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Title: A Computationally Inexpensive Approach in Multiobjective Heat Exchanger Network Synthesis

Year: 2010

Version:

Please cite the original version:

Hartikainen, M., & Miettinen, K. (2010). A Computationally Inexpensive Approach in Multiobjective Heat Exchanger Network Synthesis. In M. Collan (Ed.), Proceedings of the 2nd International Conference on Applied Operational Research - ICAOR'10 (pp. 99-109). Uniprint.

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A Computationally Inexpensive Approach in Multiobjective Heat Exchanger Network Synthesis

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June 26, 2010

Abstract

We consider a heat exchanger network synthesis problem formulated as a multiobjective optimization problem. The Pareto front of this problem is approximated with a new approximation approach and the preferred point on the approximation is found with the interactive multiobjective optimization method NIMBUS. Using the approximation makes the solution process computationally inexpensive. Finally, the preferred outcome on the Pareto front approximation is projected on the actual Pareto front.

Keywords: heat exchanger network synthesis, multiobjective optimization, Pareto front approximation, interactive decision making, NIMBUS

1 Introduction

Multiobjective optimization means optimizing multiple objectives at the same time (11). In multiobjective optimization problems there is no well defined single optimal solution, but we can identify a set of so-called Pareto optimal solutions where none of the objectives can be improved without impairing some other. A vector containing the values of all objectives as its components is called an outcome and an outcome given by a Pareto optimal solution is called a Pareto optimal outcome. The set of Pareto optimal solutions can be called the Pareto front.

The many mathematically equal Pareto optimal solutions cannot be ordered without preference information related to outcomes on the Pareto front and the person giving this

information is called a decision maker. We can say that the aim of multiobjective optimization approaches is to help the decision maker in finding the outcome that is the most preferable. Different approaches to multiobjective optimization problems are summarized e.g., in (1; 9; 11).

The heat exchanger network synthesis problem is an important problem concerning heat exchange and the efficient use of energy in it. In (10), this problem is formulated in a new way as a multiobjective optimization problem and solved with an approach where GAMS (the General Algebraic Modeling System, see <http://www.gams.com/>) and the interactive multiobjective optimization method NIMBUS (12; 14) are combined. The use of the NIMBUS method enables the examination of the trade-offs between different objectives of the problem.

The drawback in the interactive method is, however, the fact that the problem is computationally expensive and the decision maker has to wait a relatively long time to get feedback for his/her preferences. This is a common issue, when the problem formulation includes a simulator and function evaluations take time. To keep waiting times feasible a local optimizer is used in (10) to generate Pareto optimal solutions within NIMBUS. Local optimizers, however, have the risk of getting caught in local optima instead of global ones.

In (8), an idea inspired by (4) for solving computationally expensive multiobjective optimization problems is introduced. In this paper, it is proposed that the Pareto front should be approximated in a way that enables examining this Pareto front approximation with existing interactive multiobjective optimization methods. It is argued that the computational expense of the approximation phase which takes place before introducing the decision maker in the solution process does not matter as much as the time-consuming computation done while the decision maker is waiting. In that paper it is argued that an *inherently nondominated Pareto front approximation*, as defined therein, is a good approximation to be used because it does not mislead the decision maker in what is attainable in the problem and what is not. In (7), a method for constructing such an inherently nondominated Pareto front approximation is presented based on the Delaunay triangulation.

In this paper, we present an application of the Pareto front approximation approach in heat exchanger network synthesis. We start with a small set of Pareto optimal outcomes. An inherently nondominated Pareto front approximation is constructed based on these outcomes with the approach given in (7). After this, the Pareto front approximation is parametrized to get a multiobjective optimization problem related to the approximation as defined in (8) and the preferred outcome on the Pareto front approximation is found with the WWW-NIMBUS[®] implementation of the NIMBUS method. The parametrized multiobjective optimization problem based on the approximation is computationally much less costly than the original problem. This is a benefit compared to (Laukkanen et al, 2010). Finally, the preferred solution on the Pareto front approximation is projected on the actual Pareto front by the means of an achievement scalarizing function (18).

The rest of this paper is organized as follows. In Section 2, we briefly describe the heat exchanger network synthesis problem considered. We introduce the tools used, that is our approximation algorithm and NIMBUS, in Section 3. Section 4 is devoted to generating

a Pareto front approximation for the problem and to finding the preferred point on the approximation with the help of NIMBUS. Finally, conclusions are drawn in Section 5.

