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Mathematical Foundation of Pinch Analysis

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Techniques of Process Integration can be applied to conserve resources such as energy, freshwater, cooling water, hydrogen, solvent, etc. Process Integration methodologies are broadly classified into two categories: methodologies based on the numerical optimization techniques and methodologies based on the conceptual approaches of Pinch Analysis. In this paper, a generalized problem definition for Pinch Analysis problems is mathematically analyzed and a rigorous methodology to solve this problem is discussed. There are three important graphical methodologies also proposed in the literature: Limiting Composite Curve, Material Recovery Pinch Diagram, and Source Composite Curve. In this paper, fundamental derivation of these graphical representations and interrelation between them are established mathematically.

1. Introduction

Process Integration is a system oriented and integrated approach to industrial process design (both grassroots and retrofits) with special emphasis on efficient utilization of various resources and reducing environmental pollution. Process Integration is a branch of generalized process systems engineering. Methodologies of Process Integration are broadly classified into two categories: methodologies based on the numerical optimization techniques and algebraic methodologies based on the conceptual approaches of Pinch Analysis. Numerical optimization based approaches serve as a good synthesis tool in handling complex systems with different complex constraints and employs standard optimization packages to solve these problems. However, major drawbacks associated with these methodologies are model formulation and convergence efficiency. It is utmost important to develop the generalized superstructure in the mathematical modeling of the problem to embed the global optimal solution. Failure to embed global optimal solution in the superstructure implies failure to identify global optimal solution. Use of standard optimization packages leads to inefficient solution procedure as these generalized optimization routines fail to exploit the special structure of the resource conservation problems. Standard numerical techniques, though robust and can handle generalized optimization problems, can be made more efficient by exploiting special structures of some specific problems.
Methodologies based on conceptual approaches of Pinch Analysis help in getting a physical insight of the problem through its graphical representations and simplified tableau-based algebraic calculation procedures. Pinch Analysis was originally developed as a thermodynamic tool to conserve thermal energy through systematic design of heat exchanger networks in process plants (Linnhoff et al., 1982). Subsequently, the problem definition as well as the scopes of Pinch Analysis have been extended to conserve precious resources in various resource allocation networks (RAN), for example, mass exchanger networks (El-Halwagi, 1997), water conservation networks (Wang and Smith, 1994), cooling water networks (Kim and Smith, 2001), hydrogen conservation networks in refineries (Alves and Tolwer, 2002), material reuse networks in process plants (Kazantzi and El-Halwagi, 2005), power system planning with constraints on CO_2 emission (Tan and Foo, 2007), renewable system design for isolated energy systems (Bandyopadhyay, 2011), Chilled water network (Foo et al., 2014), smart grid networks (Giaouris et al., 2014), etc. In recent years, mathematically rigorous analyses of RAN are reported. Savelski and Bagajewicz (2000) proved necessary conditions for optimizing RAN. El-Halwagi et al. (2003) used dynamic programming to develop a rigorous graphical approach. Pillai and Bandyopadhyay (2007) developed a mathematically rigorous solution procedure.

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To enhance physical insight of the problem, different graphical representations have been proposed in literature. Three of the most important graphical representations are Limiting Composite Curve (LCC), Material Recovery Pinch Diagram (MRPD), and Source Composite Curve (SCC). LCC was originally proposed by Wang and Smith (1994) to reduce fresh water requirement in water conservation networks. It is interesting to note that MRPD was introduced independently by El-Halwagi et al. (2003) and Prakash and Shenoy (2004) to reduce fresh water and hydrogen requirements in water and hydrogen conservation networks. On the other hand, SCC was proposed by Bandyopadhyay (2006) to reduce generation of waste in resource conservation networks. Mathematical basis of these graphical representations as well as interrelations between them is established in this paper. The mathematical foundation, established in this paper, help in extending scope of the applicability of Pinch Analysis to handle more complex resource conservation problems.

2. Problem definition and mathematical results

The general problem of Pinch Analysis may be mathematically stated as follows (Bandyopadhyay, 2006):

- A set of N_s internal sources (streams) is given. Each source produces a flow F_{si} with a given quality q_{si}.
- A set of N_d internal demands (units) is also given. Each demand accepts a flow F_{dj} with a quality that has to be less than a predetermined maximum limit of q_{dj}.
- There is an external source, called resource, with a given quality q_{rs}.
- There is an external demand, called waste, without any maximum quality limit.

There is no flow limitation associated with the resource and the waste. Flows are denoted by non-negative real numbers. Quality is defined as a real number and follows inverse scale. In other words, a source with higher numerical value of quality is inferior to another source with lower numerical value. The objective is to minimize total flow requirement from the resource. A network representing the generalized Pinch Analysis problem is shown in Figure 1.

