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Multi-period steam turbine network optimisation. Part I: Simulation based regression models and an evolutionary algorithm for finding D-optimal designs

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Abstract

In this work, a methodology for building multi-period optimisation model of steam turbine network is presented. The optimisation model can estimate and evaluate the effect of changes to the thermal energy demand of processes. The subject is divided into two parts. In Part I, a method for finding regression models for steam turbine networks using a simulation model and an evolutionary algorithm for finding D-optimal designs is presented. In Part II, the method presented in Part I is used to develop and solve a multi-period MINLP model of a steam turbine network in a utility system. There are two major problems that are addressed in Part I; Firstly, the evolutionary algorithm for finding D-optimal design is applied to try to determine which values should be simulated in order to generate the data for the regression model. Secondly, a theoretical model of steam turbine performance is used to model the feasible operation of the steam turbine. This is necessary to be able to make an efficient evolutionary algorithm for finding D-optimal designs. The use of regression models makes it possible to build optimisation models of utility systems that are compact and transparent. There is a natural trade-off between the flexibility of a model and the accuracy. The major drawback of the methodology, is that the models developed must be considered 'ad hoc'-models, and are not as flexible compared to models where all the process units are modelled in full detail. An advantage of the methodology developed in this work is that it gives more possibilities of finding an acceptable simplification of the optimisation problem, as the methodology is not bound by a certain set of thermodynamic rules or specific mathematical form of the relations in the models.

Part II demonstrates how the methodology can be applied when building a multi-period optimisation model to estimate and evaluate how changes to the processes will affect the utility system.

Keywords: Multi-period optimisation; Steam turbine network; D-optimal design

1. Introduction

A common problem in the process industry is to correctly estimate and evaluate how changes to the process will affect the utility system. Utility systems generates heat (usually as steam) and electricity, and are an important and essential part of many industrial processes. A good utility system will potentially reduce both the negative environmental impact of the processes and reduce the costs of operation. The operation of steam turbines is an important part of a utility system, and subsequently the optimisation of steam turbine networks is an important part of improving the efficiency of the utility system. The methodology developed in this work can be useful when evaluating how process changes will affect the optimal operation and design of the utility systems. In this work, a methodology for building multi-period optimisation model of steam turbine network is

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Nomenclature

μ	$\mu = k_2 c_{n2}/\sqrt{2\Delta h_s}$
ξ	matrix containing all candidate points
a	regression model coefficient
b	regression model coefficient
$C(n,p)$	the number of combinations of size p from a collection of size n, i.e. $C(n,p) = \frac{n!}{p!(n-p)!}$
c	velocity vector (m/s)
h	specific enthalpy (kJ/kg)
k	flow-through factor
m	mass flow (kg/s)
n	polytropic exponent, number of candidate points
p	pressure (bar), number of variables in a model
R^2	the square of the Pearson correlation
S	set of all possible model matrices
v	specific volume (m^3/kg)
W	work/load (MW)
X	model matrix
x	variable
y	response variable

Superscripts and subscripts

$*$	optimal
$'$	transpose of a matrix
k	number of factors in a 2^k design
0	design state
α	state before turbine stage
ω	state after turbine stage
n	normal component of vector
s	isentropic

presented. The methodology will be useful for consultants and process engineers involved in energy efficiency in the process industry, as the methodology can be used when evaluating how process changes will affect the optimal operation and design of the utility systems. The optimisation model can estimate and evaluate the effect of changes to the thermal energy demand of processes. The novel part of this work is the combination of the regression models, mathematical programming and evolutionary algorithm with physical insight of the steam turbine behaviour.

The work is based on the earlier work [1,2]. The subject is divided into two parts. In Part I, a method for finding regression models for steam turbine networks using a simulation model and an evolutionary algorithm for finding D-optimal designs is presented.

In Part II, the method presented in Part I is used to develop and solve a multi-period optimisation model of a steam turbine network in a utility system. The optimisation model is used to model and evaluate how different process changes will affect the performance of the utility system.

