PROCESS DESIGN AND CONTROL

Input Design for Large-Scale Sheet and Film Processes

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Manipulated variable moves are computed to maximize the information contained in experimental data collected from sheet and film processes. The experimental design procedure minimizes the confidence ellipsoid of the critical model parameters over the manipulated variables subject to their physical constraints. For a simulated blown film process, the model is 1 order of magnitude more accurate than that identified from the industrial standard bump test experiments. The improved accuracy results in a 37% reduction in closed-loop thickness variations. This indicates that substantial benefits can be achieved by incorporating the optimal experimental design algorithm into industrial sheet and film process control algorithms.

1. Introduction

Sheet and film processes constitute a class of processes important to the polymer, pulp and paper, and photographic industries (Braatz et al., 1996; Rawlings and Chien, 1996; Smook, 1992). Such processes include papermaking, polymer extrusion, and adhesive coating (see Figure 1). Sheet and film processes are characterized by large dimensionalities (up to 200 manipulated and 1000 controlled variables), tightly constrained input moves (min−max and second-order spatial constraints), poorly conditioned interaction matrices (condition number approaching infinity), poor signal-to-noise ratios (which can be less than one for thin films), and a limited number of experimental runs allowed for model identification purposes (sometimes no more than five) (Braatz et al., 1996). The development of high-quality models for such processes poses a challenging identification problem (Campbell and Rawlings, 1996; Featherstone and Braatz, 1995, 1997b; Kjaer et al., 1994; Kristinsson and Dumont, 1996).

In past work it was shown that the industrial bump tests that are applied to sheet and film processes are not sufficiently informative to adequately identify the process directionality (Featherstone and Braatz, 1997b). Here the main goal is to determine whether the optimal experimental design can result in substantial control benefits by providing experimental input−output data as informative as possible. The experimental design procedure minimizes the confidence ellipsoid of the most critical model parameters over the manipulated variables subject to their physical constraints. A simulated annealing algorithm computes a suboptimal solution of the nonconvex optimization problem. This algorithm appears to be the first to include the effect of constraints in the experimental input design for processes with high condition numbers (Andersen and Kummel, 1992a,b; Koung and MacGregor, 1993, 1994; Li and Lee, 1996a,b). The algorithm is applied to a simulated blown film extruder and compared to the results from a standard industrial input design. The new algorithm provides an order-of-magnitude improvement in model quality, which results in a 37% reduction in thickness variability.

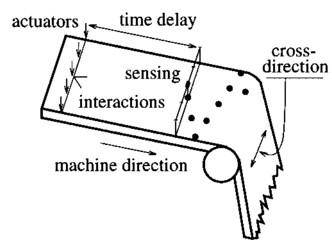

Figure 1. Generic web forming process (not drawn to scale).

2. Experimental Design—A Brief Review

The optimal design of experiments was extensively studied in the 1970s−80s (Box and Draper, 1975; Draper and Hunter, 1966; Federov, 1972; Goodwin and Payne, 1977; Silvey, 1980; Titterington, 1975; Welch, 1984; Zarrop, 1979). Several experimental design objectives have been studied, perhaps the most popular being *D*-optimality, *G*-optimality, and *A*-optimality (Atkinson and Donev, 1992; Silvey, 1980). *D*-optimality is the criterion that best satisfies our purposes and was also used by Koung and MacGregor (Koung and MacGregor, 1993, 1994) for the design of identification experiments for the robust control of 2×2 processes.

A *D*-optimal experimental design minimizes the volume of the confidence ellipsoid of the parameter vector subject to the physical constraints on the manipulated variables. The optimization problem with the *D*-optimality objective subject to constraints is nonconvex and can be shown to be NP-hard (Welch, 1984). This means

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that the computational requirements to achieve the true optimum become prohibitive as the dimension of the problem increases. While several algorithms for the construction of suboptimal designs have been proposed (Draper and Hunter, 1966; Wynn, 1970; Cook and Nachtscheim, 1980; Welch, 1982, 1984; Bates, 1983; Snee, 1985; Bohachevsky et al., 1986; Haines, 1987), these algorithms are computationally expensive and are not guaranteed to converge to the globally optimal experimental design.

