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PREFACE

In a very short time since its announcement in November 1987, the National Research Council report, "Frontiers in Chemical Engineering: Research Needs and Opportunities," has become accepted as the point of departure in any discussion on the future of our profession. The report hails four principal frontiers: starting new technologies, maintaining leadership in established technologies, protecting and improving health, safety, and the environment, and developing systematic knowledge and generic tools. This report is required reading for all serious chemical engineers who are concerned about the future.

There are three chapters in this volume of *Advances in Chemical Engineering*. The chapter, "Analysis and Synthesis of Resilient Heat Exchanger Networks" by Colberg and Morari of Caltech, is concerned with the development of new generic tools. It provides an overview on the macroscale design of systems that are resilient and flexible to uncertainties and variations in system variables, such as flow rates and fouling of heat exchanger surfaces.

The chapter, "Catalytic Hydrodemetallation" by Quann and Ware of Mobil, Hung of Chevron, and Wei of MIT, is devoted to maintaining leadership in an established technology, namely oil refining. There are two topics with the greatest potential impact on our ability to increase the supply of clean premium transportation fuels of gasoline and kerosene: the liquefaction of ubiquitous and refractory methane and the upgrading of heavy and resid oils. This chapter provides a timely review of a principal problem in resid upgrading.

The chapter, "Safety Matrix: People Applying Technology to Yield Safe Chemical Plants and Products" by Davis of Dow Chemical, is concerned with protecting and improving safety in chemical plants. Dow Chemical has dramatically improved its safety record and seized a leadership position among chemical companies in the past decade. This improvement is not an accident, but the result of a dedicated attitude and systemic application that should be exported to the entire chemical industry. The lessons here would make us all winners and demonstrate that the chemical engineers are the solutions rather than the problems.

James Wei

ANALYSIS AND SYNTHESIS OF RESILIENT HEAT EXCHANGER NETWORKS

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I. Introduction

Research on the synthesis of economically optimal heat exchanger networks (HENs) has been performed for over 15 years (Nishida *et al.*, 1981). As a result of this research, two general conclusions have emerged: (1) the optimum network generally features minimum or close to minimum utility consumption, and (2) the optimum network generally has a minimum or close to minimum number of units (exchangers, heaters, and coolers).

As aids in synthesizing economically optimal HENs, targets have been developed to predict *before* synthesis the minimum utilities required (Hohmann, 1971; Raghavan, 1977; Linnhoff and Flower, 1978) and the minimum units required (Hohmann, 1971) for given values of the stream supply and target temperatures and heat capacity flow rates and an assumed value of minimum approach temperature ΔT_m. Thus most recent HEN synthesis algorithms decompose the synthesis problem into at least two stages: (1) targeting of minimum utilities and minimum units and (2) synthesis of a HEN structure with minimum utility consumption and with minimum or close to minimum number of units.

Most recent synthesis algorithms are also based upon the principles of the thermodynamic "pinch" (Linnhoff *et al.*, 1979; Umeda *et al.*, 1978). Recognition of the pinch provided great physical insight into the problem of HEN synthesis. The reader is assumed to be familiar with the principles of the pinch and with general methods for HEN synthesis [e.g., pinch design method (Linnhoff *et al.*, 1982; Linnhoff and Hindmarsh, 1983), structural optimization methods for selection of a minimum set of stream matches (Papoulias and Grossmann, 1983), and determination of the most economical network structure (Floudas *et al.*, 1986) from the predicted matches].

The difficulty with these synthesis methods is that they generate HENs for *fixed* nominal values of the stream supply temperatures and flow rates and for assumed nominal values of the heat transfer coefficients. In an industrial HEN, the supply temperatures and flow rates will vary (because of unpredictable environmental disturbances or because of predictable feedstock and throughput changes), and the heat transfer coefficients are highly uncertain (due to fouling, etc.). The HEN synthesized for nominal conditions must be *resilient* (flexible) to changes in supply temperatures and flow rates and to uncertainties in heat transfer coefficients.

In general, the entire process plant should be resilient. However, in a tightly energy-integrated plant, it is especially important that the HEN be resilient—if the HEN cannot operate, then neither can the plant.

In the past, HEN resilience was often assumed if the HEN could operate for perceived "worst" cases (i.e., combinations of highest and lowest temperatures and flow rates. However, as the next section of this chapter demonstrates, the worst cases for resilience may not agree with intuition (e.g., nonlinearities may cause the worst case for resilience to occur at intermediate values of temperature and flow rate).

