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PARAMETER OPTIMIZATION OF A PAPER MACHINE MODEL

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Abstract: In this paper, the problem of calibrating a paper machine dryer section model to measurement data is treated. The model, which is dynamic, nonlinear and of large scale, is implemented in Modelica and Dymola. The purpose of the model is to evaluate, in simulation, new control structures before application to the plant. This approach requires a well calibrated model in order for simulation results to be valid also on the real plant. In this paper, the problem is addressed by parameter optimization. A custom application integrating code generated by Dymola and packages for numerical optimization has been developed. Results are satisfactory, in that the mismatch between the calibrated model response and measured data is small.

Keywords: Parameter optimization, Large scale optimization

1. INTRODUCTION

Detailed modeling of large scale plants has received increased industrial interest in recent years. This is due mainly to the availability of languages and tools enabling development of large, hierarchical and modular models. Using this methodology, the user is relieved from the burden of managing potentially cumbersome programming API:s for e.g. numerical simulation codes, and may instead focus on embedding expert knowledge using better suited abstractions.

There are several benefits of developing detailed models of large scale industrial plants.

Typically, operation of industrial processes are costly, and it is therefore usually difficult to motivate extensive experiments, e.g. to evaluate control performance. Modeling is therefore attractive, since it enables a wide range of applications, including simulation, control design and evaluation, bottle-neck analysis and operator training, which may not be possible to implement on the real plant.

It is desirable that the behavior of the model is similar to that of the real plant, in order for results obtained from the model to be applicable on the plant. It is usually necessary to modify the original model to obtain a better match with measurement data. A common method to minimize the plant-model mis-match is to select one or more parameters of the model, and then tune these until a satisfactory model response is obtained. This procedure of tuning parame-

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ters while leaving the structure of the model unchanged is referred to as gray-box identification, see (Bohlin and Isaksson, 2003). Parameter tuning may in simple cases be done by hand, but more complex problems requires structured methods for finding the parameter set which yields the best result. One such method is parameter optimization, which, in addition to selection of parameters to optimize also includes definition of a performance criterion to minimize.

In this paper, preliminary results concerning parameter optimization of a paper machine dryer section model is reported. The model describes the dryer section of PM7 located at Husum, Sweden and is implemented in Modelica, see (Modelica Association, 2005). The structure of the model is typical for a high-fidelity model built from first principles in that it is non-linear and contains a large number of dynamic states, algebraic variables and parameters.

2. MODELING OF THE DRYER SECTION

The dryer section consists of a large number of steam heated cast iron cylinders that are used to dry the paper. The wet paper is pressed against the cylinder surfaces with aid from dryer fabrics. The moisture in the paper is controlled by changing the steam pressures in the cylinders. Around the dryer section there is a hood where the air in- and outflow is controlled. As the paper is dried, water evaporates from the sheet and the air supply is used to remove the moisture.

In the dryer section, many of the paper's final properties such as web strength, shrinkage and curl/twist are set. One of the most important quality parameter for paper is the moisture content. In the dryer section the water content in the paper web is reduced from 50-65% when entering the dryer section from the press section to the final 3-10%. The dryer section consumes 2/3 of the energy needed to run a paper machine.

The PM7 paper machine is a multi-cylinder machine producing copy paper at the M-real mill in Husum, Sweden. The PM7 drying cylinders are divided into six groups, consisting of one, two, two, three, ten and twelve cylinders respectively. The dryer section of the machine is divided into a pre-dryer and an after dryer section with the surface sizing in the middle. The objective of the after-dryer section is only to dry the mixture added by the surface sizing and it cannot take care of moisture problems from the pre-dryer section.

In order for a model to be useful, it be should accurate enough for the particular application. E.g., linear models are commonly used to describe the behavior of the plant in the close vicinity of a particular operating point. Typically, the moisture controller of a paper machine is based on several linear models to take some of the non-linearities of the plant into account. A different approach is taken in (Slätteke, 2006), where a paper machine drying section is developed using first principles for the sub-components of the plant. Connection of the sub-components then yields a model which captures the full nonlinear behavior of the drying section. This bottom-up method yields a model which describes in detail the dynamic behavior of the plant, which makes it well suited for simulation studies and control evaluation.