2. Background

There are traditionally two approaches to find the optimal operation and to improve utility systems. One approach is the *thermodynamic approach*, where the thermal efficiency is the focus. See for instance the work by Nishio et al. [3] or by Chou and Shih [4] for examples of this approach. A problem with the thermodynamic approach is that the methodologies have difficulties with handling trade-offs, for example between the investment costs and thermal efficiency. The other approach is to use mathematical programming (optimisation), which can handle trade-offs more efficiently. For an overview of how optimisation have been applied in process systems engineering see the paper by Biegler and Grossmann [5]. However, for sufficiently large and complex systems the mathematical programming approach runs into problems. Mathematical formulations of process synthesis problems are often nonlinear and contain integer variables (so-called mixed integer nonlinear programming (MINLP) problems). MINLP problems can be solved to a global optimum with algorithms that exist today. However, for complex problems these algorithms soon become prohibitively inefficient. Some MINLP problems are NP-complete (nondeterministic polynomial) problems, which means that no efficient algorithm has been found for these problems. When solving large problems of these kinds it is therefore necessary to simplify the problems, or to decompose them into smaller sub-problems. As a result of the simplifications, the mathematical programming problems might not be accurate enough to be useful in the design of a real plant. A lot of work has been made to overcome these problems. Manninen and Zhu [6] and Hostrup et al. [7] reduced the model sizes by using thermodynamic insights and analysis. Iyer and Grossmann [8] simplified the optimisation problem by using only linear relations. Using only linear relations means that the nonlinearities must be simplified or ignored, which can reduce the accuracy of the models significantly. Another example is the work by Bruno et al. [9]. They developed a rigorous MINLP model for the synthesis of power plants. The focus was on the design and involved fixing the steam pressure levels. One way of formulating optimisation models of steam turbine networks is to use the concepts developed by Mavromatis and Kokossis [10,11]. They used ideas from pinch and total-site analysis combined with the *Willan's line*. The Willan's line [12,13] is a line that describes the relationship between the mass flow rate and the load. The Willan's line works well for each turbine stage if the output is controlled by a regulation valve. However, for a steam turbine with a regulation stage, the relationship between the mass flow and the load is not linear, and the Willan's line is no longer valid [14]. It is also common to use only one Willans line to model the whole turbine. This is a poor approximation if the turbine is a complex turbine with many extractions. For a discussion of the accuracies of detailed models and the Willans line see the work by Tveit et al. [15]. Another source of nonlinearities is the variation of the steam temperature after the valve.

An approach to modelling steam turbine networks without over-simplification (e.g. fixing pressures) is to use regression model(s). As shown in the work by Tveit [2], using regression models in the mathematical programming models does not necessarily mean a loss of accuracy compared to models where all units included in the system are modelled in detail. However, there might be a considerable difference in the size and numerical complexity of the models in favour of the regression based models. Simulation models are often superior to the optimisation models when it comes to modelling existing processes. This is due to the simplifications that are necessary to make a robust and solvable optimisation model. Simulation models are often used for verification of the results from an optimisation model. As data for regression models are not always available from the existing plant, it makes sense to use the simulation model to generate the data needed. Many commercial process simulation software packages also come with an integrated option for optimisation. A standard method for process flowsheet optimisation is the SQP-algorithm (*Successive Quadratic Programming*) [16]. This algorithm is suitable for integration with simulation software, as information from the simulation model can be used directly in optimisation with continuous variables. However, optimisation models with discrete variables cannot easily be solved using process simulation software. To solve these problems it is necessary to build an optimisation model in addition to the simulation model.

A normal approach to generate data from simulation models is to change one variable at the time and keep the other variables constant. This means creating a grid of size n^k, where n is the resolution and k is the number of variables. It can be appreciated that even for a few variables, due to the combinatorial complexity, the time it takes to complete a grid, makes it necessary to choose the values to be simulated more carefully. One option is to take advantage of the methods developed in the field of *experimental design*. As the name suggests, experimental design is in general used in experimental work. In many cases an experiment is timely and costly, thus lots of work has been put into the development of methods that reduce the amount of times different combinations of an experiment has to be performed.

