed that the cost burden of P2 gradually decreases from its Shapley value as all shutdown probabilities start to increase from zero. This is due to the fact that P2 in the defective coalition tends to be penalized by the largest amount of extra utility cost. On the other hand, from the enlarged figure on the right, one can clearly see that this cost-allocation trajectory is actually a loop. The aforementioned trend reverses at the point outside the core when $\alpha_1 = \alpha_2 = \alpha_3 = 0.5$, and then returns to the starting point, i.e., the original cost-allocation scheme suggested by the conventional Shapley values, as the dropout risks approach 100%.

10. Conclusions

A rigorous synthesis procedure has been developed in this work to produce a realistic cost-sharing plan for interplant heat integration in

[1] For interpretation of color in Fig. 11, the reader is referred to the web version of this article.

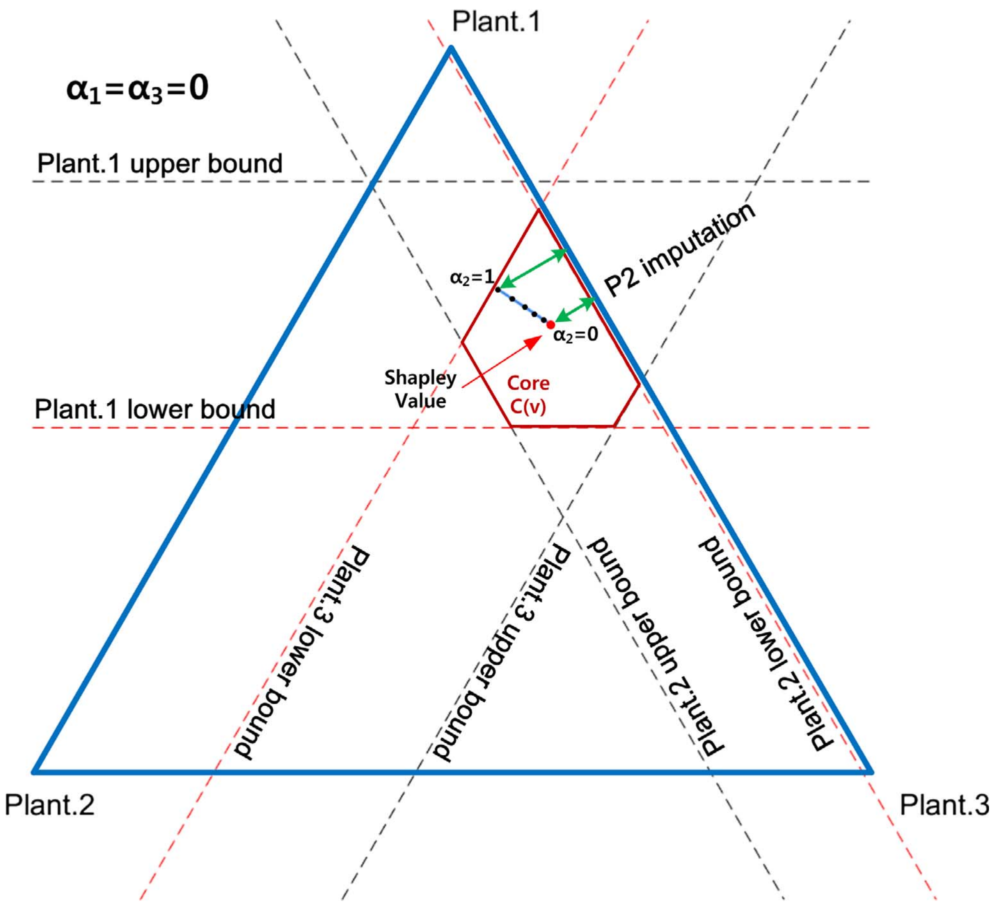

Fig. 13. Cost-allocation trajectory when P2 is at risk.