Simulated annealing is a well-known algorithm for computing good local optima (Bohachevsky et al., 1986; Haines, 1987; Corana et al., 1987; Goffe et al., 1994). Goffe et al. (1994) compared the simulated annealing algorithm to three common optimization algorithms (a simplex algorithm, a conjugate gradient algorithm with numerical derivatives, and a quasi-Newton algorithm with numerical derivatives) on four econometric parameter identification problems. They found that the simulated annealing algorithm was able to find the global optimum in several cases, and for difficult functions, it performed better than the other algorithms. They also found it to be a very robust algorithm and not likely to fail or have numerical difficulties. The largest problem they studied had 62 parameters. Bohachevsky et al. (1986) reported that their generalized simulated annealing method produced a better experimental input design than the one found by Bates (1983). Haines (1987) also reported favorable results when applying the simulated annealing algorithm to the construction of exact optimal designs. Although the simulated annealing algorithm does not guarantee a solution that is globally optimal, it allows the search to move away from local optima and continue over a wider area. The computational expense is less than an exhaustive search and can incorporate a large number of parameters (Bohachevsky et al., 1986; Corana et al., 1987; Goffe et al., 1994). On the basis of these advantages, we propose to use a modified version of the simulated annealing algorithm to compute suboptimal experimental designs for sheet and film processes. Before the experimental design procedure is discussed, we will summarize the model description and define nomenclature commonly used in parameter estimation and optimal design.

3. Process Gain Estimation

The interaction matrix for a sheet and film process is the mapping from the manipulated variables to the sheet/film profile (see Figure 1). The manipulated variables are typically slice or die lip positions, while the sheet/film profile measurements are typically in terms of basis weight, thickness, or moisture content. Detailed process descriptions with typical interaction matrices are provided elsewhere (Braatz et al., 1996; Featherstone and Braatz, 1997b).

Sheet and film process models can be written in the form (Featherstone and Braatz, 1997b):

$$\mathbf{P}(s) = \mathbf{U}\Lambda(s)\,\mathbf{V}^{\mathrm{T}} \tag{1}$$

where the matrices $\mathbf{U}$ and $\mathbf{V}$ are unitary. The elements of the diagonal matrix $\Lambda(s)$ are transfer functions, and their values at steady state ($s = 0$) are referred to as the *gains* of the sheet/film process (Featherstone and Braatz, 1997b). Featherstone and Braatz (Featherstone and Braatz, 1997b) showed that the accuracy of the gains directly specifies the closed-loop performance achievable by a model-based controller. More specifically, the sign of a process gain must be accurately known for the controller to reliably suppress disturbances in the direction of the column of $\mathbf{V}$ associated with the process gain.

Here we will focus only on the steady-state model because the scalar dynamics for sheet and film processes are trivial to identify in practice. The measured process output at steady state for the ith experiment is assumed to be described by

$$\mathbf{y}_i = \mathbf{P}\mathbf{u}_i + \epsilon_i \tag{2}$$

where $\mathbf{P}$ is the $n \times n$ steady-state process interaction matrix, and the measurement noise ϵ_i has a normal distribution, an expected value of zero ($E(\epsilon_i) = 0$), and a positive-definite covariance matrix $\mathrm{cov}(\epsilon_i) = \mathbf{S}$. The noise covariance matrix takes into account potential spatial correlation of noise processes across the machine (Rawlings and Chien, 1996).

Substituting (1) into (2), rearranging, stacking vectors, and taking the expected value gives

$$E(\tilde{\mathbf{y}}) = \mathbf{X}\lambda \tag{3}$$

where $\tilde{\mathbf{y}} = [\mathbf{y}_1, ..., \mathbf{y}_n]^{\mathrm{T}}$, $\lambda^{\mathrm{T}} = [\lambda_1, ..., \lambda_n]^{\mathrm{T}}$, and the *input matrix* $\mathbf{X}$ is a function of $\mathbf{u}_i$. The least-squares estimate of λ is $\hat{\lambda} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\tilde{\mathbf{y}}$ with $\mathrm{cov}(\tilde{\mathbf{y}}) = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{S}\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}$ (Ljung, 1987).

