A ROLE FOR RESPONSE SURFACE BASED OPTIMIZATION IN SYSTEM DYNAMICS STUDIES

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Abstract

Traditional system dynamics studies rely heavily upon heuristics and experience. Notwithstanding, mathematical optimization techniques have been introduced as important elements for a successful study. Different views abound regarding the relevance of qualitative heuristics compared to mathematically rigorous optimization tools. We argue that the role of optimization in system dynamics studies is not to replace experience-based knowledge, but instead to augment, facilitate and expand the heuristic exploration of a model. Accordingly, our approach involves narrowing the design space (using response surfaces) and the subsequent direct investigation of the simulation model (using heuristics).

Response surfaces received considerable attention in optimization due to their capability to replace complex models with analytic equations, thereby increasing computational efficiency. However, doubts exist as to whether a response surface approximation of an approximation of reality is useful. We demonstrate the usefulness of response surfaces in system dynamics studies with a case study involving a high-level model of an industrial ecosystem; our intent in using response surfaces is not to replace the simulation models with analytic equations, but instead to direct attention to regions within the design space with the most desirable performance. Recommended changes to a system are based directly on the simulation model, not on response surfaces, averting the added level of approximation inherent in response surfaces. Additionally, final results are composed of ranges of values for parameters, not single, point values (allowing for added flexibility in policy setting).

1 Motivation

System dynamics as a philosophy and feedback control modeling as an implementation of this philosophy are powerful in helping humans understand complex systems. The approaches and methods associated with system dynamics have traditionally been heavily reliant upon the heuristic exploration of possible changes to a system. Nevertheless, optimization techniques have been introduced and used in system dynamics studies dating back to the early 1980's. While some practitioners may have seen a future in which heuristics are completely abandoned in system dynamics studies, most of those exploring the role of optimization emphasized that mathematically rigorous optimization techniques should be *coupled* with heuristics to form a powerful approach for model improvement. Along these lines, our approach is a combination of mathematical tools and heuristics.

In particular, the mathematical tools we use are design of experiments, response surfaces, and a multiobjective decision model. In using response surfaces, a simulation model is approximated as an analytic equation in which the relevant responses are functions of significant control variables. Response surface techniques do not acknowledge that system dynamics models typically are constructed with a high degree of approximation from reality -- moreso than a model that is analytic or based on extensive historical data. While system dynamics models can be constructed of systems that are analytic or based on extensive historical data, a strength of system dynamics lies in the ability to approximate the behavior and structure of poorly understood systems. The usefulness of a response surface approximation of an already highly approximated system dynamics model is questionable. Hence, our approach applies response surfaces to guide the search for an improved system, yet the final recommendations are based directly on the simulation model.

Additionally, our approach to "optimization" does not involve finding one "optimal" solution, but instead finding a range of *satisficing* solutions. A satisficing solution is one that is "good enough," not necessarily optimal (Simon, 1996). A major reason for searching for satisficing solutions is that the optimal conditions in a model are most likely not optimal conditions in the real world, especially when modeling poorly understood systems. Therefore, in finding a range of solutions, more play between the model and reality can be accounted for and still achieve the desired responses. We begin by introducing previous work on the use of optimization in system dynamics studies.

2 Optimization and System Dynamics Modeling

The inclusion of mathematical tools in the process of improving the behavior of system dynamics models has been examined by several different people from varying perspectives. Multiple authors, including Keloharju and Coyle, have worked in the area of optimizing the parameters of a model. Keloharju emphasizes the increased efficiency with which a parameter space can be explored using optimization techniques when compared to purely heuristic techniques (Keloharju and Wolstenholme, 1989). He does, however, maintain that human skill remains important in the formulation of the model. Interestingly, he finds that several control variable combinations lead to very similar responses, an idea that supports the search for ranges of solutions introduced in this paper. Coyle's work is noteworthy in that he includes structural changes to the model through carefully formulating structural changes with parameters (Coyle, 1985). He, too, emphasizes the role of optimization as a *complementary* tool to the traditional heuristic approaches of system dynamic studies.