A more sophisticated approach to analyzing HEN resilience is to use "shifting" arguments. By considering the effects of temperature and flow rate disturbances as they are shifted and/or propagated toward the heaters and coolers (which can absorb the disturbances), one can gain physical insight into the problem of HEN resilience. However, the shifting arguments are difficult to apply quantitatively to HENs with several degrees of freedom (several exchangers more than the minimum required and/or stream splits), and it is difficult to study interactions between multiple disturbances.

In this chapter more systematic methods for HEN resilience analysis and three procedures for synthesis of resilient HENs are reviewed. Section II demonstrates how simple, empirical HEN resilience tests can fail and establishes the need for more systematic HEN resilience analysis methods. Section III presents several rigorous analysis methods, states the conditions when they are linear, and includes special nonlinear forms. Section IV reviews three procedures for synthesis of resilient HENs: (1) synthesis based on a resilience target (Colberg *et al.*, 1988); (2) "multiperiod" synthesis–analysis–resynthesis algorithm (Floudas and Grossmann, 1987b), which is an extension of the structural optimization synthesis algorithm for fixed stream conditions; and (3) synthesis using "downstream (disturbance) paths" (Linnhoff and Kotjabasakis 1986).

The scope of this chapter is limited to resilience of HENs in the steady state. Obviously, it is important that a HEN be controllable and that it be resilient to dynamic changes in temperature and flow rate (Morari *et al.*, 1985). However, dynamic resilience will not be addressed. Also, many of the resilience concepts reviewed here were developed for general chemical processes (Grossmann and Morari, 1983; Swaney and Grossmann, 1985a; Grossmann and Floudas, 1987; Linnhoff and Kotjabasakis, 1986). However, in this chapter they will be applied specifically to HENs.

II. Empirical versus Systematic Methods for HEN Resilience

A. Why Empirical Methods Can Fail: Motivating Examples

The conventional procedure for introducing resilience in a HEN (or general process plant) is to use empirical overdesign. That is, a nominal or "conservative" basis is selected for designing and optimizing the HEN. Empirical safety factors based on past experience are applied to the equipment sizes and extra units are also often introduced. However, although this empirical procedure will in general add resilience and flexibility of operation to a HEN, it has the following drawbacks:

1. Not much insight is gained on how much (if any) resilience is added for a given degree of overdesign.
2. The "most conservative" or "worst case" basis for design may not be the one the designer would intuitively expect.
3. Conditions that give rise to infeasible operation may not be detected since interactions among different exchangers are not explicitly taken into account.
4. The resulting overdesigned network may not operate efficiently and may not be optimal from an economic viewpoint.

The following two examples demonstrate these drawbacks of empirical overdesign.

Example 1 (from Grossmann and Morari, 1983). Traditional industrial practice generates resilient HENs by designing them for what are perceived to be "extreme" operating conditions. Naturally, if these extremes are selected properly, the HEN will perform satisfactorily for the whole range of expected conditions. This example demonstrates that the proper selection of "extremes" is far from trivial and that seemingly logical choices can lead to extremely poor systems.

The HEN shown in Fig. 1a was designed for the problem data shown. There are no other designs with fewer heat transfer units, and the approach temperatures fall nowhere below 10 K; therefore this structure is likely to be close to optimal economically. However, it is known that the heat capacity flow rate of stream S_{h1} can be as large as 1.85 kw/K at times. The natural approach of the design engineer would be to test his design for this extreme condition. The test reveals that the network structure also performs satisfactorily at this flow rate (Fig. 1b). It appears logical to expect that the structure can handle all flow rates in the range 1–1.85 kW/K.

Figure 1c reveals that this is not the case. *Even if exchanger 1 had infinite area* (ie., infinite overdesign factor), for a heat capacity flow rate of 1.359 kW/K the outlet temperature of stream S_{h1} cannot be decreased below 344 K. With a reasonable approach temperature difference of 10 K (Fig. 1d), the minimum attainable outlet temperature for stream S_{h1} is 375.4 K, corresponding to a target temperature violation of 52 K. If S_{h1} were the feed stream to a reactor, this design error could have serious consequences.