3. D-optimal design

The problem of optimal experimental designs is to choose the best reduced set of points from all the possible candidate points. There exists several symmetric designs for fitting first-order and second-order models, e.g. the 2^k-design and several variations of the central composite design (CCD) [17]. Where it is not possible to use the traditional symmetric designs, since the experimental region is irregular, or the model is non-standard, or the sample size requirements are unusual, other criteria for selecting the design must be applied. It will be seen in Section 4 that the feasible regions for steam turbine operations are not symmetrical. There are several design optimality criteria (e.g. *A-optimality* and *D-optimality*). Perhaps the most used is the D-optimality criterion. An introduction to D-optimal designs can be found in the paper by Aguiar et al. [18]. The symmetric designs mentioned above are all D-optimal designs.

The D-optimal design aims to minimise the volume of the hyper-ellipsoid that describes the confidence interval for each coefficient. When this volume becomes smaller, the coefficients will be more precise, and subsequently the estimation is more precise. Let ξ_n be an $(n \times p)$ matrix that contains all the candidate points, and p is the number of variables in the model, as shown in Eq. (1).

$$\xi_n = \begin{bmatrix} x_{1,1} & x_{2,1} & \cdots & x_{p,1} \\ x_{1,2} & x_{2,2} & \cdots & x_{p,2} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1,n} & x_{2,n} & \cdots & x_{p,n} \end{bmatrix} \tag{1}$$

If the purpose of the experiment is to fit the model shown in Eq. (2) and the number of experiments are limited to four, then four candidate points must be selected from ξ_n.

$$y = a_1 + a_2x_1 + a_3x_2 + b_2x_1^2 + b_3x_2^2 \tag{2}$$

If, for instance, the selected candidate points are numbered 1, 4, 12 and 17, Eq. (3) shows the resulting matrix, ξ_4, containing the candidate points and the so-called *model matrix*, X.

$$\xi_4 = \begin{bmatrix} x_{1,1} & x_{2,1} \\ x_{1,4} & x_{2,4} \\ x_{1,12} & x_{2,12} \\ x_{1,17} & x_{2,17} \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{1,1} & x_{2,1} & x_{1,1}^2 & x_{2,1}^2 \\ 1 & x_{1,4} & x_{2,4} & x_{1,4}^2 & x_{2,4}^2 \\ 1 & x_{1,12} & x_{2,12} & x_{1,12}^2 & x_{2,12}^2 \\ 1 & x_{1,17} & x_{2,17} & x_{1,17}^2 & x_{2,17}^2 \end{bmatrix} \tag{3}$$

The *dispersion matrix* is defined as $(X'X)^{-1}$. The D-criterion states that the optimal design matrix, X^*, is the model matrix, X, that minimises the determinant of the dispersion matrix:

$$|(X^{*\prime}X^{*})^{-1}| = \min_{X \in S} |(X'X)^{-1}| \tag{4}$$

where S is the set of all $C(n,p)$ possible model matrices.

Among several exchange algorithms for finding D-optimal designs, *Fedorov's* algorithm is most known [19]. An overview of some exchange algorithms can be found in the paper by Nguyen and Miller [20]. As the number of candidates increases, the number of possible combinations becomes prohibitively large to be solved using the exchange algorithms, and other strategies for solving the problem must be applied. Stochastic search methods based on natural processes like genetic algorithms and simulated annealing have successfully been applied to this problem. For instance, Broudiscou et al. [21] used a genetic algorithm for selecting the D-optimal design, while Duffull et al. [22] used simulated annealing.

In Section 5, an evolutionary algorithm for finding D-optimal designs for developing regression models for steam turbine behaviour based on simulations is presented. An important part of the algorithm is the modelling of the feasible region for the steam turbine operation. In the next section, an mathematical expression of this feasible region is presented.