Kleijnen includes design of experiments and response surface methodology in his approach to optimizing the parameters of a model (Kleijnen, 1995). Kleijnen introduces these tools as being "objective, efficient, and effective" and applies them in a moderately standard manner. Kleijnen does not discuss the high levels of approximation of reality incurred when a simulation model is approximated by a response surface. For those not familiar with regression and design of experiments, Rotmans and Vrieze provide a "textbook" review of these techniques, applying them to a simulation model (Rotmans and Vrieze, 1990). Rotmans and Vrieze prefer the use of a central composite design (CCD), which is also used in this paper, when applying design of experiments techniques to their simulation model. As an additional source, the use of orthogonal arrays versus latin hypercubes in the sensitivity analysis of system dynamics models is discussed by Clemson, et. al (Clemson, et al., 1995). They point to response surfaces as being more appropriate when "all parameter interactions need to be studied," which is the case in optimization .

One final class of approaches to enhancing the analysis and improvement of a system dynamics model is that of modal control, in which the eigenvalues of the motion equations are used to synthesize new policy options (Macedo, 1989). The main strength of using modal control theory is that new policy structures can be generated mathematically, as opposed to the heuristic methods of Coyle, Kleijnen, and Keloharju. Drawbacks of modal control theory include the necessary linearization of the model, the amount of computation, and the design of realistic policies from the synthetically generated policies (Mohapatra and Sharma, 1985). Macedo has introduced a mixed approach in which modal control and traditional optimization are sequentially applied in the improvement of a model (Macedo, 1989). While not focused on in this work, Macedo's method appears to be promising.

The approach taken in this paper is similar to that of Keloharju in that the optimization of parameters is the primary focus. However, the implementation of design of experiments and response surface techniques draws upon the work of Kleijnen. A hidden assumption of Kleijnen, that a response surface approximation of a simulation model (which is an approximation of reality) can be used to determine realistic options for parameter settings, is addressed and handled in the work presented in this paper. Additionally, our focus is not on determining one "optimal" solution set of parameter settings, but instead to determine a range of solutions in which system behavior is acceptable. It is in these two points of contrast to earlier research that the contributions of this work are founded.

3 Frame of Reference: Robust Concept Exploration

In recent years, design of experiments and response surfaces have gained in popularity as tools for aiding the exploration of concepts (Box and Draper, 1987; Khuri and Cornell, 1987; Myers and Montgomery, 1995). The basic notion is to relate responses to controllable variables through analytic equations that are constructed through statistical methods. These analytic equations allow for quicker exploration of multiple concepts than do the simulation codes from which they are built.

The Robust Concept Exploration Method (RCEM) is a formalization of the steps followed in using response surfaces in the design of a system. The RCEM is composed of four steps, starting with the identification of design parameters (STEP 1). Next, screening experiments are conducted using design of experiments techniques to reduce the problem size (STEP 2). Following the screening experiments, response surfaces are created to map significant design parameters to response behaviors (STEP 3). Finally, a multiobjective decision support tool (the compromise DSP) is formulated using the response surfaces and solved to facilitate concept exploration and the identification of top-level design specifications (STEP 4).

The causal loop diagram in Figure 1 shows the flow of information during the RCEM process. Important to note is that final solutions are based directly on the response surface approximations of the original simulation code.