By switching the cooler from stream S_{h2} to S_{h1} the network can be made resilient (Fig. 1e). In all exchangers the approach temperatures exceed 10 K over the whole range of flow rate variations $1 \leq w_{h1} \leq 1.85$ kW/K and therefore capital costs remain reasonable. The example shows that

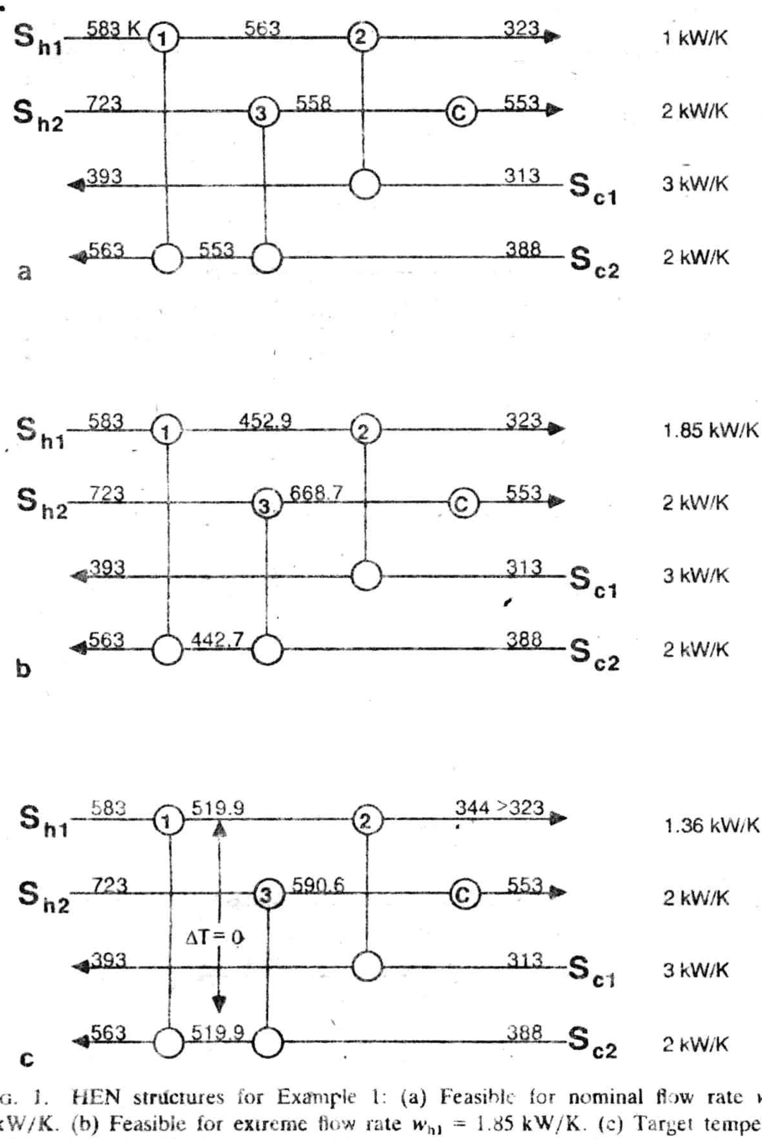

FIG. 1. HEN structures for Example 1: (a) Feasible for nominal flow rate w_{h1} = 1.0 kW/K. (b) Feasible for extreme flow rate w_{h1} = 1.85 kW/K. (c) Target temperature violation of 21 K with intermediate flow rate w_{h1} = 1.359 kW/K (with ΔT_m = 0 K). (d) Target temperature violation of 52 K with intermediate flow rate w_{h1} = 1.359 kW/K (with ΔT_m = 10 K). (e) Resilient for $1.0 \le w_{h1} \le 1.85$ kW/K. (f) Resilient for modified example (T^S_{c2} = 393 K).