The process treated this work is presented in detail in (Ekvall, 2004), and only a brief description is given here. In modeling of the PM7 dryer section, the work by (Slätteke, 2006) is used. Based in this work, Slätteke has developed a library containing common components of a dryer section, such as steam heated cylinders, lumped models for the paper web in contact with a cylinder and in the free draw as well as control system structures. The library enables rapid development of dynamic models of paper machine dryer sections. The library is implemented in Modelica.

Using this library, a dryer section model for PM7 has been developed. For simulation, the software Dymola has been used. The final DAE model has about 1750 variables, of which 250 are continuous time states, and 700 parameters.

The optimization software, described in Section 3, does not support all features of Modelica. Most notably, state and time events are not supported. This implies that no Modelica constructs that results in events in the simulation model can be used. In addition, the software is currently designed to calculate sensitivities for state variables (as opposed to algebraic variables) only. Hence, all variables used in optimization problems must be state variables in order for sensitivity information to be obtained.

Accordingly, the original model was modified to take these restrictions into account. In order to force the desired variables to be state variables the `selectState` modifier was used. The model contained only one event generating sub-model; a PID controller with a saturation function. In this case, the saturation function was simply replaced by a smooth approximation. The influence on the simulation result was neglectable.

3. SOFTWARE TOOLS

The dryer section model has been implemented, as mentioned above, in Modelica and Dymola. The parameter optimization problem, however, was solved by integrating several software packages into a custom application which utilized the C-code representing the model generated by Dymola. The results were then fed back to Dymola and verified on the original simulation model.

The software packages used in the development of the custom application are:

- a C programming interface to access routines generated by Dymola, dsblock. Using this interface, custom applications can be developed for e.g. simulation or like in this case, optimization. The interface provides basic routines for obtaining information about model parameter and initial state values, evaluation of the right side of the resulting ODE (DAE) and the associated Jacobian.
- a DAE-solver, DASPK 3.1 (Maly and Petzold, 1996). This code solves DAE:s as well as calculates sensitivities required for optimization. The code is written in Fortran and was translated to C using f2c.
- an NLP-code, IPOPT (Wächter and Biegler, 2006). This code implements a primal-dual interior point method and was used to solve the NLP resulting from the parameter optimization problem.
- a package for managing the communication between the Dymola C interface and DASPK, which has been developed in order to enable convenient development of optimization applications based on models generated by Dymola. This package, in the following referred to as ssDASPK, provides e.g. simulation and sensitivity calculation for use in custom applications.

These packages were compiled and linked with the code representing the model generated by Dymola, into an application which was used to set up and solve the optimization problem. The structure of the application is shown in Figure 1.

4. PARAMETER OPTIMIZATION

Model parameter values can be determined in several ways. Some parameters are available in tables, and are not associated with uncertainty, whereas others may be determined from experiments. Mechanical systems may for example be disassembled and its components can be measured and weighted. Yet some parameters may
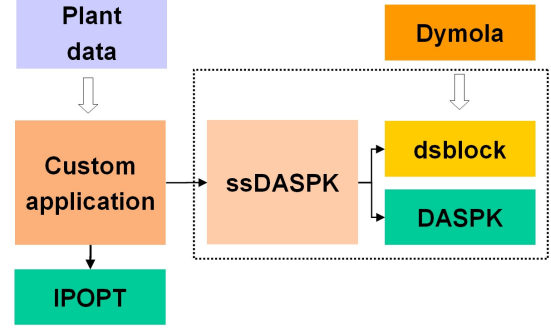

Fig. 1. Software application structure.

be inherently hard to find accurate values for. In the dryer section model, typically heat transfer coefficients fall into this category.