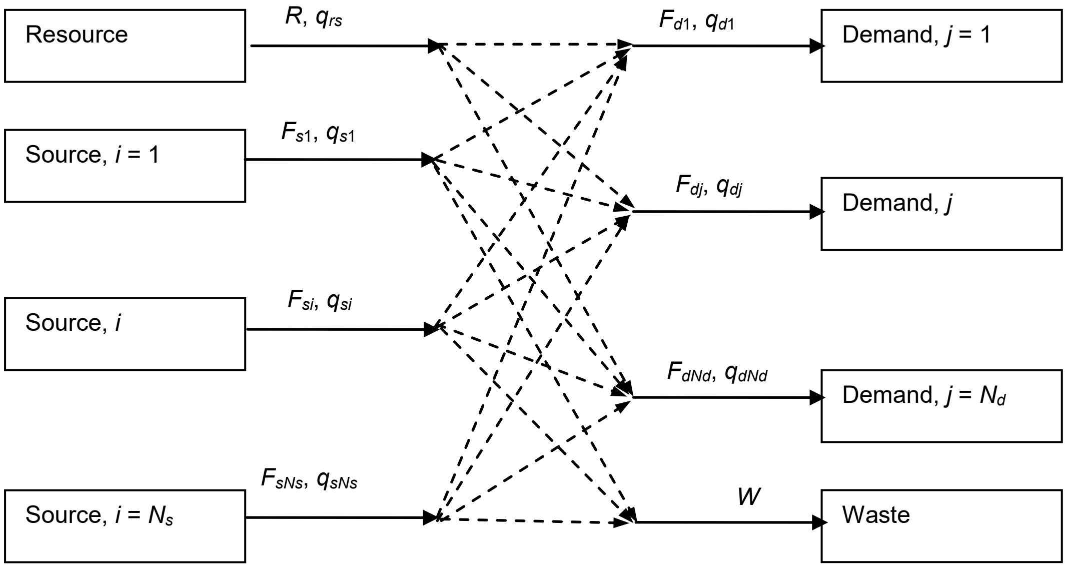

Figure 1: Network representation of Pinch Analysis problem

Before mathematical equations can be written for the generalized mathematical problem, it is important to define the condition of summability of flows and qualities. Whenever two streams with flows F_1 and F_2 and qualities q_1 and q_2, respectively, are added to produce a mixed stream with flow, F_3 and quality, q_3, following relationships are assumed to be true:

$$F_1 + F_2 = F_3 \tag{1}$$

$$F_1 q_1 + F_2 q_2 = F_3 q_3 \tag{2}$$

The product of quality with flow is defined as quality load. Eq(1) and Eq(2) essentially define that flows and quality loads are conserved. In literature, these equations are also known as mixing rules.

Let f_{ij} denote the flow transferred from source i to demand j. Similarly, f_{rsj} and f_{iw} represent the flow transferred from the resource to demand j and flow transferred from source i to the waste, respectively. Mathematical optimization problem can be written as:

$$\text{Minimize, } R = \sum_{j=1}^{N_d} f_{rsj} \tag{3}$$

Subject to following constraints:

$$\sum_{j=1}^{N_d} f_{ij} + f_{iw} = F_{si} \qquad \forall i \tag{4}$$

$$f_{rsj} + \sum_{i=1}^{N_s} f_{ij} = F_{dj} \qquad \forall j \tag{5}$$

$$f_{rsj} q_{rs} + \sum_{i=1}^{N_s} f_{ij} q_{si} \le F_{dj} q_{dj} \qquad \forall j \tag{6}$$

It should be noted that this is a linear programming problem with ($N_s + N_d + N_s \times N_d$) flow variables, ($N_s + N_d$) equality constraints, and N_d inequality constraints.
Total waste generation of the problem can be expressed in terms of total resource requirement:

$$W \equiv \sum_{i=1}^{N_s} f_{iw} = R + \Delta \tag{7}$$

where $\Delta = \sum_{i=1}^{N_s} F_{si} - \sum_{j=1}^{N_d} F_{dj}$, a constant for a given problem. Based on the overall flow balance of the problem and Eq. (7), following lemma can easily be proved (Pillai and Bandyopadhyay, 2007).

Lemma 1: Minimization of resource requirement (3) subject to the constraints (4)–(6) is equivalent to the minimization of waste generation (7) subject to the same constraints.