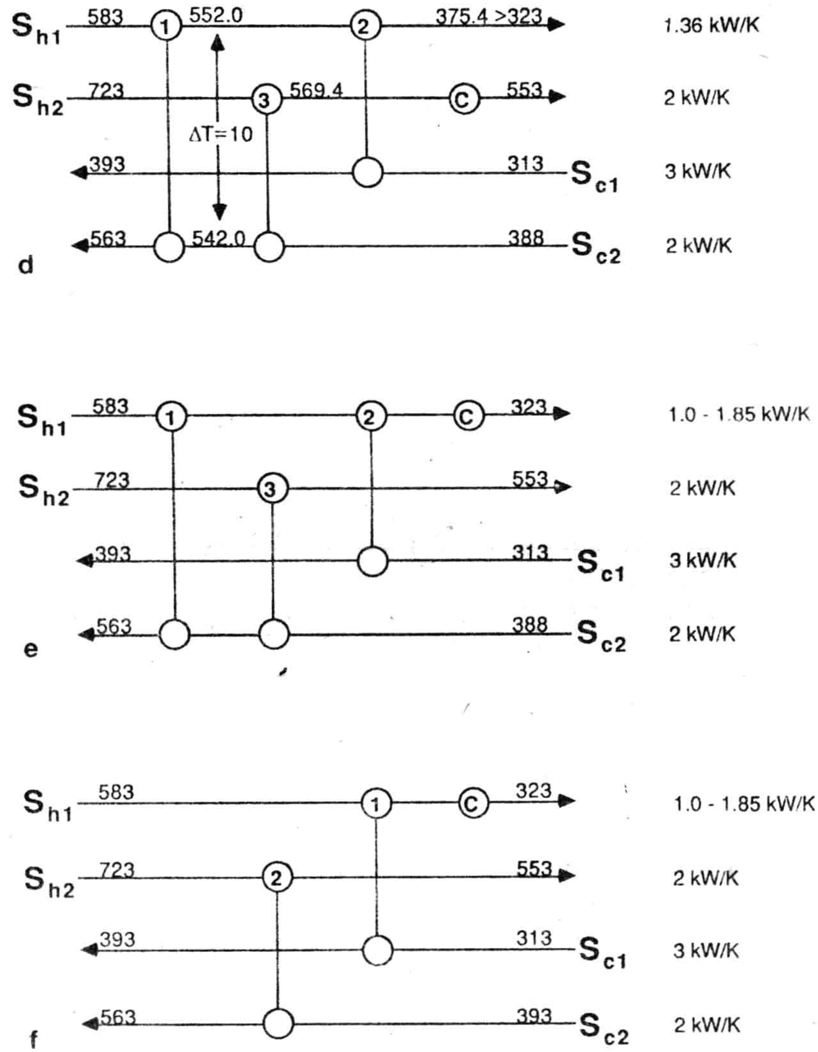

FIG. 1 (*Continued*)

resilience may not be obtained with additional exchangers or excessive oversizing, but simply by a proper redesign of the network structure.

Let us also look at the slightly modified problem in which the inlet temperature of stream S_{c2} is increased to $T_{c2}^{S} = 393$ K. The network structure in Fig. 1a suffers from the same deficiencies as before. A resilient structure is shown in Fig. 1f. It involves only three heat exchangers, while the other structure had four. Selecting networks with a larger number of transfer units not only increases capital costs, but can *decrease* resilience. Resilience cannot be achieved by *ad hoc* addition of equipment, but by systematic design techniques based on a thorough understanding of the physicomathematical problem.

Example 2 (from Grossmann and Morari, 1983). In order to illustrate the problem of overlooking effects of interactions, consider the HEN shown in Fig. 2a. Note that in this case the outlet temperatures of streams S_{h1} and S_{c2} have been specified as inequalities: stream S_{h1} must be cooled down to at least 410 K, while stream S_{c2} must be heated up to at least 430 K.

Assume that the areas of exchangers 1 and 2 are sized for nominal values of heat transfer coefficients $U_1 = U_2 = 800$ W/m^2 K and that the resulting areas are oversized by 20%. If such a design were implemented in practice, the following situation might occur.