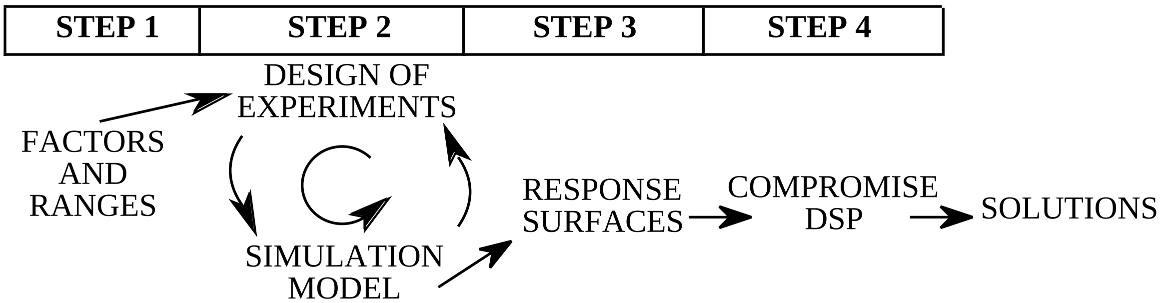

Figure 1 Robust Concept Exploration Method

When the simulation code is based on concrete relationships (such as those from physics or thermodynamics) or from extensive historical data, using response surface approximations to generate final solutions has been shown to be effective (Koch, et al., 1996; Myers, et al., 1989; Simpson, et al., 1997). From a system dynamics perspective, however, models commonly are constructed with a higher level of approximation from reality -- not based on concrete relationships, but instead on human interactions, aggregated trends, and less precise information. The usefulness of a response surface approximation of a highly approximated simulation model has not been directly addressed. Our approach to using response surfaces with system dynamics emerges from this dilemma.

4 Our Approach

A response surface *approximation* of a simulation model that is already an *approximation* of reality leads to ***two layers of approximation*** between the solutions and the real world. If possible, there is a need to eliminate one level of approximation. One way to remove a level of approximation is by adding a feedback loop to the baseline RCEM. With this approach, shown in Figure 2, response surfaces and a compromise DSP are used as *attention-directing* tools, forming an information feedback loop (Bailey, 1997).

Instead of taking the solutions directly from a compromise DSP, the results from a compromise DSP (which are based on response surface approximations of the simulation model) are fed back to the simulation model. The regions near the compromise DSP solutions are explored with the simulation model in search of a region of acceptable solutions. The response surfaces are still extremely useful in identifying a promising region of the design space, but not in identifying final solutions. The process of creating the response surfaces is termed the *comprehension loop* because the relationships between responses and control variables are identified and *learned* in this loop.

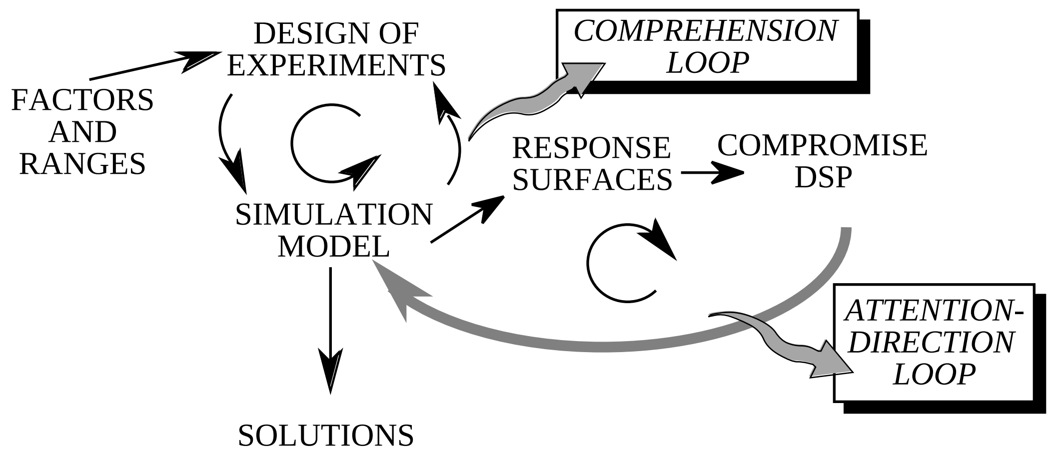

Figure 2 Augmented RCEM

The added step in the augmented RCEM (shown in Figure 2) involves returning to the simulation program and using the solutions from the compromise DSP formulations as guides to explore the design space. Ranges of control variables for further exploration are determined with two heuristic principles (Bailey, 1997):

1. If a compromise DSP solution for a control variable is not on a bound, then two points, one to either side of the compromise DSP solution, are selected for further exploration.
2. If a compromise DSP solution for a control variable is on a bound, then two points within the bound are explored. Instead of exploring one point on each side of the compromise DSP solution, two points are explored on the side of the compromise DSP solution within the bound.