It essentially suggests that resource minimization and waste minimization are equivalent. Based on the mathematical relations between flows and qualities, few interesting properties of the overall problems may be derived. Using Eq(5) and Eq(6), following lemmas can easily be proved.

Lemma 2: If all the quality vales are added with a constant, the optimization problem remains unchanged.

Lemma 3: If all the quality vales are multiplied by a positive real constant, the optimization problem remains unchanged.

Lemma 2 suggests that quality may be represented by non-negative real numbers. Lemma 3 essentially suggests that quality values can be normalized without affecting the overall result. Similar scaling property may be stated for the flow variables. However, in that case, total resource requirement and total waste generation is also get scaled accordingly.

Lemma 4: If all the flow values, associated with internal sources and demands, are multiplied by a positive real constant, minimum total resource requirement is also multiplied by the same constant.

It is important at this juncture is to define the Pinch Quality. Pillai and Bandyopadhyay (2007) defined Pinch Quality as 'the minimum quality at which waste is generated at optimum.' This implies that $f_{iw} \neq 0$ for $q_{si} = q_p$ and $f_{iw} = 0$ for $q_{si} < q_p$. It should be noted that by definition, Pinch Quality is always controlled by internal sources.
A Pinch divides the entire process into two parts: an above Pinch portion and a below Pinch portion. All internal sources with quality greater than the Pinch Quality ($q_{si} > q_p$), internal demands with maximum acceptable quality greater than the Pinch Quality ($q_{dj} > q_p$), and the waste are part of the above Pinch portion. Below Pinch portion consists of rest of the sources, demands and resource. Following two lemmas suggest that there should not be any Cross Pinch flow transfer (Pillai and Bandyopadhyay, 2007).

Lemma 5: At optimum, no flow is transferred from a below Pinch source to an above Pinch demand.
Lemma 6: At optimum, no flow is transferred from an above Pinch source to a below Pinch demand.

Using these lemmas, the overall flow and quality load balances for the below Pinch portion (inclusive of the Pinch Point) may be expressed as:

$$R + \sum_{\substack{i=1 \\ q_{si} \le q_p}}^{N_s} F_{si} = \sum_{\substack{j=1 \\ q_{dj} \le q_p}}^{N_d} F_{dj} + W_{at\ pinch} \tag{8}$$

$$R\, q_{rs} + \sum_{\substack{i=1 \\ q_{si} \le q_p}}^{N_s} F_{si} q_{si} \le \sum_{\substack{j=1 \\ q_{dj} \le q_p}}^{N_d} F_{dj} q_{dj} + q_p W_{at\ pinch} \tag{9}$$

Combining these two equations, limit for the resource requirement can be expressed as:

$$R \ge \sum_{\substack{j=1 \\ q_{dj} \le q_p}}^{N_d} F_{dj} \frac{(q_p - q_{dj})}{(q_p - q_{rs})} - \sum_{\substack{i=1 \\ q_{si} \le q_p}}^{N_s} F_{si} \frac{(q_p - q_{si})}{(q_p - q_{rs})} \tag{10}$$

Corresponding minimum waste generation can be calculated using Eq. (7).

$$W \ge \sum_{\substack{i=1 \\ q_{si} > q_p}}^{N_s} F_{si} - \sum_{\substack{j=1 \\ q_{dj} > q_p}}^{N_d} F_{dj} + \sum_{\substack{i=1 \\ q_{si} \le q_p}}^{N_s} F_{si} \frac{(q_{si} - q_{rs})}{(q_p - q_{rs})} - \sum_{\substack{j=1 \\ q_{dj} \le q_p}}^{N_d} F_{dj} \frac{(q_{dj} - q_{rs})}{(q_p - q_{rs})} \tag{11}$$

At a given source quality, the lower limit of the resource requirement and waste generation may be calculated using Eq(10) and Eq(11). Since the Pinch Quality is not known a priori, resource requirement and waste generation predicted using these equations can be calculated for every source quality. The Maximum of these lower limits must give the minimum resource requirement and waste generation. This proves the following fundamental theorem of Pinch Analysis.

Theorem 1: The Maximum of the resource requirements, calculated using Eq(10) for different source qualities gives the minimum resource requirement of the overall optimization problem.