4. Feasible region for steam turbine operation

For a turbine stage there is a relationship between the mass flow, m, the entrance state (e.g. pressure, p_α, and specific volume, v_α) and the back pressure, p_ω. Eq. (5) shows an expression of this relationship for a fixed blade construction [23].

$$\left(\frac{m}{m_0}\right)^2 = \frac{\bar{\mu}^2 p_\alpha v_{\alpha 0}}{\bar{\mu}_0^2 p_{\alpha 0} v_\alpha}\left(\frac{1-\frac{p_\omega}{p_\alpha}^{\left(\frac{n+1}{n}\right)}}{1-\frac{p_{\omega 0}}{p_{\alpha 0}}^{\left(\frac{n+1}{n}\right)}}\right) \tag{5}$$

where the subscript '0' refers to the design state, n is the polytropic exponent and $\mu = k_2 c_{n2}/\sqrt{2\Delta h_s}$. c_{n2} is the normal component of the velocity vector of the steam at the exit, Δh_s is the isentropic enthalpy difference for the stage and k_2 is the flow-through factor. Under the assumptions that the polytropic exponent, n, is constant and equal to 1 and μ is constant and that the steam is ideal steam (i.e. $p_\alpha v_\alpha = p_{\alpha 0} v_{\alpha 0}$), Eq. (5) can for superheated steam be written as

$$\left(\frac{m}{m_0}\right)^2 = \frac{p_\alpha^2}{p_{\alpha 0}^2}\left(\frac{1-\left(\frac{p_\omega}{p_\alpha}\right)^2}{1-\left(\frac{p_{\omega 0}}{p_{\alpha 0}}\right)^2}\right) \tag{6}$$

Solving Eq. (6) for p_α gives:

$$p_\alpha = \sqrt{\left(\frac{m}{m_0}\right)^2 (p_{\alpha 0}^2 - p_{\omega 0}^2) + p_\omega^2} \tag{7}$$

From Eq. (7) it is possible to calculate the extraction pressure in a turbine as a function of the mass flow through the next stage. Many processes require the steam to be above a certain pressure, so the mass flow through the turbine stages is bounded from below. The lower bound can be calculated using Eq. (8).

$$m_{\text{lower},i} = \max\left\{\frac{\sqrt{-(p_{\alpha 0,i}^2 - p_{\omega 0,i}^2)(p_{\omega,i}^2 - p_{\alpha,\text{lower},i}^2)}\, m_{0,i}}{p_{\alpha 0,i}^2 - p_{\omega 0,i}^2}, m_{i+1}\right\} \tag{8}$$

where $p_{\alpha,\text{lower},i}$ is the lowest acceptable inlet pressure for the stage and m_{i+1} is the mass flow to the next stage. By using the above expressions it is possible to define the feasible region for the mass flows, bounded by the extraction pressure. An example is shown in Section 6. For a real process the situation is more complicated, as it is possible to by-pass the steam turbine and reduce the high pressure steam to lower pressures using a valve. This will give more controllability, but the exergy losses will increase and the overall system efficiency will decrease. It is also common to have selective extractions (i.e. steam can be supplied from multiple extractions and steam from the stage with the lowest extraction pressure above the required pressure is used).

5. Evolutionary algorithm for selecting D-optimal designs

Genetic algorithms was first developed by Holland [24], while evolution strategies were developed by Rechenberg and Schwefel (see for instance the book by Schwefel [25]). An overview of evolutionary algorithms is given in the paper by Whitley [26]. The evolutionary algorithm developed in this paper can be seen as a hybrid of the genetic algorithms and evolution strategies, as it applies ideas from both.

A flowchart for the evolutionary algorithm for finding D-optimal designs for regression model of the steam turbine behaviour is shown in Fig. 1.

The first step is to find an initial population. The next step is to generate a new generation by modifying individuals. The individuals to be modified are taken from the previous generation, where the probability of an individual to be selected is proportional to its fitness. The fitness is the value of the determinant of the dispersion matrix.