Our focus will be on sequential estimation, since the other cases are similar. The volume of the confidence ellipsoid for the parameter vector λ based on the first N experiments is quantified by the *information matrix* (Beck and Arnold, 1977; Silvey, 1980)

$$M(\{\mathbf{u}_i:\ i = 1, ..., N\}) \equiv \mathbf{X}^{\mathrm{T}}\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{S}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{X} \tag{4}$$

which is the inverse of the covariance matrix for the gain estimates.

4. Problem Formulation for Constrained Input Design

For identification and control purposes, the most critical parameters for sheet and film processes are the process gains (Featherstone and Braatz, 1997b). The D-optimality criterion minimizes the volume of the confidence ellipsoid for the process gain estimates (Atkinson and Donev, 1992):

$$\max_{\mathbf{u}_N} \det M(\{\mathbf{u}_i:\ i = 1, ..., N\}) \tag{5}$$

where the optimization is only over experimental designs that are physically realizable. Also, the objective function is modified to exclude process gain estimates whose signs are known with confidence after previous experimental data are available. The following is a brief description of the constraints, the objective function modification, and the method used to solve the optimization problem.

Constraints. To prevent excessive process upsets during experimental data collection, constraints are imposed on the process inputs and outputs. For sheet and film processes the constraints on the manipulated variables at each time instance are usually of the forms

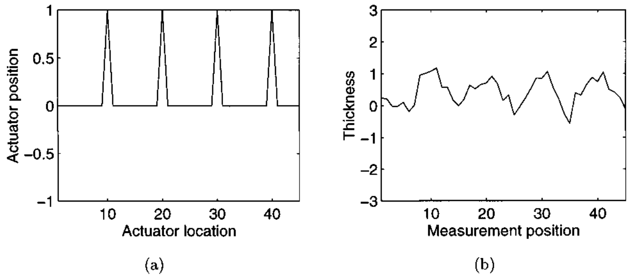

Figure 2. Blown film example: (a) the standard step experiment input manipulations; (b) a representative open loop output response.

(Braatz et al., 1996; Braatz and VanAntwerp, 1997; Chen and Wilhelm, 1986)

$$-a \le u_j \le a, \quad \forall j \text{ (min−max constraint)} \quad (6a)$$

$$-b \le u_j - u_{j-1} \le b, \quad \forall j \text{ (1st-order constraint)} \quad (6b)$$

$$-d \le u_{j+1} - 2u_j + u_{j-1} \le d, \quad \forall j \text{ (2nd-order bending moment constraint)} \quad (6c)$$

After the first experiment, output constraints can be included by applying (2) with the estimated $\mathbf{P}$ to rewrite the output constraints as input constraints. The optimization problem for *D*-optimal sheet and film identification design is posed as (5) subject to the constraints (6).

Modification of the Objective Function. For the first experiment, no modification of the objective function is necessary. However, in subsequent experiments, the sign of some process gains may be known with sufficient confidence. For control purposes, further reduction of the confidence interval associated with these gains will not significantly improve the achievable closed-loop control performance (Featherstone and Braatz, 1997b). Therefore, these gains are excluded in the objective function. This formulation still allows input manipulations in any direction, as allowing inputs in directions associated with known gains can allow input designs to more easily satisfy the constraints.

At a given level of confidence, the confidence interval around each estimated gain is tested for inclusion of zero. If the confidence interval does not include zero, then the sign of the gain is known within the selected confidence level. After the first experiment, a 99.99% confidence interval was used in the accuracy tests. This conservative level of confidence was used to prevent any poorly identified gain from being mistakenly excluded from the objective function after only one experiment. For gain estimates based on more than one optimally designed experiment, the level of confidence was reduced to 99.9%.