The points used for further analysis (called *exploration points*), therefore, surround the compromise DSP solution in orthogonal directions. Values for the deviation variables are found at the exploration points with the original simulation program (*not* the response surface models) and are then compared to the compromise DSP, or *baseline*, solution. Consider the example shown in Figure 3, in which, for simplicity, a two-dimensional design space is explored (in the case study, the design space is ten-dimensional).

The compromise DSP solution is found and inputted into **Step 1**. Points orthogonal to the compromise DSP solution are found for each of the two variables in **Step 2**. In **Step 3**, the deviation from the desired responses (referred to as *deviation variables*) at each one of the solution exploration points is determined with the simulation model (shown in Figure 3 as vertical columns). Finally, in **Step 4,** these deviation variables are compared to the deviation variables for the compromise DSP solution. If the deviation variables are within a certain percentage of the compromise DSP solution, then that point is included in the solution range. A designer must determine the allowable amount of fluctuation for each deviation variable (in the case study presented here, a ten percent fluctuation is allowed). If the responses are for very precise system (i.e., a laser used in surgery), a smaller percent fluctuation is appropriate.

There are two main points of interest worth discussing concerning the solution exploration strategy:

1. the exploration points are determined heuristically; and,
2. the solution ranges are based on main effects (Bailey, 1997).

The heuristic determination of the exploration points leads to more flexibility in the solution exploration scheme. After formulating a decision support problem, developing a simulation model, building response surfaces, and analyzing results from compromise DSPs, a designer has considerable knowledge concerning the sensitivity of the control variables. Setting concrete rules for exploration point determination limits the process more than enhances it.

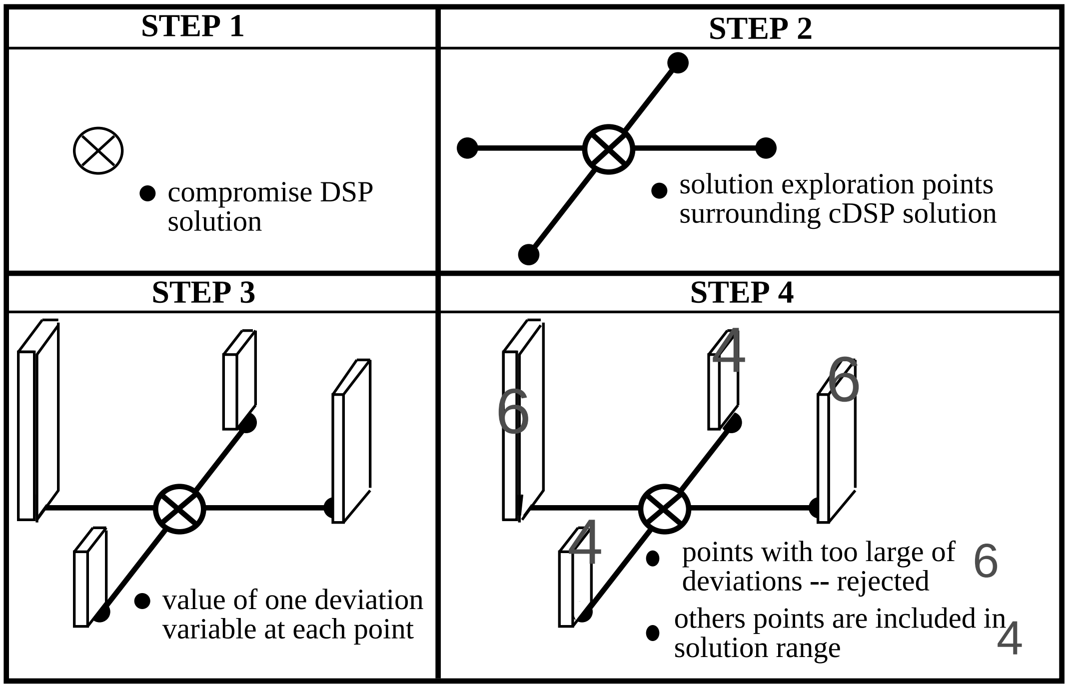

Figure 3 Solution Exploration Process

The sole use of main effects in developing ranged sets of solutions is based on the premise that the interactions and second-order effects do not have as much influence over the behavior of the system when small perturbations are made in the control variable values. Large changes in control variable values are not made because interaction effects can begin to more strongly influence the system behavior.