When selecting parameters to optimize, parameters which are uncertain are attractive choices. However, it should be kept in mind, that the parameter optimization procedure does not necessarily produce the physically correct parameter values. Rather, the selected parameters are used to compensate for all types of model-data mismatch given a particular performance criterion. This implies that the actual parameter values obtained from optimization should not be interpreted as the true physical values, but rather those that achieves the best model-data match. On the other hand, it is usually desirable to ensure that parameters have physically feasible values.

4.1 Problem Definition

Setting up a parameter optimization problem requires insight into which aspects of the model are most important. In this case, both the dynamic and static model response is of importance. However, in a first step, only the static behavior has been considered. Specifically, cylinder and paper temperatures of the paper machine have been measured during stationary operation conditions. The aim of the optimization has been to improve the stationary response of the model in the sense that the difference between simulated temperatures and measured temperatures, in stationarity, should be minimized.

A reasonable cost function to minimize is then

$$J = \sum_{i \in \mathcal{S}} \gamma_i (x_i^m - x_i^s)^2 \qquad (1)$$

where $\mathcal{S}$ are the indices of the temperature states of interest, γ_i are weights, x_i^m measured temperatures (in stationarity) and x_i^s simulated temperatures (in stationarity). During the optimization all weights were set to 1.

Table 1. Optimization parameters

Parameter	Nom.	Min.	Max.
α [W/(m^{2}K)]	500	400	5000
K_G [m/s]	0.06	0.02	0.1
α_{p0} [W/(m^{2}K)]	400	200	1000
α_{pK} [W/(m^{2}K)]	1200	400	1600

Four parameters were selected for optimization:

- The heat transfer coefficient between steam and condensate in a cylinder, α
- The mass transfer coefficient K_G which is used in the expression defining evaporation of water from the paper surface
- The heat transfer coefficient between cylinder and paper is given by the expression $\alpha_p = \alpha_{p_0} + \alpha_{p_K}u$, where u is the moisture of the paper, see (Wilhelmsson, 1995). α_{p_0} and α_{p_K} were optimized.

Table 1 summarizes nominal, maximum and minimum values for the parameters.

4.2 Solving the Problem

Traditionally, optimization problems incorporating constraints imposed by dynamic systems have been addressed by dynamic programming, (Bellman, 1957) or the maximum principle, (Pontryagin *et al.*, 1962). During the last two decades, however, a new family of methods, referred to as direct methods have emerged. These methods are based on discretization of the original optimization formulation, transforming the infinite dimensional problem into a finite dimensional one. The discretized problem is then solved by means of algebraic non-linear programming.

There are two main approaches to direct discretization. Simultaneous methods are based on full discretization of the control and state spaces, yielding very large NLP to solve, see (Biegler *et al.*, 2002) for an overview. There exist, however, efficient solvers for this type of problems. Sequential methods, on the other hand, are based on discretization of the control space only, resulting in a smaller number of parameters in the resulting NLP, see (Vassiliadis, 1993). Optimization of Dymola models has previously been considered in the work (Franke *et al.*, 2003), where the Simulink interface provided with Dymola was used to access the model. The main difference between the approach used in (Franke *et al.*, 2003) and this work lies in the methods of accessing the model, where the `dsblock` interface has the advantage of offering evaluation of a symbolic Jacobian.

The algorithm used to solve the problem in this work is in line with a sequential method. The dynamics of the model is represented by a DAE system of index 1, which is generated by Dymola from the Modelica code. The DAE system can be written on the form

$$\dot{x} = f(x, y, p)$$
$$0 = g(x, y, p) \tag{2}$$

where x represents the (dynamic) state, y are the algebraic variables and p are the parameters.

In order for a (gradient based) NLP algorithm to have fast convergence, it is important to provide to the algorithm not only the cost function, but also its gradient with respect to the optimization parameters. Calculation of high accuracy gradients for dynamical systems generally involves calculation of the state sensitivities with respect to parameters, $\partial x/\partial p$. This can be done by integration of the sensitivity equations. In this work, DASPK was used for this purpose.