Constrained Input Design via Simulated Annealing. A simulated annealing algorithm (Corana et al., 1987; Goffe et al., 1994) was used to solve the optimization problem. Basically, the simulated annealing algorithm searches for the global optimum of an n-dimensional function by allowing both up- and downhill moves and focusing on the most promising area as the optimization proceeds. As the constraints (6) are not the box constraints which are used in most simulated annealing algorithms (Bohachevsky et al., 1986; Corana et al., 1987; Goffe et al., 1994), modifications were necessary to handle the first- and second-order spatial constraints (6). A detailed description of the algorithm, with details regarding the parameters used and computation times, is provided in the first author's thesis (Featherstone, 1997).

5. Example: Blown Film Process

The following example is based on a simulated blown film process and illustrates the experimental design procedure for a realistic large-scale sheet and film process. Identification experiments were performed to develop two models: one based on using the standard industrial step experiments and the other based on the proposed experimental design procedure. Control simulations were performed on the original process to compare the achievable closed-loop performance by the two models.

Consider the true process transfer function matrix $\mathbf{C}(s)$ to be

$$\mathbf{C}(s) = \frac{e^{-s}}{s+1}\cdot \underbrace{\begin{bmatrix} c_1 & c_2 & \cdots & c_{m-1} & c_m & \cdots & c_m & c_{m-1} & \cdots & c_2 \\ c_2 & c_1 & c_2 & \cdots & c_{m-1} & c_m & \cdots & \ddots & \ddots & \vdots \\ \vdots & c_2 & c_1 & c_2 & \cdots & c_{m-1} & \ddots & \ddots & \ddots & c_{m-1} \\ c_{m-1} & \vdots & c_2 & c_1 & c_2 & \cdots & \ddots & \ddots & \vdots & c_m \\ c_m & c_{m-1} & \vdots & c_2 & \ddots & \ddots & \vdots & c_{m-1} & c_m & \vdots \\ \vdots & c_m & c_{m-1} & \vdots & \ddots & \ddots & c_2 & \vdots & c_{m-1} & c_m \\ c_m & \vdots & \ddots & \ddots & \cdots & c_2 & c_1 & c_2 & \vdots & c_{m-1} \\ c_{m-1} & \ddots & \ddots & \ddots & c_{m-1} & \cdots & c_2 & c_1 & c_2 & \vdots \\ \vdots & \ddots & \ddots & \cdots & c_m & c_{m-1} & \cdots & c_2 & c_1 & c_2 \\ c_2 & \cdots & c_{m-1} & c_m & \cdots & c_m & c_{m-1} & \cdots & c_2 & c_1 \end{bmatrix}}_{n\times n} \quad (7)$$

where m is the spatial extent of interactions, n is the number of actuator and sensor lanes across the machine, s is the Laplace transform variable, and the interaction parameters are

$$c_1 = 1.0; \quad c_2 = 0.9; \quad c_3 = 0.6; \quad c_4 = 0.2; \quad c_5 = 0.1; \quad c_6 = -0.1; \quad c_7 = 0.05; \quad c_8 = c_m = 0.0 \quad (8)$$

In practice, the process parameters c_i are really nonlinear functions of the polymer being processed, the die gap opening, the temperature, etc. These nonlinear interactions are quite complex, and current modeling efforts are focused on the axial (bubble) shape, assuming constant properties at surface and a rigid die gap opening (Sidiropoulos et al., 1996; Perdikoulias and Tzoganakis, 1996; Kurtz, 1995; Wong, 1995; Liu et al., 1995; Pearson and Richardson, 1983). Koop (1993) has studied the deformation of an elastic ring under pointwise radial load but does not consider the actual blown film process. Therefore, a linear model was assumed which is only representative of a possible interaction matrix. The condition number of the interaction matrix is singular, which poses difficulties for most identification and control procedures.