2 Heat Exchanger Network Synthesis

The heat exchanger network synthesis is a problem for the efficient use of energy. According to (10), the objective of research in heat exchanger network synthesis is to

...design a heat exchanger network that minimises the total annualised cost, given sets of hot streams, cold streams, hot utilities and cold utilities. Each hot and cold stream has a specific heat capacity flowrate, a start- and target temperature.

For more detailed treatment of the topic see (10) and references therein. Different optimization based solution approaches are given e.g., in (2; 10; 16). Even though the problem has conflicting objectives, only in (10) it is clearly formulated as a multiobjective optimization problem.

A way to model the heat exchanger network synthesis, called the SynHeat model, is introduced in (19). Based on this model, a multiobjective optimization problem with four objectives

$$\begin{array}{ll}
 \min & \text{Cold utility consumption} \\
 \min & \text{Hot utility consumption} \\
 \min & \text{Number of heat exchanger units} \\
 \min & \text{Total heat exchanger surface area} \\
 \text{s.t.} & \text{Energy balance for each stream} \\
 & \text{Energy balance for each stage} \\
 & \text{Calculation of hot and cold utility requirements} \\
 & \text{Assignment of inlet temperatures} \\
 & \text{Feasibility of temperatures} \\
 & \text{Logical constraints for process stream matches and utility matches} \\
 & \text{Calculation of approach temperatures}
 \end{array}$$

was formulated in (10). For details, see the appendix of (10). In this paper, we to consider a slight modification of the above with three objectives

$$\begin{array}{ll}
 \min & \text{Number of heat exchanger units} \\
 \min & \text{Total heat exchanger surface area} \\
 \min & \text{Hot utility consumption} \\
 \text{s.t.} & x \in S,
 \end{array} \tag{1}$$

where S is the set given by the constraints in the above multiobjective optimization problem. The most important reason not to consider the cold utility consumption objective is that it has been noticed to correlate with the hot utility consumption and it suffices to examine only

one of them. Also an advantage of having three objectives is that then we can conveniently illustrate the approximated Pareto front. Let us however stress that the usability of our approximation approach does not depend on the number of objectives.

3 Background: Approximation and NIMBUS

Before solving the synthesis problem, we briefly describe the methods used. In other words, we introduce the approximation method used as well as the NIMBUS method.

A Pareto front approximation is defined by (17) to be a set A in the objective space considered a surrogate of the Pareto front. Approximating the Pareto front of a multiobjective optimization problem is an interesting problem from both the application and the theoretical viewpoint. Surveys of approximation methods can be found in (Hartikainen et al., 2010 b) and in references therein. However, as noted in (8), most of the Pareto front approximations have not been designed with decision making at mind but mainly for representing Pareto optimal solutions.

In (8), inherent nondominance is introduced as a desirable property for a Pareto front approximation and it is shown that an inherently nondominated approximation of the Pareto front is a good basis for decision making. A set A in the objective space is defined to be inherently nondominated, if there does not exist vectors $a, b \in A$ so that a dominates b . A vector a is said to dominate another vector b , if a is at least as good as b in all objectives and strictly better in at least one. If P is a set of Pareto optimal outcomes for the multiobjective optimization problem, an inherently nondominated set A is called an inherently nondominated Pareto front approximation based on P , if also $P \subset A$. Furthermore, an inherently nondominated set A is called a B -maximal inherently nondominated Pareto front approximation for some other set B if there does not exist an inherently nondominated set $\tilde{A} \subset B$ so that $A \subsetneq \tilde{A}$. In (8), also an approach to solve multiobjective optimization problems using a inherently nondominated Pareto front approximation was proposed, where a parametrized problem is formed with the approximation so that e.g., interactive multiobjective optimization methods can be applied for decision making on the approximation.

In (7), an approach to construct a \mathcal{D} -maximal inherently nondominated approximation is given, where \mathcal{D} is a Delaunay triangulation of a given subset of Pareto optimal outcomes P . The Delaunay triangulation is a complex (i.e., collection of polytopes with certain additional properties (6)) so that the body (i.e., the union of all polytopes in the complex) is the convex hull of the outcomes in P and also some other properties are satisfied. The Delaunay triangulation is a useful concept in computational geometry (5). It is shown in (7) that an inherently nondominated complex is such that there are no two polytopes in the complex so that one dominates the other. It is said that a polytope K^1 in the objective space dominates another polytope K^2 also in the objective space, if there exists vectors $s^1 \in K^1$ and $s^2 \in K^2$ so that s^1 dominates s^2 . In (7), it is shown that, if all the objectives of the multiobjective optimization problem are to be minimized and k is the number of objectives, the domination

between polytopes K^1 and K^2 can be found by solving optimization problems

$$\begin{aligned} \min & \max_{i=1,\dots,k} (s_i^1 - s_i^2) \\ \text{s.t. } & s^1 \in K^1, s^2 \in K^2 \end{aligned} \quad (2)$$

and

$$\begin{aligned} \min & \sum_{i=1}^k (s_i^1 - s_i^2) \\ \text{s.t. } & s^1 \in K^1, s^2 \in K^2 \\ & s_i^1 \leq s_i^2 \text{ for all } i = 1, \dots, k. \end{aligned} \quad (3)$$