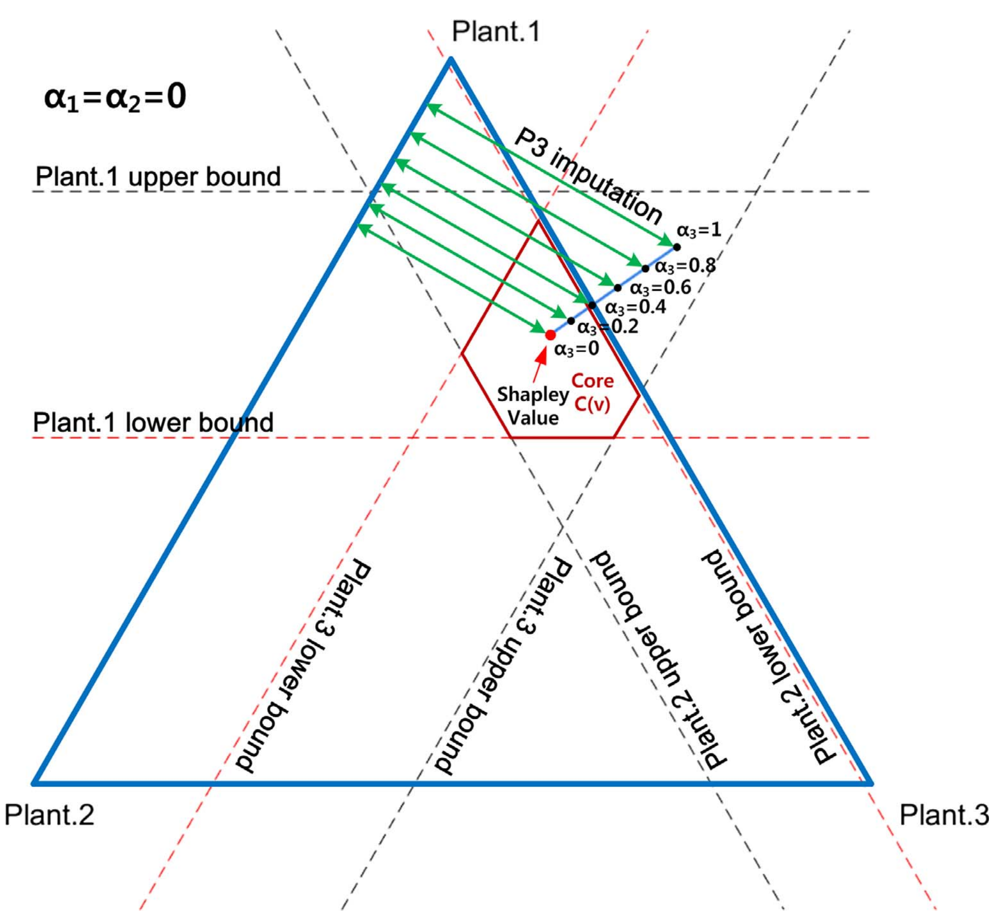

Fig. 14. Cost-allocation trajectory when P3 is at risk.