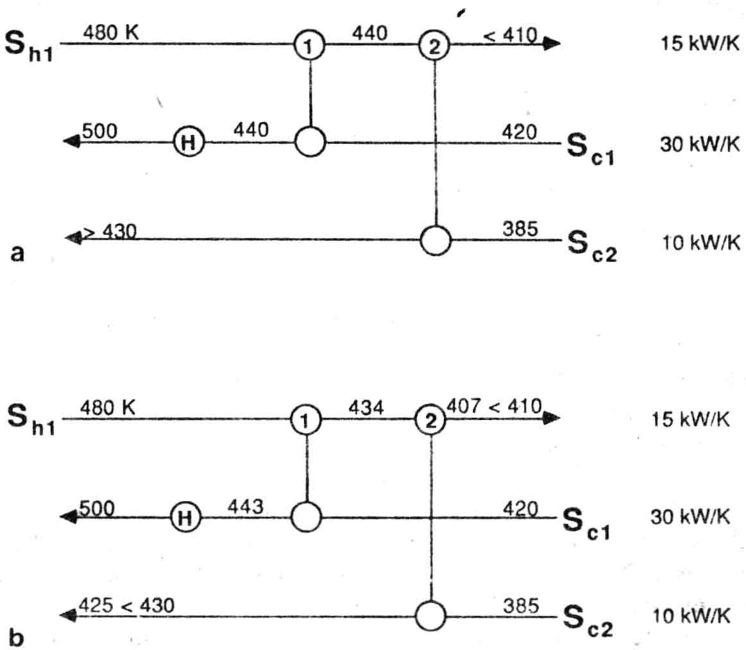

FIG. 2. HEN structure for Example 2: (a) Feasible with nominal heat transfer coefficients. (b) Infeasible with heat transfer coefficients +20% and −20% of their nominal values in exchangers 1 and 2, respectively.

Suppose that U_1 is 20% higher than its nominal value while U_2 is 20% lower. For such a case, as shown in Fig. 2b, the exit temperature of stream S_{h1} from exchanger 1 would drop from the expected 440 K down to 434 K owing to the larger heat transfer coefficient. However, with this change the temperature driving force in exchanger 2 is reduced, which when coupled with the lower heat transfer coefficient causes the outlet temperature of stream S_{c1} from this exchanger to be 425 K, or 5 K below the minimum temperature that was specified. Therefore, for this realization of heat transfer coefficients the network attains infeasible operation since it violates the temperature specification. This example illustrates the danger of overlooking interactions when using empirical overdesign.

It should be noted that this design satisfies the temperature specifications when both heat transfer coefficients are 20% lower than their nominal values, which intuitively would be regarded as the "worst" condition. Thus, this example also shows that identifying "worst" conditions for feasible operation may not always be obvious from intuition.

Another point of the example is related to the choice of areas such that temperature specifications are not violated for any deviation of U_1 and U_2 within ±20% of their nominal values. For instance, if one were to insist on oversizing the area of exchanger 1 by 20%, then the area of exchanger 2 would have to be oversized by 108%. On the other hand, if one were to oversize exchanger 2 by 23%, then exchanger 1 would not have to be oversized, but rather it could be *undersized* by 16%! This shows that the choice of a resilient design which is also economically optimal may not be obvious in general. Hence, the need for a systematic treatment of resilience and flexibility in process design should be evident.

B. Systematic Methods: Basic Problem Descriptions

The previous examples clearly demonstrate the need for more systematic methods to treat HEN resilience. In particular, systematic methods are needed to determine how much, if any, resilience is gained for a given degree of overdesign, or whether resilience can be improved by simple structural changes; to rigorously handle process interactions and to correctly identify "worst case" operating conditions; and to synthesize the structure and determine the minimal amount of oversizing to yield an economically optimal, resilient HEN.

Before describing some basic problems in systematic analysis and synthesis of resilient HENs, we need to establish a common vocabulary of clearly defined terms. (Most of these definitions are adopted from Grossmann and Morari, 1983.)

Analysis means the study of the properties (economics, resilience, etc.) of a given design.

Design is the selection of variables (e.g., heat exchanger areas, maximum heater and cooler loads) which lead a given design structure (HEN topology or general process flow sheet) to have specified properties.

Synthesis is the generation of the process structure. The structural variables (existence or absence of a process unit—e.g., exchanger—or interconnection between process units) can be represented by binary integer variables.

Feasible refers to a process (HEN structure) which satisfies all physical constraints (nonnegative exchanger loads) and performance specifications (target temperatures, minimum approach temperature, specified energy recovery).

Control is the manipulation of a degree of freedom (e.g., heater, cooler or exchanger load, stream split fraction) in order to make a process feasible and/or economically optimal in the steady state. In this chapter, "control" is used in a static sense only; process dynamics are not considered.

Uncertainty range is the range of uncertain variables in a design problem. The uncertainty range can consist of "external" uncertainties (e.g., supply temperatures and flow rates) and/or "internal" uncertainties (e.g., heat transfer coefficients). The uncertainty range is typically specified in terms of finite upper and lower bounds on each of the uncertain variables.[1]

Flexible refers to a process which remains feasible for every value of the uncertain variables in the uncertainty range despite *desired* changes to the process (e.g., supply temperature and flow rate variations due to feedstock changes).