A benefit of exploring the regions surrounding each control variable is the development of a ranged set of solutions, as opposed to a singular, point solution. With the augmentation made to the RCEM, design freedom is maintained while design knowledge is increased with the solution exploration process. The use of response surfaces and the compromise DSP as *attention directing* tools (instead of solution determining tools) is a significant step taken to maintain design freedom while gaining information about the system. Instead of using these tools to narrow the design space to one final solution, response surfaces and the compromise DSP are used to expand the information about the design space, which is narrowed to a final range of solutions after an additional step.

The simulation slot in the augmented RCEM (see Figure 3) is where domain-dependent information enters the concept exploration process. The simulation model presented in this paper is of a system of industries in Kalundborg, Denmark.

5 Case Study: A System of Industries in Kalundborg, Denmark

Over the past thirty years in Kalundborg, Denmark, a system of industries has developed in which by-products and wastes from one company are used by other companies in the system. For instance, industrial gypsum collects in the scrubbers at Asnæs, a coal and gas burning power plant. This industrial gypsum is sold to Gyproc, where it is used instead of mined gypsum to make wallboard. A series of such interactions exists in Kalundborg and is described in more detail in (Bailey, et al., 1997; Ehrenfeld and Gertler, 1997; Frenay, 1995).

A simulation model of a section of Kalundborg (including the industries with the most interactions with other industries) was built, validated, and used to generate data in STELLA (Chichakly, et al., 1994). While the model and its validation is described in great detail in (Bailey, 1997), only a brief description is presented here. In Figure 4, a simplified version of the flow diagram of the simulation model is shown.