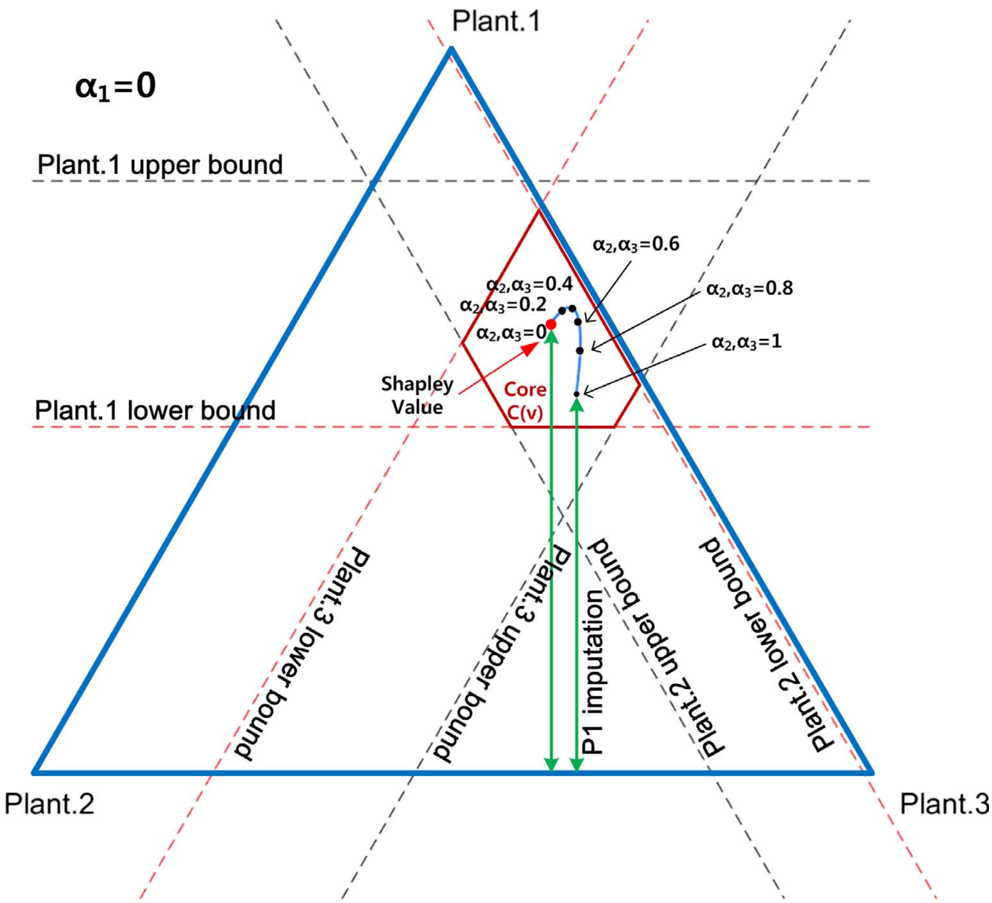

Fig. 15. Cost-allocation trajectory when both P2 and P3 are at risk.

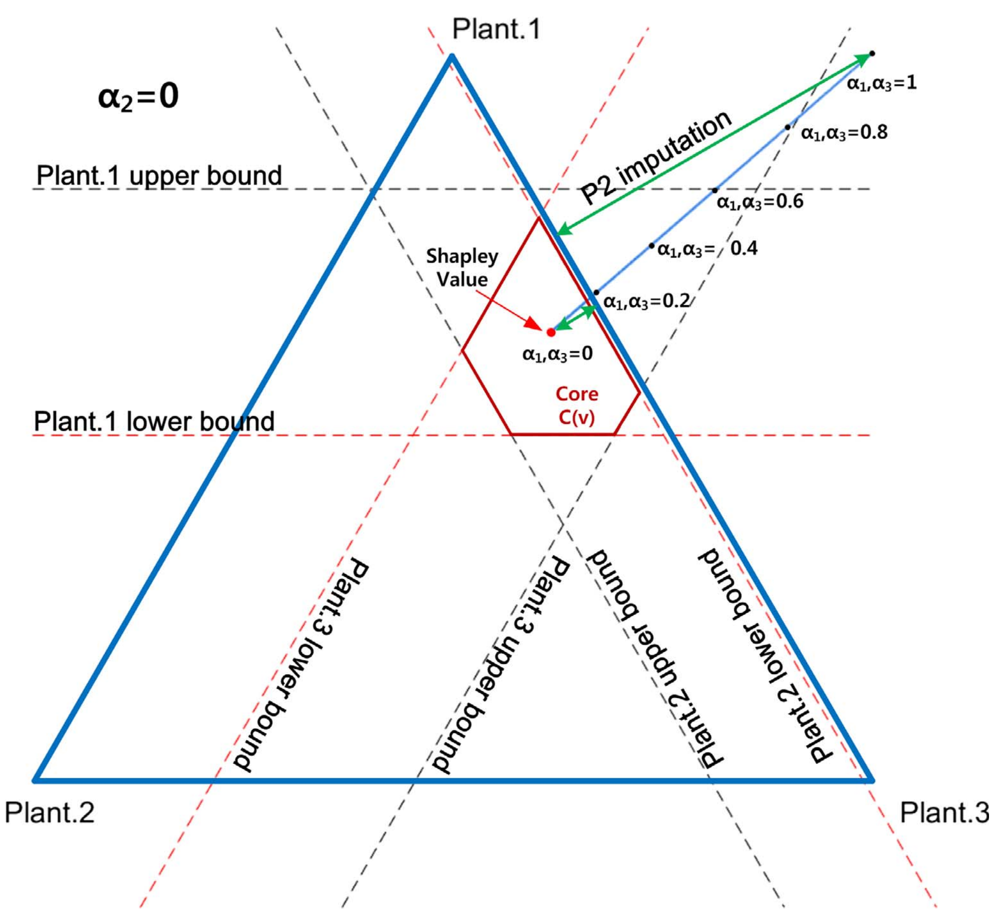

Fig. 16. Cost-allocation trajectory when both P1 and P3 are at risk.