Identification. For this example, the measurement noise in each sensing location was considered to be

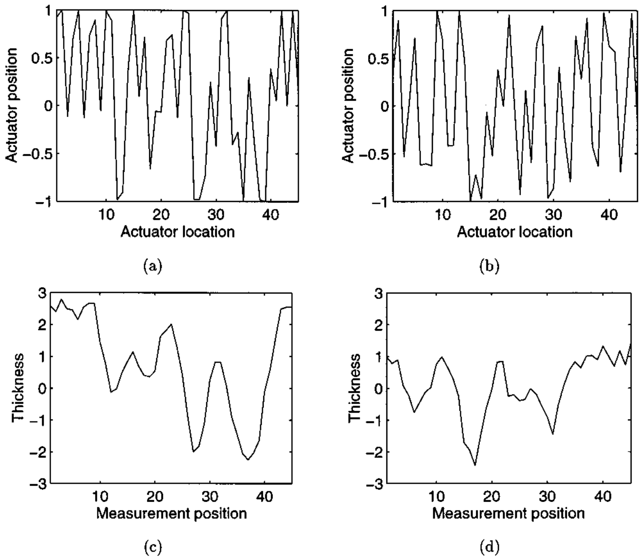

Figure 3. Blown film example: the input manipulations (a, b) and open loop output responses (c, d) of the first and fifth optimally designed experiment, respectively.

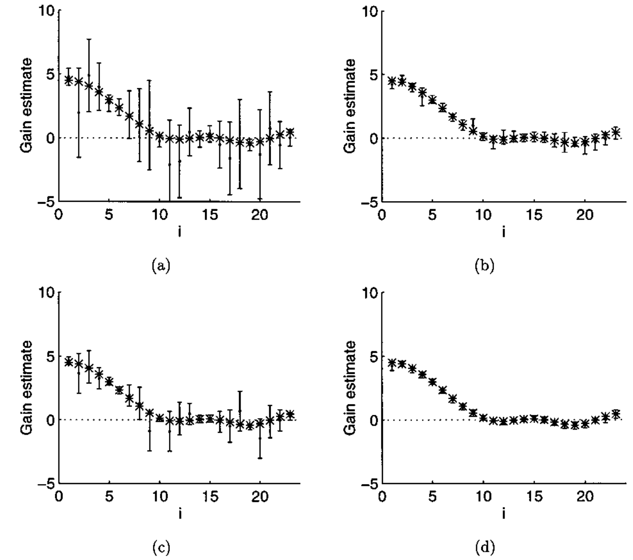

Figure 4. Plant gains λ_i (shown using *) and the 95% confidence intervals associated each estimated model gain $\hat{\lambda}_i$ (shown using ·) based on (a) one standard step experiment, (b) one optimally designed experiment, (c) five standard step experiments, and (d) five optimally designed experiments.

independent and have a variance of 0.04. This is a realistic noise description for many plastic film extrusion processes. Using the industrial standard input design (Heaven et al., 1993), the step input was performed in a number of actuator locations which are separated so that the resultant bump response profiles do not overlap. For the blown film process example, the step input was specified as

$$\mathbf{u}_s = \mathbf{e}_{10} + \mathbf{e}_{20} + \mathbf{e}_{30} + \mathbf{e}_{40} \tag{9}$$

where

$$\mathbf{e}_k^{\mathrm{T}} = [0 \quad ... \quad 0 \quad 1 \quad 0 \quad ... \quad 0]^{\mathrm{T}} \tag{10}$$

with the 1 in the kth position. The standard step input satisfies the constraints (6) with $a = 1$ and $b = d = 2$. A representative output in response to the standard step experiment is shown in Figure 2.

The optimally designed experiments were computed while satisfying the same constraints applied to the standard step experiment. The input manipulations and output responses for the first and fifth optimally designed experiments are shown in Figure 3. The results of the identification experiments are contained in Figure 4, which shows the 95% confidence interval for each estimated gain along with the true value when the number of experiments is either one or five (only the unique 23 process gains are shown—the other 22 gains are repeated (Featherstone, 1997)).