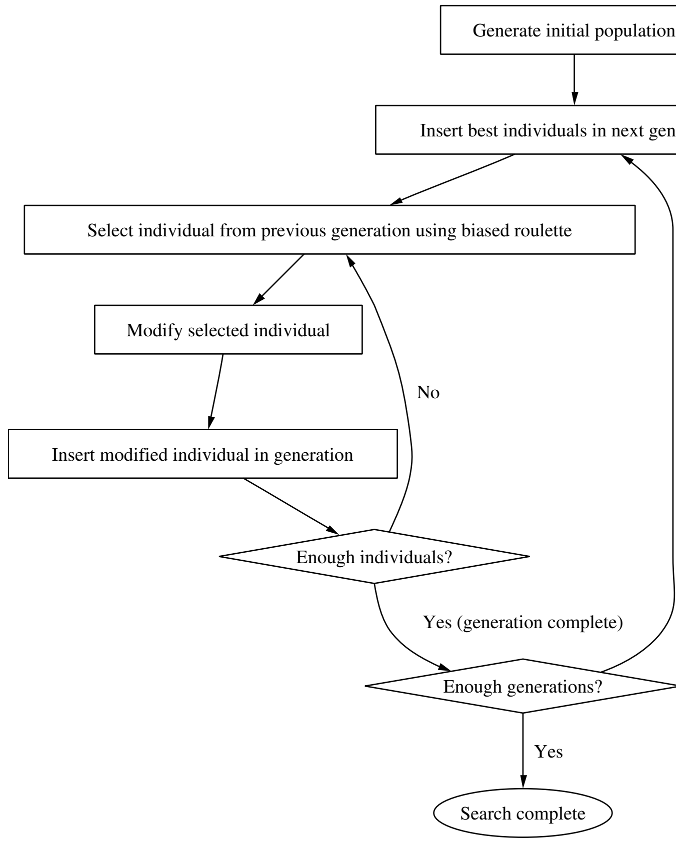

Fig. 1. Flowchart of the evolutionary algorithm for finding D-optimal designs.

5.1. Initial population

A generation consists of the individuals, which are matrices containing candidate points, different information about the individuals, (i.e. the fitness and the relative fitness), and different information about the generation (i.e. maximum, minimum and average fitness of the individuals).

The initial population is generated by selecting the mass flows at random, but making sure that the selected mass flows are feasible. The mass flow for the last turbine stage is selected first. A random number between the lower and upper bound of the mass flow of the last stage is selected. The inlet pressure to the stage is calculated using Eq. (7). The lower bound for the mass flow into the previous stage is calculated using Eq. (8), and a random number between the upper and newly calculated lower bound can be selected. This continues until the first turbine stage is reached, where the lower bound for the mass flow is the flow into the second stage. When the sufficient amount of individuals are generated, the fitness, relative fitness, maximum, minimum and average fitness for the individuals are calculated, and the generation is complete.

5.2. Construction of the next generation

In order to make sure that the best solution in the next generation is not worse than the previous generation, a strategy often referred to as *elitism* is applied. This involves that a given fraction of the best individuals in a generation is copied to the next. The next procedure is to select the individuals for reproduction. This is done using a method similar to a biased roulette wheel. The probability of an individual to be selected for reproduction is as mentioned proportional to the individuals relative fitness. See for example the book by Goldberg [27] for a detailed explanation.

In the classical genetic algorithm a crossover operator is applied. The crossover means that the new individual is generated by selecting two ‘‘parents’’, and converting them into a string of chromosomes (e.g. a binary string) and mix the chromosomes. This strategy cannot efficiently be used in this case, since the offspring resulting from the crossover might not be feasible. Instead a mutation strategy similar to the one used for generating the initial population is applied. This strategy is more related to evolutionary strategies. The strategy also starts from the last turbine stage and then continues forward, but in this case the random numbers used for selecting the mass flows are normally distributed centred on the current value of the mass flow. There is a chance that the normal distributed random number is infeasible, so this must be checked for calculation. If no feasible point is found after a preset value, the search terminates, and the mass flow is selected using the strategy for the initial population. When a sufficient amount of individuals are generated, fitness, relative fitness, maximum, minimum and average fitness for the individuals are calculated, and the generation is complete.

The search can be terminated if the objective function has not improved during a fixed amount of generations, or when a predetermined number of generations has been reached. The last termination strategy is applied here. The result of the algorithm is the matrix containing the mass flow with the smallest determinant of the dispersion matrix.