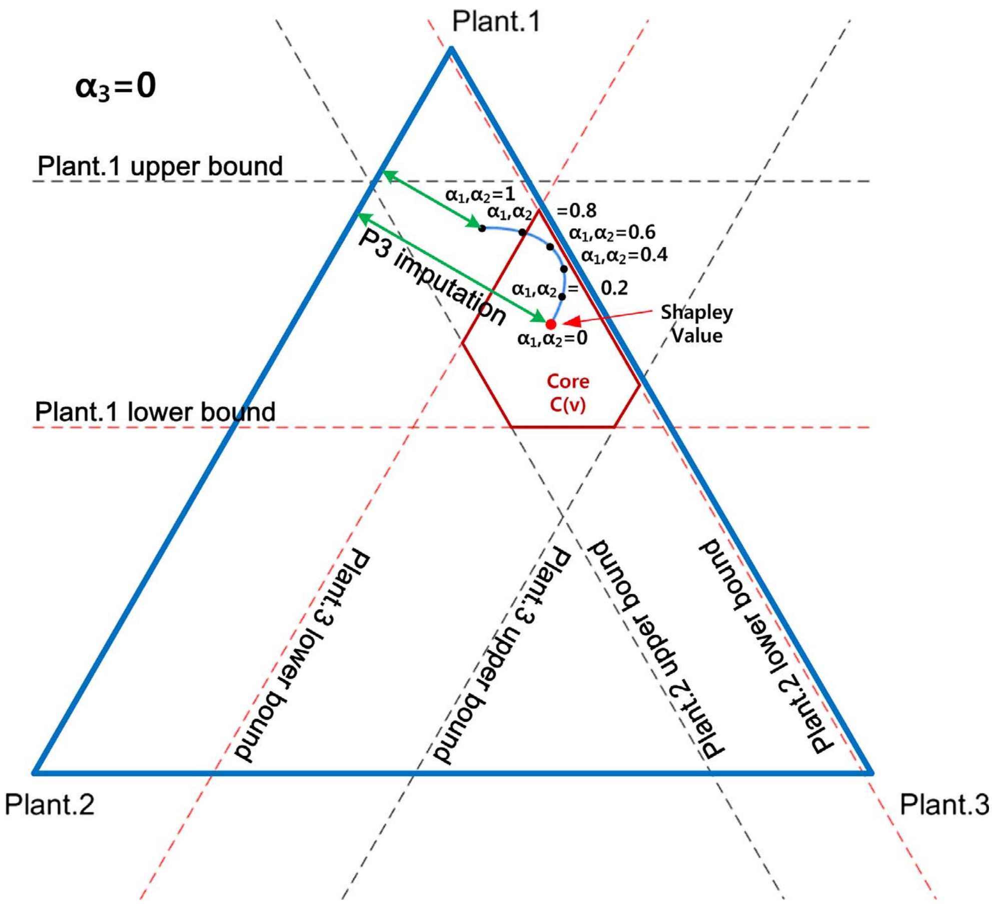

Fig. 17. Cost-allocation trajectory when both P1 and P2 are at risk.