The polytope K^1 dominates the polytope K^2 if and only if one of the following holds: (i) the optimal value in problem (2) is less than zero or (ii) the optimal value in problem (2) is exactly zero and the optimal value in problem (3) is less than zero.

The dimension of a polytope $K \subset \mathbb{R}^k$ is defined to be the minimal dimension of a linear subspace L for which there exists a points $z \in \mathbb{R}^k$ so that $K \subset z + L$. According to (6), the dimension of a polytope K with vertices $z^1, \dots, z^a \in \mathbb{R}^k$ is the rank of the matrix

$$\begin{bmatrix} 1 & z_1^1 & \dots & z_k^1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & z_1^a & \dots & z_k^a \end{bmatrix}$$

minus one. A Delaunay triangulation contains polytopes of different dimensions. In (7), it is shown that polytopes with dimension equal to the number of objectives are not inherently nondominated. For this reason, we can remove these polytopes straight away and, thus, we let \mathcal{D} from now on be the Delaunay triangulation containing only the polytopes with dimension less than the number of objectives.

In (7), an approach to construct a \mathcal{D} -maximal inherently nondominated Pareto front approximation is proposed based on removing polytopes from the Delaunay triangulation. In this paper, we construct the approximation for problem (1) by removing polytopes from the triangulation \mathcal{D} according to the rules (R1) and (R2) given in (7). Assume that the a -polytopes (i.e., polytopes with a vertices) in the Delaunay triangulation \mathcal{D} are $K^{a,1}, \dots, K^{a,t^a}$. A polytope $K^{a,j}$ is removed from the triangulation \mathcal{D} , if (R1) there exists a point $p \in P$ that dominates or is dominated by the polytope or the polytope dominates itself or (R2) there exists a b -polytope $K^{b,j'} \in \mathcal{D}$ with either $b > a$ or ($b = a$ and $j' < j$) that is not removed from the triangulation and that dominates or is dominated by the polytope $K^{a,j}$.

Before we describe how the Pareto front is approximated, we briefly introduce NIMBUS. We use NIMBUS in this paper, because it was used also by (10) as it has been successfully applied in various design and planning problems (15). NIMBUS is an interactive multiobjective optimization method (12; 14; 11). In interactive methods (9; 11; 15), the decision maker expresses his/her preferences iteratively and before every iteration the decision maker is given additional information about the problem related to the preferences that he/she has given previously. This iterative procedure enables the decision maker to learn about the problem (15) and also the decision maker is able guide the search to the areas of the Pareto front that are most interesting to him/her.

Interactive methods differ by the types of preference information asked from the decision maker and by the ways this preference information is used. The NIMBUS method uses classification of objectives to indicate how the current solution should be changed; given a Pareto optimal solution to the multiobjective optimization problem the decision maker can classify the objective functions into classes $I^<$, $I^{\leq}(z)$, $I^=$, $I^{\geq}(z)$ and $I^>$ defined, respectively, as classes of objective functions that the decision maker wants to improve as much as possible, wants to improve to the limit z , is allowed to remain unchanged, is allowed to deteriorate until limit z and is allowed to change freely for a while. This preference information is then converted into several different single-objective subproblems with the help of different scalarization functions as proposed in (14). These subproblems are then solved to generate different Pareto optimal outcomes which are then shown to the decision maker who can see how well the designed changes could be attained. The decision maker can choose any of these outcomes as the starting point of the next round of iteration. This iteration procedure can either start with an outcome given by the decision maker or from a so-called neutral outcome and it is repeated as long as the decision maker is satisfied with the outcome at hand. Further information of this so-called synchronous NIMBUS with other means to direct the search process is given in (14).

The WWW-NIMBUS[®] is a web based implementation of the NIMBUS method introduced in (13; 14). WWW-NIMBUS[®] is free for academic use at <http://nimbus.mit.jyu.fi/>.