6. Small example

The methodology is illustrated using a simulation model in *Prosim* [28] of a back pressure steam turbine with two extraction levels. The objective is to generate a model of the steam turbine using the simulation model and the algorithm for finding D-optimal designs. Fig. 2 shows a picture of the simulation model.

The extraction pressure is dependent on the mass flow of the following stage. Fig. 3 shows the feasible region for the mass flows through the last two stages of the steam turbine.

The form of the regression model is given in Eq. (9). The model connects the mass flow through the turbine to the shaft work.

$$W = a_1 + \sum_{i=2}^{4}(a_i m_i + b_i m_i^2) \tag{9}$$

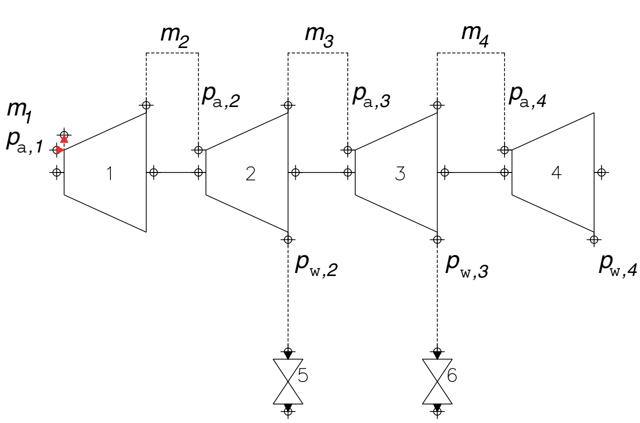

Fig. 2. Back pressure steam turbine with regulation stage and two extraction levels; The live steam temperature and pressure are 450 °C and 70 bar, respectively. The extraction pressures are 20 bar and 10 bar and the back pressure is 3 bar.

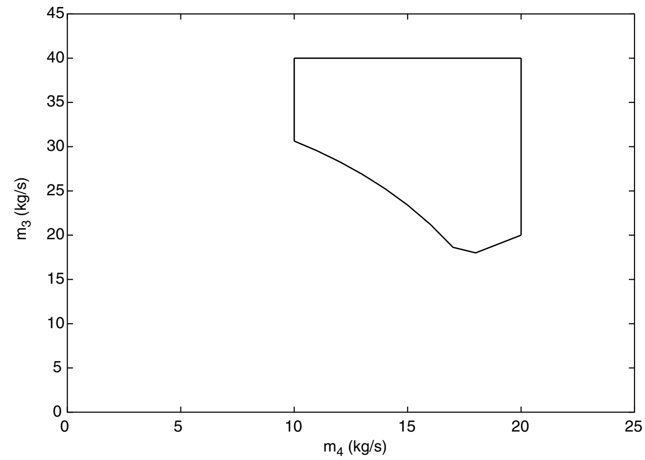

Fig. 3. Feasible region for the mass flows through the two last stages.

where the subscript $i = 2,\ldots,4$ numbers the mass flows according to the numbering in Fig. 2. The regression model will be based on 50 simulation points. The evolutionary algorithm presented in Section 5 is implemented in *Matlab* [29]. The number of individuals in a generation is set to 100 and the number of generations is set to 250. Fig. 4 shows how the objective function is improving with the generations for five different runs of the evolutionary algorithm.

The 50 points resulting from the evolutionary algorithm are simulated and the resulting turbine shaft work, W, is recorded for each simulation run. The coefficients for Eq. (9) are found using the least absolute deviation criterion. The resulting linear optimisation model is shown in Eq. (10).

$$\begin{aligned} &\min\left(\sum_{j=1}^{50} r_j^+ + r_j^-\right) \\ &\text{s.t.}\ \ W_j = a_{1,j} + \sum_{i=2}^{4}(a_i m_{i,j} + b_i m_{i,j}^2) + r_j^+ - r_j^- \quad \forall j \in (1,2,\ldots,50) \\ &\quad r_j^+, r_j^- \geqslant 0 \end{aligned} \tag{10}$$

where j refers to the results from the simulations. The optimisation model is formulated and solved using *GAMS* [30] with CPLEX as the LP-solver. The resulting coefficients are listed in Table 1.