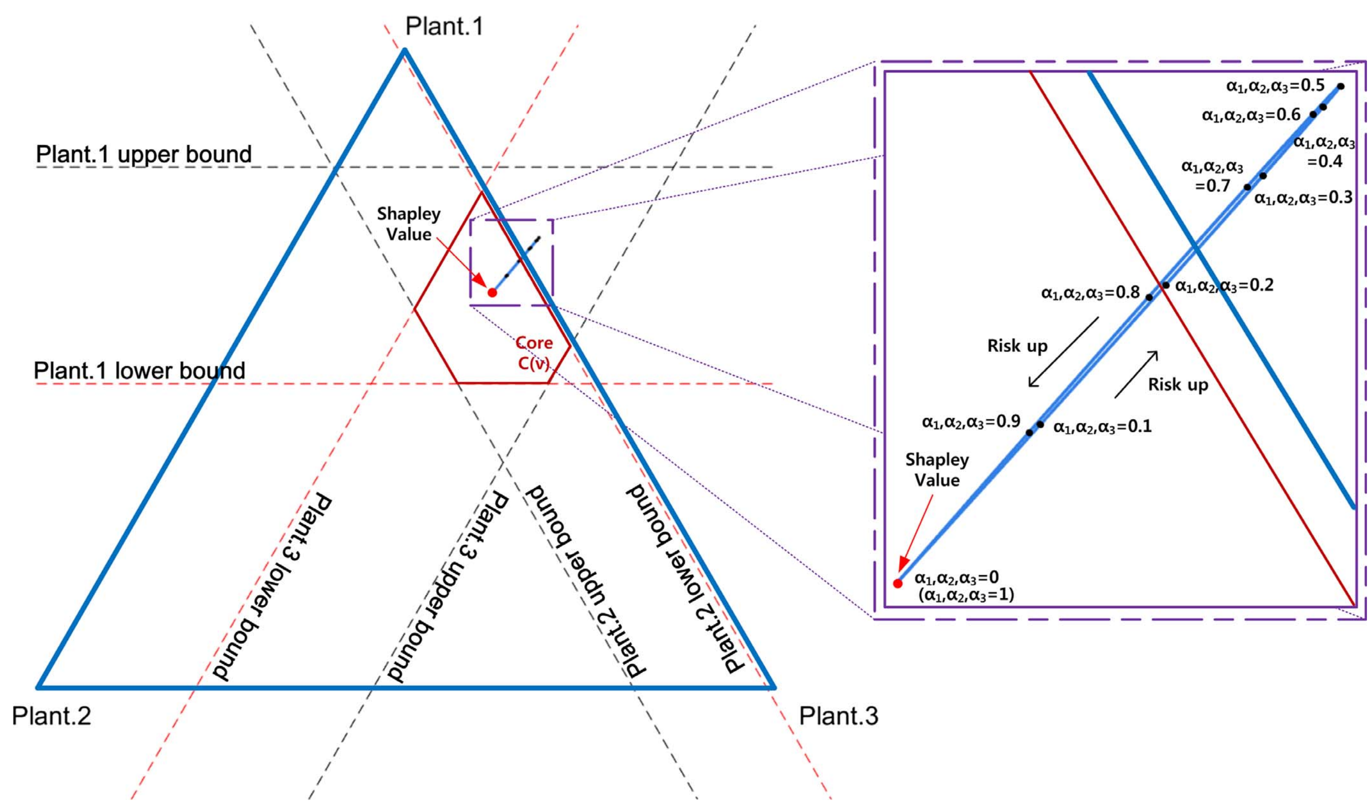

Fig. 18. Cost-allocation trajectory when all plants are at risk.

the spirit of a cooperative game. Specifically, to ensure feasibility and fairness, a novel computation strategy is devised to determine the core and also the risk-based Shapley values of all players. As a result, a definite portion of the total annual cost of the multi-plant HEN can be calculated for assignment to each plant by considering both its cost contribution level and also the potential fallouts of unexpected plant shutdowns. The proposed methodology is illustrated in detail in a simple example.

Acknowledgment

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Appendix A. Appendix: MINLP model for optimal interplant HEN designs

As mentioned previously in Section 2, the conventional MINLP model [1] has been modified in this work to generate the optimal interplant HEN designs. A concise summary of the resulting model formulation is given in the sequel. Note that only the proposed changes are explained for the sake of illustration brevity, while the definitions of all symbols used in this model can be found in the nomenclature section.

- Model Constraints:

1. Overall heat balance for each process stream

$$(TIN_i-TOUT_i)F_i = \sum_{k\in ST}\sum_{j\in C} q_{i,j,k} + \sum_{n\in CU} q_{i,n}, \forall\, i \in H; \tag{A1}$$

$$(TOUT_j-TIN_j)F_j = \sum_{k\in ST}\sum_{i\in H} q_{i,j,k} + \sum_{m\in HU} q_{j,m}, \forall\, j \in C. \tag{A2}$$

2. Heat balance at each stage

$$(t_{i,k}-t_{i,k+1})F_i = \sum_{j\in C} q_{i,j,k}, \forall\, i \in H, \forall\, k \in ST; \tag{A3}$$

$$(t_{j,k}-t_{j,k+1})F_j = \sum_{i\in H} q_{i,j,k}, \forall\, j \in C, \forall\, k \in ST. \tag{A4}$$