After one experiment using the step input (9), it is apparent from Figure 4 that many of the gains are incorrectly identified and that most gains have large confidence intervals. Comparing parts a and b of Figure 4, the first optimally designed experiment has significantly tighter confidence intervals for all the parameters. In fact, on average the parameter estimates $\hat{\lambda}_i$ are 1290% more accurate for the optimally designed experiment (Featherstone and Braatz, 1997a).

Seventeen gains are identified with confidence for the five optimally designed experiments, whereas only ten gains are confidently identified for the five standard step experiments (Figure 4). Not all the gains have a smaller variance than after the step experiments, due to the exclusion of the already confidently known gains in the objective function during the optimization. The step experiments identify $\hat{\lambda}_1$, $\hat{\lambda}_{19}$, and $\hat{\lambda}_{23}$ more accurately than the optimally designed experiments. This has no consequence in the controller design, because the gains are identified with significant confidence in both models. The optimally designed experiments are concerned with obtaining better estimates for the gains whose signs are not accurately identified. On average the estimated gains are 1120% more accurate for the optimally design experiments (Featherstone and Braatz, 1997a).

Time Domain Simulations. The two models were used to design the controllers in the simulation studies; one based on the five step experiments (model 1) and the other on the five optimally designed experiments (model 2). The controllers were designed using the SVD controller design method of Braatz and co-workers (Featherstone and Braatz, 1997b; Hovd et al., 1996; Braatz and VanAntwerp, 1996), which provides a controller designed to be robust to the inaccuracies quantified by the identification algorithm as well as model structure errors (the control weights and other details in the design are available in the first author's thesis (Featherstone, 1997)). The controller provides the best performance achievable for the model with the quantified model inaccuracies. The simulations demonstrate how much improvement in closed-loop performance is obtained by the more accurate model obtained from the experimental design procedure (see Figure 5).

The model based on the five optimally designed experiments has a larger number of gains known with confidence, allowing the robust controller to perform input moves in more directions than with the model based on the standard step experiments (33 directions for the optimally designed model compared to 19 for the step model). This results in a smoother final profile response. The standard deviation of the profile as a result of the controller based on the better model is 37% smaller. It should be reiterated that the better model was not obtained by more experiments or by weakening the constraints. The better model was obtained by

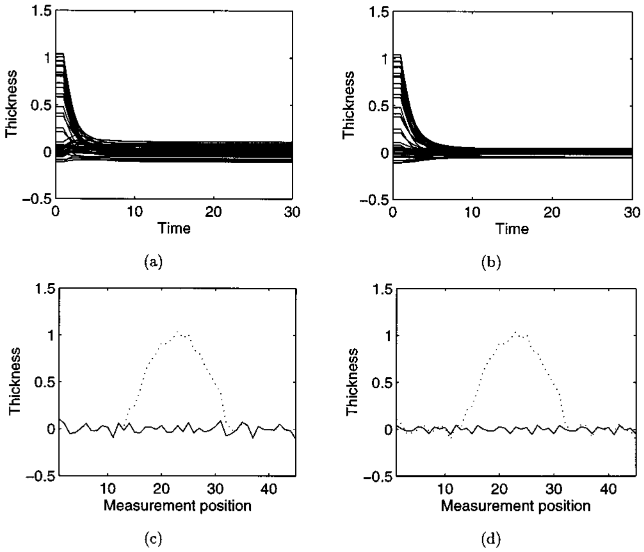

Figure 5. Time domain profile response (a, b) and steady-state controlled variable profile (c, d) based on the model from five standard step experiments and five optimally designed experiments, respectively [final profile (—); initial disturbance (···)].

using the optimal experimental design rather than the standard industrial bump tests.

6. Conclusions

Manipulated variables were computed that optimize the information in data collected from sheet and film processes. For a simulated blown film process, the model was an order of magnitude more accurate than that obtained using the industrial standard bump test experiments. The improved accuracy resulted in a 37% reduction in closed loop thickness variations. This indicates that substantial benefits can be achieved by incorporating the optimal experimental design algorithm into industrial sheet and film process control algorithms.

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