The values from the simulations are compared to the values calculated by the regression model. The average absolute deviation between the simulated values and the values calculated by the regression model is 1.51% and the square of the Pearson correlation, R^2, is 0.996. The regression model is now complete, and can be included in an optimisation model.

7. Discussion and conclusions

A methodology for finding regression models of steam turbine networks is developed successfully.

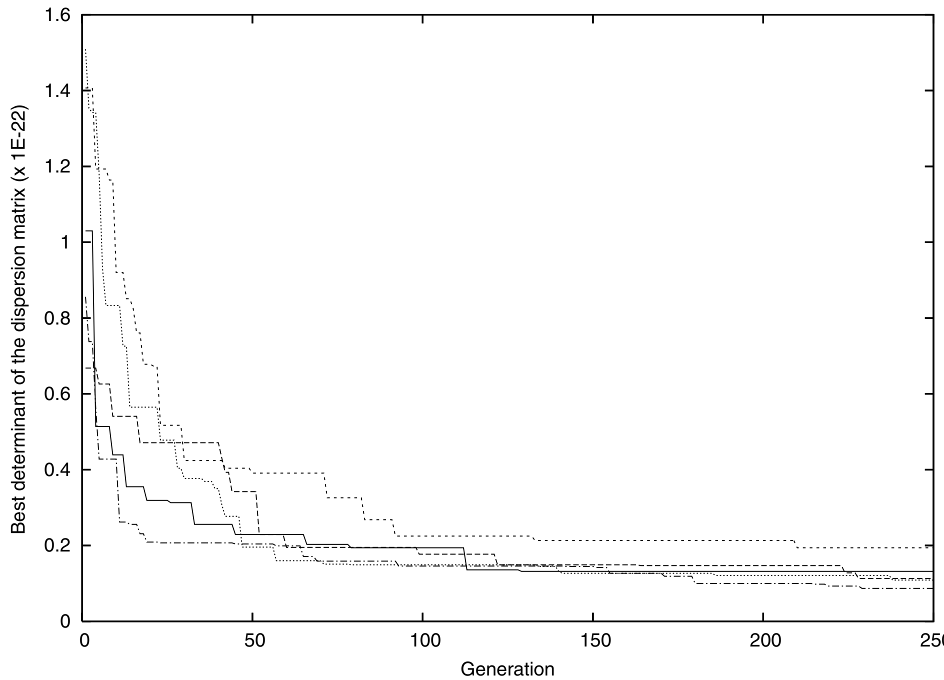

Fig. 4. The best determinant of the dispersion matrices found in each generation for five runs of the evolutionary algorithm.

Table 1
Coefficients for the regression model in Eq. (9)

i	a_i	b_i
1	−21.042	
2	1.591	-1.419×10^{-2}
3	−0.155	3.261×10^{-3}
4	−0.232	8.119×10^{-3}

The methodology involves simulation models and an evolutionary algorithm for finding D-optimal designs. The simulation model is used to generate data, based on the design generated by the evolutionary algorithm. The use of regression models makes it possible build optimisation models of utility systems that are compact and transparent. There is a natural trade-off between the flexibility of a model and the accuracy. The major drawback of the methodology is that the models developed must be considered 'ad hoc'-models, and are not as flexible compared to models where all the process units are modelled in full detail. In this respect, developed models based on the work by Bruno et al. [9] can more easily be used for a wider range of objectives. However, this flexibility comes at the cost of accuracy. An advantage of the methodology developed in this work is that it has greater flexibility of chosing the desired accuracy of the models. Compared with the earlier work by Manninen and Zhu [6], Hostrup et al. [7], and Iyer and Grossmann [8], the methodology gives more possibilities of finding an acceptable simplification of the optimisation problem, as the methodology is not bound by a certain set of thermodynamic rules or specific mathematical form of the relations in the models.

Part II will demonstrate how the methodology can be applied in a multi-period optimisation model.

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