The problem may now be written

$$\min_p J = \min_p \sum_{i \in S} \gamma_i (x_i^m - x_i^s)^2$$

subject to $\tag{3}$

$$\dot{x} = f(x, y, p)$$
$$0 = g(x, y, p)$$

This formulation has the benefit of having few optimization variables – only the parameters p are optimized – but also involves integration of the sensitivity equations up to steady state, which is computationally expensive.

However, since only the stationary response of the model is considered in this work, the dynamic constraint $\dot{x} = f(x, y, p)$ can actually be written $0 = f(x, y, p)$. This yields a purely algebraic optimization problem, which eliminates the need to integrate the sensitivity equations. The optimization problem may now be written

$$\min_{p, x, y} J = \min_{p, x, y} \sum_{i \in S} \gamma_i (x_i^m - x_i^s)^2$$

subject to $\tag{4}$

$$0 = f(x, y, p)$$
$$0 = g(x, y, p)$$

This problem is obviously algebraic, but has, on the other hand, a larger number of optimization variables including parameters, state variables and algebraic variables.

Both methods were evaluated, and it was found that the algebraic formulation rendered significantly shorter execution times. For the algebraic formulation, execution times ranged from approx 0.5-3 min depending on problem set up. The termination tolerance in IPOPT was set to 10^{-4}. The dynamic formulation needs, however, to be used if dynamic aspects of the model are included in the performance index.
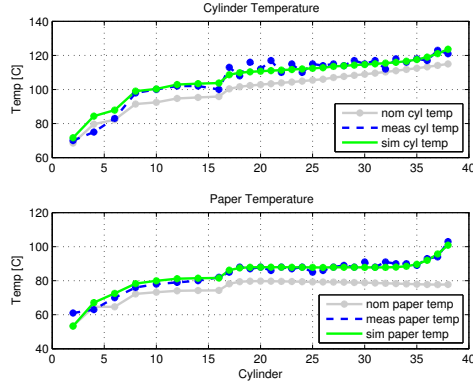
Fig. 2. Stationary temperature profiles in the case of four parameters. The x-axis shows cylinder numbers.

5. RESULTS

Solving the problem (4) yields the optimal parameter values $\alpha = 703.14$, $K_G = 0.037531$, $\alpha_{p_0} = 955.52$ and $\alpha_{p_K} = 843.72$. The optimal cost was 447.5, compared to the cost 4787 for the nominal parameter values. The optimal temperature profiles are shown in Figure 2. For comparison, the nominal profiles are plotted. As can be seen, there is a significantly improved fit between simulated and measured responses. It can be noted, however, that there is still a temperature mismatch for some cylinders.

In order to further improve model fit to data, the number of optimization parameters could be increased. There are two main reasons why additional parameters may achieve a better fit. Firstly, the initial assumption that all cylinders of the dryer section share the same parameter set may not be true. This is because the cylinders are operated under different conditions (pressures, temperatures etc.). Secondly, additional optimization parameters may give improved compensation for unmodelled phenomena, such as e.g. varying air condition along the dryer section.

In this case, the structure of the model offers a natural way to introduce additional parameters. The cylinders of the dryer section are organized into steam groups, where all cylinders of a group are operated at the same pressure. It then seems reasonable to assume that cylinders within a group share the same characteristics, and could share the same parameter set. The model consists of six steam groups, which yields 24 optimization parameters.

Now, the introduction of additional parameters may lead to an over-parametrized model. This may lead to a situation where the model is fitted to a particular data set, including potential measurement errors. In order to avoid
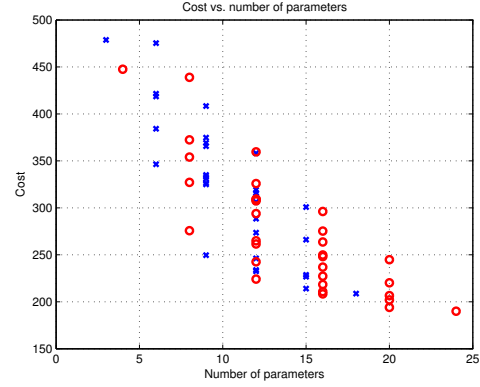