3. Cold and hot utility loads

$$(t_{i,NOK+1}-TOUT_i)F_i = \sum_{n\in CU} q_{i,n}, \forall\, i \in H; \tag{A5}$$

$$(TOUT_j-t_{j,1})F_j = \sum_{m\in HU} q_{j,m}, \forall\, j \in C. \tag{A6}$$

4. Utility selections

Notice that, in this modified model, the sums on the right sides of Eqs. (A5) and (A6) are used to respectively replace the cold and hot utility loads on hot stream i and cold stream j in the original formulation. In addition, note that these sums also appear in the second terms on the right sides of Eqs. (A1) and (A2). To facilitate selection of only one utility among all possible options, the following logic constraints must be imposed:

$$\sum_{n\in CU} z_{i,n} \leqslant 1, \forall\, i \in H; \tag{A7}$$

$$\sum_{m\in HU} z_{j,m} \leqslant 1, \forall\, j \in C. \tag{A8}$$

Note that $z_{i,n}, z_{j,m} \in \{0,1\}$ in the above constraints.

5. Match selections

$$q_{i,j,k}-\Omega_{i,j}z_{i,j,k} \leqslant 0, \forall\, i \in H, \forall\, j \in C, \forall\, k \in ST; \tag{A9}$$

$$q_{i,n}-\Omega_{i,n}z_{i,n} \leqslant 0, \forall\, i \in H, \forall\, n \in CU; \tag{A10}$$

$$q_{j,m}-\Omega_{j,m}z_{j,m} \leqslant 0, \forall\, j \in C, \forall\, m \in HU. \tag{A11}$$

Note that $z_{i,j,k} \in \{0,1\}$. Note also that $\Omega_{i,j}$, $\Omega_{i,n}$ and $\Omega_{j,m}$ are model parameters which must be computed in advance according to the following formulas:

$$\Omega_{i,j} = min\{F_i(TIN_i-TOUT_i), F_j(TOUT_j-TIN_j)\}, \forall\, i \in H, \forall\, j \in C;$$

$$\Omega_{i,n} = F_i(TIN_i-TOUT_i), \forall\, i \in H, \forall\, n \in CU;$$

$$\Omega_{j,m} = F_j(TOUT_j - TIN_j)\ ,\forall\ j \in C\ ,\forall\ m \in HU.$$

Temperature precedence on each process stream

$$TIN_i = t_{i,1}\ ,\forall\ i \in H; \tag{A12}$$

$$t_{i,k} \geqslant t_{i,k+1}\ ,\forall\ i \in H\ ,\forall\ k \in ST; \tag{A13}$$

$$t_{i,NOK+1} \geqslant TOUT_i\ ,\forall\ i \in H; \tag{A14}$$

$$TOUT_j \geqslant t_{j,1}\ ,\forall\ j \in C; \tag{A15}$$

$$t_{j,k} \geqslant t_{j,k+1}\ ,\forall\ j \in C\ ,\forall\ k \in ST; \tag{A16}$$

$$t_{j,NOK+1} = TIN_j\ ,\forall\ j \in C. \tag{A17}$$

6. Temperature approach in each heat exchanger

$$dt_{i,j,k} \leqslant t_{i,k} - t_{j,k} + \Gamma_{i,j}(1 - z_{i,j,k})\ ,\forall\ i \in H\ ,\forall\ j \in C\ ,\forall\ k \in ST; \tag{A18}$$

$$dt_{i,j,k+1} \leqslant t_{i,k+1} - t_{j,k+1} + \Gamma_{i,j}(1 - z_{i,j,k})\ ,\forall\ i \in H\ ,\forall\ j \in C\ ,\forall\ k \in ST; \tag{A19}$$

$$dt_{i,j,k} \geqslant \Delta T_{min}\ ,\forall\ i \in H\ ,\forall\ j \in C\ ,\forall\ k \in ST. \tag{A20}$$

The model parameter $\Gamma_{i,j}$ in the above inequalities can be determined as follows:

$$\Gamma_{i,j} = max\{0, TIN_j - TIN_i, TOUT_j - TIN_i, TIN_j - TOUT_i, TOUT_j - TOUT_i\} + \Delta T_{min}$$

where $i \in H$ and $j \in C$.