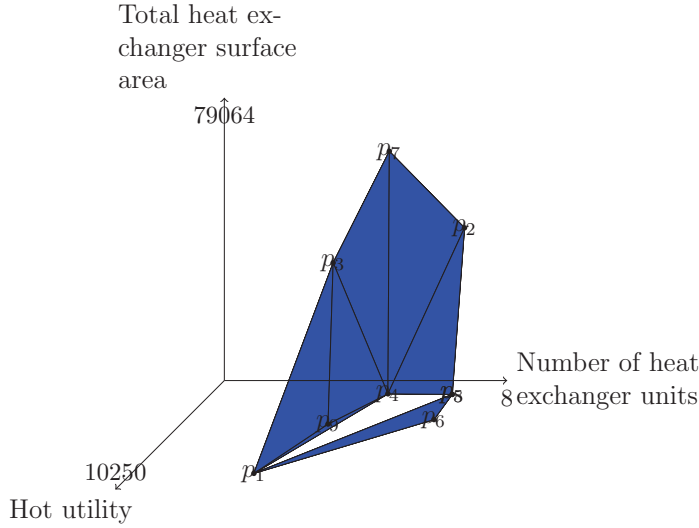
4 Approximation and Solution Process in Heat Exchanger Network Synthesis

In this section, we solve the heat exchanger network synthesis problem and for that we first generate an inherently nondominated Pareto front approximation for it. We assume we are given nine Pareto optimal outcomes (forming the set P) summarized in Table 1.

Table 1: The Pareto optimal outcomes for the multiobjective heat exchanger network synthesis problem

Point	Number of heat exchanger units	Total heat exchanger surface area	Hot utility consumption
p^1	4	1897	10250
p^2	8	52175	1755
p^3	5	52175	5371
p^4	6	4913	3028
p^5	8	4734	3028
p^6	8	2608	4920
p^7	6	79064	2882
p^8	8	4734	3028
p^9	5	4153	5902

Figure 1: The body of the \mathcal{D} -maximal inherently nondominated Pareto front approximation



The Deulaunay triangulation of this set P contains 75 polytopes. Twelve of these polytopes are three-dimensional and they are removed as explained before, because the number of objectives is three in this case. By solving optimization problems (2) and (3) for each pair of polytopes in the complex \mathcal{D} we determine which polytopes dominate each other and by following rules (R1) and (R2) one can see which polytopes are removed from the triangulation \mathcal{D} . Solving problems (2) and (3) for each pair is easily implemented on any programming language and here we have used GNU Octave (3). The polytopes in the resulting \mathcal{D} -maximal inherently nondominated Pareto front approximation are summarized in Table 2 and the body of the resulting approximation is drawn in Figure 1.

Table 2: The polytopes in the \mathcal{D} -maximal inherently nondominated Pareto front approximation

Polytope	Vertices	Polytope	Vertices	Polytope	Vertices
\mathcal{P}_1	p^6	\mathcal{P}_2	p^7	\mathcal{P}_3	p^2
\mathcal{P}_4	p^1	\mathcal{P}_5	p^3	\mathcal{P}_6	p^4
\mathcal{P}_7	p^8	\mathcal{P}_8	p^9	\mathcal{P}_9	$p^6 p^1$
\mathcal{P}_{10}	$p^7 p^2$	\mathcal{P}_{11}	$p^3 p^7$	\mathcal{P}_{12}	$p^3 p^1$
\mathcal{P}_{13}	$p^3 p^4$	\mathcal{P}_{14}	$p^4 p^7$	\mathcal{P}_{15}	$p^4 p^2$
\mathcal{P}_{16}	$p^8 p^6$	\mathcal{P}_{17}	$p^8 p^2$	\mathcal{P}_{18}	$p^8 p^4$
\mathcal{P}_{19}	$p^8 p^1$	\mathcal{P}_{20}	$p^9 p^4$	\mathcal{P}_{21}	$p^9 p^1$
\mathcal{P}_{22}	$p^4 p^1$	\mathcal{P}_{23}	$p^9 p^3$	\mathcal{P}_{24}	$p^3 p^4 p^7$
\mathcal{P}_{25}	$p^4 p^7 p^2$	\mathcal{P}_{26}	$p^8 p^4 p^2$	\mathcal{P}_{27}	$p^8 p^6 p^1$
\mathcal{P}_{28}	$p^9 p^4 p^1$	\mathcal{P}_{29}	$p^9 p^3 p^1$	\mathcal{P}_{30}	$p^9 p^3 p^4$