Resilient processes are those which remain feasible for every value of the uncertain variables in the uncertainty range despite *undesired* changes to the process (e.g., environmental disturbances in supply temperatures, fouling of heat transfer surfaces). Mathematically, flexibility and resilience are the same problem; in this chapter, the two terms are used synonymously.

Several types of problems can be defined for the analysis and synthesis of resilient HENs. Some basic problems are verbally described here. In the next section, these problems are defined mathematically and interpreted graphically. In subsequent sections, algorithms are presented for solving these problems.

[1] In all of the resilience analysis techniques reviewed here, the uncertainty range can be extended to include variable target temperatures. In addition, if any of the uncertainties are correlated, then the uncertainty range should include only the independent uncertainties with all the dependent uncertainties expressed in terms of the independent ones.

1. *Feasibility Test*

For assumed, fixed values of the uncertain variables, can the "control variables" (degrees of freedom) be manipulated so as to make the HEN feasible (Saboo *et al.*, 1987a)? Note that feasibility of a HEN depends on several factors: assumed values of the uncertain variables, feasibility constraints (e.g., value of ΔT_m, specified level of energy recovery), values of the design and structural variables chosen by the designer *before* the feasibility test (or analogously before plant operation), and the fact that control variables are allowed to vary *during* the feasibility test (or analogously during plant operation).

Many earlier researchers neglected the fact that degrees of freedom are usually available in a process plant (HEN) which can be manipulated during plant operation so as to maintain feasibility (review by Grossmann *et al.*, 1983). By not allowing the control variables to vary, the feasibility test can be unnecessarily conservative.

2. *Resilience (Flexibility) Test*

Is the HEN feasible for *every* value of the uncertain variables in the expected uncertainty range? Note that whether a HEN is resilient depends upon the size of the expected uncertainty range (which the designer must estimate), in addition to the factors listed earlier which affect HEN feasibility. This test can be used to identify "worst case" values of the uncertain variables and to determine whether design changes make a formerly nonresilient HEN resilient in the specified uncertainty range. [Note that Halemane and Grossmann (1983) and Grossmann and Floudas (1987) call this test a "feasibility test" and that they have no specific name for the test with assumed, fixed values of the uncertain variables. In this chapter, we follow the terminology of Saboo *et al.* (1987)].

3. *Resilience (Flexibility) Index*

The resilience (flexibility) test is a yes–no test of HEN resilience in a specified uncertainty range. A more general problem is to measure the size of the largest uncertainty range for which the HEN is resilient (flexible). The resilience and flexibility indices are two different measures of the largest uncertainties (from assumed nominal values of the uncertain variables) for which a HEN remains feasible (Saboo *et al.*, 1985; Swaney and Grossmann, 1985a). Note that these indices depend upon the choice of nominal values for the uncertain variables. These indices can be used to determine how much resilience (flexibility) is gained for a given design change (overdesign or structural change) and to identify "worst case" values of the uncertain variables which limit HEN resilience.

4. *Synthesis of Resilient HENs*

The problem of synthesizing HENs which are both economically optimal and resilient can be posed in many forms. Should HEN cost be minimized only for "worst case" values of the uncertain variables (minimax strategy), or should the "expected" cost of the HEN—averaged over the expected frequency of occurrence of each value of the uncertain variables—be minimized? Should HEN feasibility be guaranteed only at the values of the uncertain variables which minimize cost or for the whole range of uncertain variables? Grossmann *et al.* (1983) review the approaches of several earlier researchers in uncertain process design. Later in this chapter, methods are presented to synthesize HENs in which the cost is minimized for several values of the uncertain variables (to approximate the minimax strategy) and which are resilient for the entire uncertainty range (Floudas and Grossmann, 1987b; Colberg *et al.*, 1988).

III. Analysis of HEN Resilience

A. General Problem Formulations

In this section, general mathematical formulations and graphic interpretations are presented for several resilience analysis problems: (1) feasibility test, (2) resilience (flexibility) test, (3) flexibility index, and (4) resilience index.