3. Graphical representations

Based on the results outlined in the previous section, different graphical representations are developed in this section. A representative example (data provide in Table 1) is considered to illustrate different graphical representations. There are four internal sources and four internal demands. In may be noted that supply quality of one internal source (S1) is better than the resource.
For a given q, for all the internal sources and demands, quality load Q_{LCC} can be defined as:

$$Q_{LCC} = \sum_{\substack{j=1 \\ q_{dj} \le q}}^{N_d} F_{dj}(q - q_{dj}) - \sum_{\substack{i=1 \\ q_{si} \le q}}^{N_s} F_{si}(q - q_{si}) \tag{12}$$

Q_{LCC} represents a piecewise linear curve on quality load-quality diagram and known as LCC (Figure 2a). A resource line, given by the following equation, can also be represented on the same diagram.

$$Q_{resource} = R(q - q_{rs}) \tag{13}$$

It should be noted that inverse of the slop of resource line represents resource requirement. Eq. (10) suggests that resource line, represented by Eq(13), must always be on the right side of the LCC and at optimum, they touch each other at Pinch Quality. Therefore, a feasible resource line, with a pivot point at (0, q_{rs}) must be rotated anti-clock wise to find the minimum resource requirement (Figure 2a). Minimum resource requirement for the illustrative example is 90 t/h with a Pinch at 0.1.
Similar to LCC, for a given q, quality load Q_{SCC} and waste line can be calculated using following expressions:

$$Q_{SCC} = \sum_{\substack{i=1 \\ q_{si} > q}}^{N_s} F_{si}(q_{si} - q) - \sum_{\substack{j=1 \\ q_{dj} > q}}^{N_d} F_{dj}(q_{dj} - q) \tag{14}$$

3.1 $Q_{waste} = Q_T - W(q - q_{rs})$ (15)

Where ΔQ_T is the total quality load surplus in the problem and is defined as:

$$Q_T \equiv \sum_{i=1}^{N_s} F_{si}(q_{si} - q_{rs}) - \sum_{j=1}^{N_d} F_{dj}(q_{dj} - q_{rs}) \tag{16}$$

Q_{SCC} represents a piecewise linear curve on quality load-quality diagram and known as SCC (Figure 2b). Eq(11) suggests that the waste line, represented by Eq(15), must always be on the left side of the SCC and at optimum, they touch each other at Pinch Quality (Figure 2b). Therefore, a feasible waste line, with a pivot point at (Q_T, q_{rs}) must be rotated clock wise to find the minimum waste generation. For the illustrative example, minimum waste generation is targeted to be 70 t/h with a Pinch at 0.1. It may be noted that the pivot point for rotating waste line to minimize waste generation is (8, 0.05) and this is not on the SCC (Figure 2b).

Table 1: Source and demand data for resource conservation problem

Sources	Flow (t/h)	Quality (fraction)	Demands	Flow (t/h)	Quality (fraction)
S1	50	0.01	D1	50	0.02
S2	100	0.1	D2	100	0.05
S3	70	0.2	D3	80	0.15
S4	60	0.3	D4	70	0.25
Resource	To be determined	0.05	Waste	To be determined	To be determined

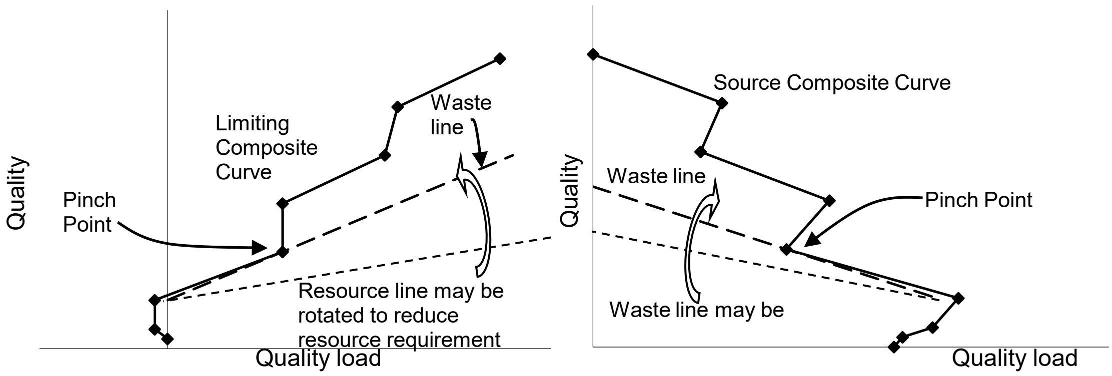

Figure 2: Quality load-quality diagrams: (a) LCC with resource line and (b) SCC with waste line