Fig. 3. Optimal cost as a function of the number of parameters. (o) corresponds to the cases with all parameters free and (x) corresponds to the cases where α_{p_K} has been assumed fixed.
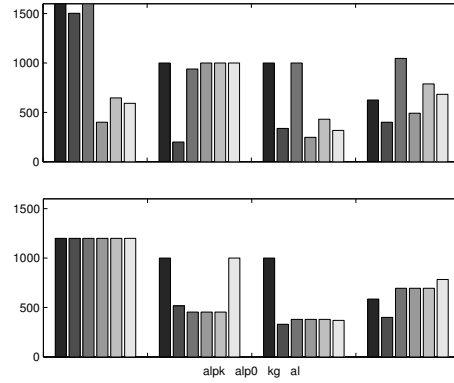

Fig. 4. Parameter values in the case of additional parameter sets. The first bar within each group corresponds to the parameter value for the first steam group etc.

this situation, the marginal benefit of introducing additional parameters should be quantified and analyzed. This has been done by assuming that neighbouring steam groups may share the same parameter set. For example, if we let steam groups one and two, three and four and finally five and six share parameter sets, three parameter sets yielding twelve parameters are obtained. Using this approach, there are 32 combinations, including the extreme cases with four and 24 parameters.

In Figure 3 the optimal cost obtained in each of the 32 cases is indicated by (o). As can be seen, the marginal benefit from introducing additional parameters is decreasing. It is also interesting to investigate the optimal parameter values for the steam groups. In the upper plot of Figure 4, the parameter values for each steam group in the case of 24 parameters are shown. As can be seen, there are large parameter variations between the steam groups, and several parameter values are equal to the bounds. Also,
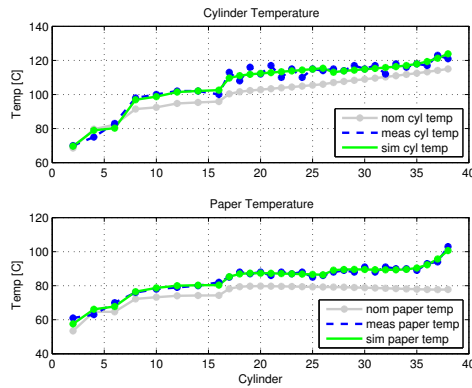
Fig. 5. Temperature profiles for the case of separate parameter sets for each cylinder group.

it can be noted that the parameters α_{p_K} and α_{p_0} seems to have an inverse relationship for some steam groups, i.e. groups two, four, five and six. This is due to the relationship $\alpha_p = \alpha_{p_0} + \alpha_{p_K}$. Clearly, this expression gives two degrees of freedom for the single parameter α_p, and when additional parameter sets are introduced, this leads to redundancy. In order to resolve this problem, α_{p_K} was fixed to its nominal value 1200. The optimal costs for the resulting cases are indicated by (x) in Figure 3. As can be seen, little is lost in terms of lowest cost for a particular number of free parameters. In the lower plot of Figure 4, the optimal parameter values corresponding to the case of 12 free parameters (four parameter sets) which yields the lowest cost are shown. This choice is made since it seems to be a reasonable trade-off between cost and number of parameters. The parameter variations between the steam groups are now smaller, although some values are still at the upper and lower bounds. The corresponding temperature profiles are shown in Figure 5. The improvement compared to the case of four parameters is clearly visible.

The issue of trading decreased cost against number of parameters deserves a more extensive treatment than has been given in this paper. However, this will further elaborated in future work, where fitting of the dynamic response of the model in combination with larger data sets will be treated.

6. CONCLUSIONS AND FUTURE WORK

In this paper, a parameter optimization scheme, applied to a paper machine dryer section has been reported. A dryer section model has been developed in Modelica. A custom application integrating software packages for simulation and optimization has been developed to solve the pa-

rameter optimization problem. The results show a good match between measured and simulated values. Future work in the project includes incorporation of dynamic quantities in the objective function, taking also dynamic properties of the model into account.

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