1. *Feasibility Test*

The physical performance of a HEN can be described by the following set of constraints (Grossmann and Floudas, 1987):

$$h(d, z, x, \theta) = 0, \qquad g(d, z, x, \theta) \leq 0 \tag{1}$$

where h is the vector of equations (mass and energy balances, energy recovery specification) which hold for steady-state operation and g is the vector of inequalities (target temperature and ΔT_{m} specifications; nonnegative load constraints) which must be satisfied if operation is to be feasible. The variables are classified as follows: d is the vector of design variables that define the HEN structure and exchanger sizes. These variables are fixed at the design stage and remain constant during plant operation. Here θ is the vector of uncertain variables (uncertain supply temperatures and flow rates, heat transfer coefficients, etc.). The vector z of control variables stands for the degrees of freedom that are available during operation and which can be adjusted for different realizations of uncertain variables θ. Finally, x is the vector of state variables which is a subset of the remaining variables and which has the same dimension as h.

For a given HEN design d and for any realization of θ during operation, the state variables can in general be expressed as an implicit function of control variables z using equalities h,

$$h(d, z, x, \theta) = 0 \Rightarrow x = x(d, z, \theta)$$

This allows elimination of the state variables, and the HEN performance specifications can be described with the following reduced set of inequality constraints:

$$g_m[d, z, x(d, z, \theta), \theta] = f_m(d, z, \theta) \leq 0 \qquad (m \in M) \tag{2}$$

where M is the index set for the inequalities. It should be noted that elimination of the state variables is done at this point for the sake of simplicity in presentation; the actual numerical algorithms for analyzing HEN resilience do not require elimination of the equality constraints.

A HEN is feasible for assumed, fixed values of uncertain variables θ if control variables z can be found to satisfy the reduced set of constraints. The HEN feasibility test can be formulated as follows to minimize the maximum constraint violations (Halemane and Grossmann, 1983):

$$\psi(d, \theta) = \min_{z} \max_{m \in M} f_m(d, z, \theta) \tag{3}$$

This minimax problem can be converted to a simpler nonlinear program (NLP) by introducing a slack variable β to measure violations of the inequality constraints:

$$\psi(d, \theta) = \min_{z, \beta} \beta \tag{4}$$

subject to

$$f_m(d, z, \theta) \leq \beta \qquad (m \in M)$$

The HEN is feasible for the assumed values of the uncertain variables θ if and only if $\psi \leq 0$.

In terms of the actual HEN feasibility constraints (including the equality constraints), NLP (4) can be expressed more explicitly as (Saboo *et al.*, 1987a)

$$\psi = \min_{u, v, \beta} \beta \tag{5}$$

subject to:

(A1) Energy balances on all exchangers, heaters, and stream splits:

$$A(u, w)t^S + B(u, v, w)v = b$$

(A2) Specified energy recovery:

$$\sum_k l_k^H = \alpha H(t^S, w)$$

(B1) ΔT_m constraints on all exchangers:

$$C(u, w)t^S + D(u, v, w)v + p \leq \beta e$$

(B2) Nonnegative exchanger and cooler loads:

$$E(u, w)t^S + Gv + r \leq \beta e$$

(B3) Nonnegative heater loads:

$$-l^H \leq \beta e$$

where t^S is the vector of supply temperatures; w the vector of inlet heat capacity flow rates;

$$\theta = \begin{bmatrix} t^S \\ w \end{bmatrix}$$

is the vector of uncertain variables (constant for feasibility test); u the vector of stream split fractions; t^I the vector of intermediate stream temperatures (between exchangers); l^H the vector of heater loads;

$$v = \begin{bmatrix} t^I \\ l^H \end{bmatrix}$$

is the vector of state and control variables (excluding stream split fractions); H the minimum heating requirement; α the factor by which heating target is relaxed from minimum heating requirement;

$$e = [1\ 1 \cdots 1]^T$$

b, G, p, r are constant vectors and matrices; A, C, E are matrices whose elements are functions of u and w; and B, D are matrices whose elements are functions of u, v, and w.

If the HEN has more than the minimum number of exchangers (say n_U more than the minimum) and n_T variable target temperatures, then $n_U + n_T$ of the intermediate stream temperatures and heater loads can be chosen as control variables. Stream split fractions are always available as control variables. These variables are adjusted to try to make the HEN feasible for the assumed, fixed values of the uncertain supply temperatures and flow rates. The HEN is feasible if and only if $\psi \leq 0$.

2. *Resilience (Flexibility) Test*

Resilience of a HEN represents its ability to accommodate uncertainty in a set of selected variables. The resilience properties of a HEN can be