Now that we have formulated an inherently nondominated approximation we can move to the next phase and show how to use it for decision making. Through a parametrization of the approximation, the multiobjective problem of choosing the preferred point on the approximation $\mathcal{A} = \{\mathcal{P}_1, \dots, \mathcal{P}_{30}\}$ can be formulated as a mixed-integer problem with three objectives

$$\begin{aligned} \min \quad f(\lambda, t) = & t_1(\lambda_1 p^3 + \lambda_2 p^4 + \lambda_3 p^7) + t_2(\lambda_1 p^4 + \lambda_2 p^7 + \lambda_3 p^2) \\ & + t_3(\lambda_1 p^8 + \lambda_2 p^4 + \lambda_3 p^2) + t_4(\lambda_1 p^8 + \lambda_2 p^6 + \lambda_3 p^1) \\ & + t_5(\lambda_1 p^9 + \lambda_2 p^4 + \lambda_3 p^1) + t_6(\lambda_1 p^9 + \lambda_2 p^3 + \lambda_3 p^1) \\ & + t_7(\lambda_1 p^9 + \lambda_2 p^3 + \lambda_3 p^4) \\ \text{s.t.} \quad & \sum_{i=1}^3 \lambda_i = 1 \\ & \sum_{i=1}^7 t_i = 1 \\ & \lambda \in [0, 1]^3 \\ & t \in \{0, 1\}^7. \end{aligned}$$

The above formulation is imputed into the WW-NIMBUS[®] implementation of the NIMBUS method and the most preferred point on the approximation can be found with NIMBUS.

At this point the decision maker is involved. The iterations of the solution process with WW-NIMBUS[®] can be seen Table 4. The chosen alternative on each iteration is underlined.

Table 3: The course of the NIMBUS optimization procedure

Iter.	Issue	Number of heat exchanger units	Total heat exchanger surface area	Hot utility consumption
0	Starting point	6.161743	3431.044	6347.206
	Classification	$I \leq (5)$	$I \geq (8000)$	$I <$
1	Alternative 1	5.829885	4783.843	3517.424
	Alternative 2	8.0	52175.59	1755.5
	<u>Alternative 3</u>	6.0	4913.04	3028.43
	Alternative 4	5.392376	4458.865	4774.958
	Classification	$I =$	$I \geq (6000)$	$I \leq (2500)$
2	Alternative 1	7.162517	8383.323	2932.537
	Alternative 2	6.153829	8548.212	2930.523
	Alternative 3	6.117182	7682.189	2953.848

Because the decision maker sees that the desired changes in iteration 2 were not possible, alternative 3 of iteration 1 is selected as the preferred outcome. During the solution process the decision maker is interested in reducing the hot utility consumption near 3000 with as few as possible heat exchanger units and as small as possible surface area. The true Pareto optimal outcome corresponding to the selected approximate outcome is obtained by using the achievement scalarizing function (18). The achievement scalarizing function is

maximized with the reference point as the preferred point on the approximation and this yields a Pareto optimal outcome to the initial problem with the number of heat exchanger units 6.00, total heat exchanger surface area 4791.71 and hot utility consumption 3043.59. The solution related to this outcome is taken as the final outcome since it is satisfactory to the decision maker. However, if this was not the case we could have added this point to the set P and repeated the approximation procedure to get a more accurate approximation.

5 Conclusions

This paper shows an application of a new Pareto front approximation approach to solving a heat exchanger network synthesis problem. In the solution process the Pareto front is first approximation and then the decision maker can find the most preferred approximated outcome with an interactive method, here interactive multiobjective optimization method NIMBUS. Finally, the preferred approximated outcome is projected on the true Pareto front.

The method has many advantages. First of all, because the starting point of the approximation, that is, the finite set of Pareto optimal outcomes P is computed before involving the decision maker, one can even use time consuming global optimization methods as in this case. Since the approximation has analytical error estimates given in (7), one can find out how good the approximation is. After having computed the Pareto front approximation it is possible to use any multiobjective optimization method to study the approximation and search for a preferred outcome. Because the parametrized problem formed based on the approximation is computationally inexpensive, the decision maker does not have to wait for new solutions being generated. In this paper, it was shown that NIMBUS can be used for that. Finally, the preferred outcome on the approximation can be projected on the real Pareto front with achievement scalarizing function (18).

6 Acknowledgments

This research was partly supported by the Academy of Finland, grant number 128495. The authors would like to thank MSc Vesa Ojalehto for his significant help with providing the Pareto optimal points and for his expertise with the GAMS model. The authors would also like to thank MEng Timo Laukkanen for the GAMS model that was used in this paper.

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