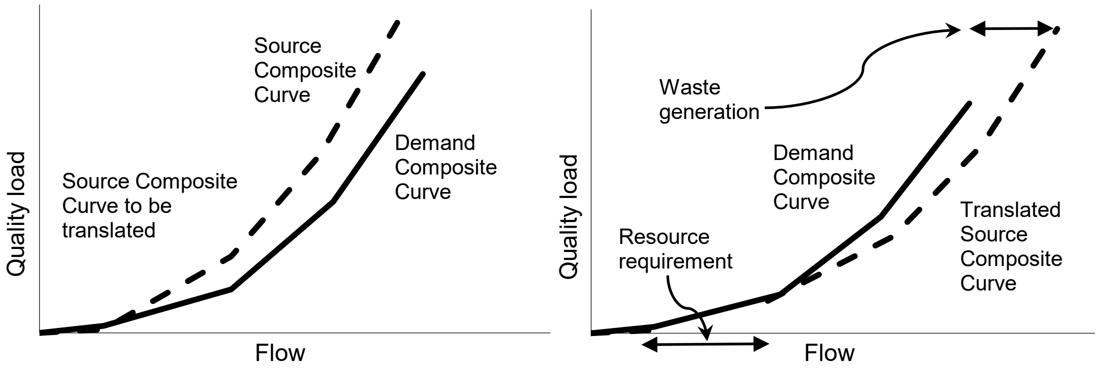

Figure 3: MRPD on flow-quality load diagram: (a) infeasible needs translation of the Source Composite Curves and (b) feasible diagram after translation

Addition of Q_{LCC} and Q_{SCC}, for a given q, leads to an interesting result. Addition of Q_{LCC} and Q_{SCC}, after some simple algebraic manipulations (not shown for brevity), leads to the following expression:

$$Q_{LCC} + Q_{SCC} = Q_T - \Delta(q - q_{rs}) \qquad (17)$$

Eq.(17) suggests that summation of LCC and SCC at any given q, is a straight line that passes through (Q_T, q_{rs}) with a negative slop of overall flow surplus. Therefore, LCC and SCC are reflection of one another about the line given by Eq. (17). The same result was proved by Sahu and Bandyopadhyay (2012) in a different way. Similarly, addition of $Q_{resource}$ line and Q_{waste} results in same expression as Eq(17) and thus, suggests that resource line of LCC and waste line of SCC are also reflection of one another about the line given by Eq(17).

Unlike LCC and SCC, MRPD is depicted on flow-quality load diagram. A Demand Composite Curve is defined as the piece-wise linear curve joining of the points ($\sum_{j=1, q_{dj}<q}^{N_d} F_{dj}$, $\sum_{j=1, q_{dj}<q}^{N_d} F_{dj} q_{dj}$) obtained by choosing q from the set of demand qualities. Similarly a Source Composite Curve may be defined as the piece-wise linear curve joining of the points ($\sum_{i=1, q_{si}<q}^{N_s} F_{si}$, $\sum_{i=1, q_{si}<q}^{N_s} F_{si} q_{si}$) obtained by choosing q from the set of source qualities. Source and Demand Composite Curves, for the illustrative example, are shown in Figure 3a. It should be noted that the slop of each line segment, both for Demand and Source Composite Curves, is quality of the next point (either a demand or a source). For the feasibility of the problem, Source Composite Curve has to

be on the right side of the Demand Composite Curve. Therefore, Composite Curves, as shown in Figure 3a, do not represent a feasible solution. Source Composite Curve has to be moved at the resource to make it feasible. As suggested by Eq(8) and Eq(9), at Pinch, both the flow and quality load balances holds equality relations and thereby suggest that the translated Source Composite Curve and Demand Composite Curve touch each other at Pinch point. Resource requirement and waste generation can both be calculated simultaneously (Figure 3b). Note that translation of Source Composite Curve for impure resource is difficult graphically. Additionally, in the illustrative example, resource quality is not even the purest and proper procedures are not discussed in literature. However, using Lemma 2, resource quality can be transformed to zero and then the Source Composite Curve can be translated along the *x*-axis to target the minimum resource requirement and waste generation.

4. Conclusions

Resource optimization in RAN can be viewed as a network flow problem. Similar to various efficient algorithms, such as transportation simplex method for transportation problems, Hungarian method for assignment problems, etc., Pinch Analysis is an efficient algorithm to solve resource conservation in RAN. In this paper, a mathematical basis for three different graphical methods of Pinch Analysis is established and their interrelation is established. Typically, Pinch Analysis can be applied to simpler problems with simpler constraints. However, the proposed mathematical foundation can be used to extend the applicability of Pinch Analysis to complex problems such as conservation of multiple resources, segregated problems, Multiple-objective Pinch Analysis, RAN with uncertainties, energy integration in water conservation networks, resource conservation with multiple quality operators, etc. Mathematical foundation, established in this paper, can help in evolving more efficient algorithms to address newer problems with mathematical rigor.

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