8. Temperature approach in each cooler

$$dtin_{i,n} \leqslant t_{i,NOK+1} - TT_{i,n} + \Gamma_{i,n}(1 - z_{i,n})\ ,\forall\ i \in H\ ,\forall\ n \in CU; \tag{A21}$$

$$dtin_{i,n} \geqslant \Delta T_{min}\ ,\forall\ i \in H\ ,\forall\ n \in CU; \tag{A22}$$

$$dtout_{i,n} \leqslant TOUT_i - TI_n + \Gamma_{i,n}(1 - z_{i,n})\ ,\forall\ i \in H\ ,\forall\ j \in C; \tag{A23}$$

$$dtout_{i,n} \geqslant \Delta T_{min}\ ,\forall\ i \in H\ ,\forall\ j \in CU. \tag{A24}$$

The model parameter $\Gamma_{i,n}$ can be determined as follows:

$$\Gamma_{i,n} = max\{0, TI_n - TIN_i, TI_n - TOUT_i, TT_{i,n} - TIN_i, TT_{i,n} - TOUT_i\} + \Delta T_{min}\ ,\forall\ i \in H\ ,\forall\ j \in CU.$$

9. Temperature approach in each heater

$$dtin_{j,m} \leqslant TT_{j,m} - t_{j,1} + \Gamma_{j,m}(1 - z_{j,m})\ ,\forall\ j \in C\ ,\forall\ m \in HU; \tag{A25}$$

$$dtin_{j,m} \geqslant \Delta T_{min}\ ,\forall\ j \in C\ ,\forall\ m \in HU; \tag{A26}$$

$$dtout_{j,m} \leqslant TI_m - TOUT_j + \Gamma_{j,m}(1 - z_{j,m})\ ,\forall\ j \in C\ ,\forall\ m \in HU; \tag{A27}$$

$$dtout_{j,m} \geqslant \Delta T_{min}\ ,\forall\ j \in C\ ,\forall\ m \in HU. \tag{A28}$$

The model parameter $\Gamma_{j,m}$ should be selected as follows:

$$\Gamma_{j,m} = max\{0, TIN_j - TI_m, TIN_j - TT_{j,m}, TOUT_j - TI_m, TOUT_j - TT_{j,m}\} + \Delta T_{min}\ ,\forall\ j \in C\ ,\forall\ m \in HU.$$

10. Maximum number of split streams in each stage

$$\sum_{j \in C} z_{i,j,k} \leqslant NST\ ,\forall\ i \in H\ ,\forall\ k \in ST; \tag{A29}$$

$$\sum_{i \in H} z_{i,j,k} \leqslant NST\ ,\forall\ j \in C\ ,\forall\ k \in ST. \tag{A30}$$

- Objective Function:

The objective function is the total annual cost (TAC) and it is supposed to be minimized in the MINLP model. This TAC is approximated in this study as the sum of the total annual utility cost ($TAUC$) and the total annualized capital cost ($TACC$), i.e., $TAC = TAUC + TACC$, while the latter two costs can be expressed explicitly as follows:

$$TAUC = \sum_{i \in H} \sum_{n \in CU} CQ_{i,n} q_{i,n} + \sum_{j \in C} \sum_{m \in HU} CQ_{j,m} q_{j,m} \tag{A31}$$

$$TACC = \sum_{i\in H}\sum_{j\in C}\sum_{k\in ST} CF_{i,j,k}z_{i,j,k} + \sum_{i\in H}\sum_{n\in CU} CF_{i,n}z_{i,n} + \sum_{j\in C}\sum_{m\in HU} CF_{j,m}z_{j,m} + \sum_{i\in H}\sum_{j\in C}\sum_{K\in ST} CA_{i,j}\left(\frac{q_{i,j,k}}{U_{i,j}(dt_{i,j,k}dt_{i,j,k+1}(dt_{i,j,k}+dt_{i,j,k+1})/2)^{1/3}}\right)^{\beta} + \sum_{i\in H}\sum_{n\in CU} CA_{i,n}\left(\frac{q_{i,n}}{U_{i,n}(dtin_{i,n}dtout_{i,n}(dtin_{i,n}+dtout_{i,n})/2)^{1/3}}\right)^{\beta} + \sum_{j\in C}\sum_{m\in HU} CA_{j,m}\left(\frac{q_{j,m}}{U_{j,m}(dtin_{j,m}dtout_{j,m}(dtin_{j,m}+dtout_{j,m})/2)^{1/3}}\right)^{\beta} \quad (A32)$$

Finally, it should be noted that the log-mean temperature difference (LMTD) of each heat-transfer unit in the above equation is calculated with the empirical formula developed by Chen [32].

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