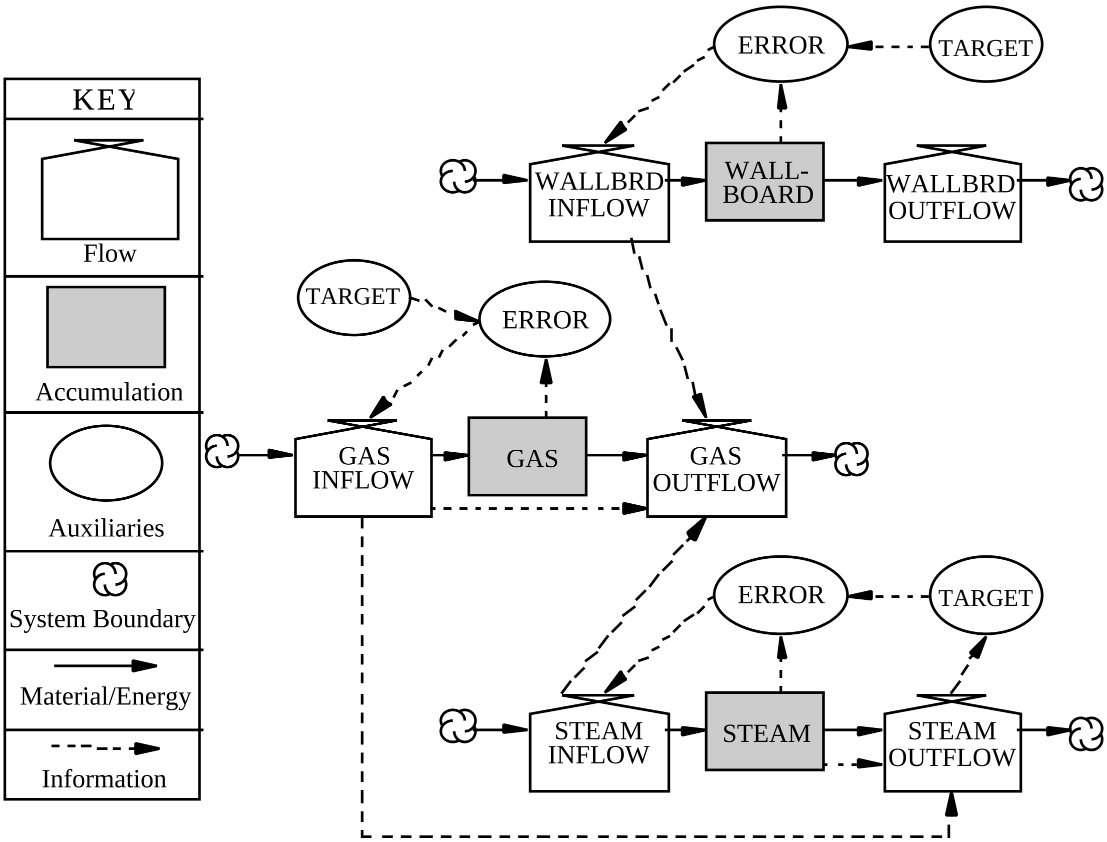

Figure 4 Simplified Flow Diagram of Kalundborg Model

There are three primary accumulations (steam, gas, and wallboard) that are each individually part of balancing loops. The targets for gas and wallboard are exogenous variables, while the target for the steam accumulation is set by current usage of steam (steam cannot be inventoried indefinitely -- it is perishable -- so current accumulation levels must be based on steam usage). The interactions between the three companies connect the three balancing loops. For instance, since steam is used in the purification of gas, an information arrow connects the gas inflow to the steam outflow.

The purpose of the concept exploration process is to design a system that is robust to a disturbance in the system. The primary responses used to evaluate system behavior are based on the three accumulations while the controllable variables deal with how the accumulations respond to a disturbance. For the purposes of this paper, only one disturbance, that of a step change in steam demand, is presented. The responses are selected to characterize the rate of recovery, mean value, and standard deviations of the accumulations as they attempt to reach the target value. Additionally, the total amount of waste generated in the system is calculated and used as a response. There are a total of eight responses used to characterize the robustness of the system and the waste generated.

The three types of control factors occur several times within the model, resulting in a total of ten control variables. These delay times, averaging times, and correction times each have physical significance in the actual system:

delay times -- time between when a discrepancy between the goal and actual levels of an accumulation occurs and when it is first acted upon;

averaging times -- times over which flows are averaged; averages of production flows are used in determining present production rates; and,

correction times -- time over which a discrepancy between the goal and actual levels of an accumulation is intended to be corrected.

All of the decisions in the simulation model relate to changing the production rate of steam, gas, or wallboard to maintain the desired accumulation levels. Additionally, the decisions are parametric in nature; they do not involve structural changes in the model. The ten control variables are related mathematically to the eight responses through response surfaces. The basis structure of the response surface formulation is presented in the next section.

5.1 Design of Experiments and Response Surface Formulation

To develop quadratic response surfaces, experiments must be conducted with the simulation model to determine the effects of each control variable and the interactions between control variables. Among the various types of experimental designs for fitting response surface models, the central composite design (CCD) is probably the most widely used for fitting quadratic response surfaces and studying second order effects (Montgomery, 1991). For each problem, a slightly different strategy will need to be used to fit response surfaces. The strategy we used is outlined here and is described in more detail in (Bailey, 1997).

First, a face-centered CCD is used to relate the ten control variables to the eight responses and screen off insignificant factors. In doing so, we found that only four of the eight response are affected by the step change in steam demand disturbance. Additionally, the number of significant control variables is reduced from ten to seven. With the problem reduced in size, a second experiment, using an inscribed CCD, is performed. The response surfaces obtained from this second round of experiments are used in the compromise DSP to search for promising regions in the design space (as defined by the control variable values). The response surfaces are judged by the R^2 value (coefficient of determination), which represents the proportion of the total variation in the response that can be accounted for by the quadratic relationship with the control variables (Simpson, et al., 1997; Walpole and Myers, 1989). An R^2 of zero means that none of the variation in response can be accounted for by the response surface while an R^2 of one means that all of the variation is accounted for by the response surface. All response surfaces used have R^2 of 0.91 or higher.

5.2 Compromise DSP Solution

The compromise DSP is the mathematical construct through which the various metrics and tools of the RCEM are integrated. It is a multiobjective decision model which is a hybrid formulation based on Mathematical Programming and Goal Programming used to find a set of system variables which satisfy system constraints while achieving a set of conflicting goals as well as possible (Mistree, et al., 1993). The systems descriptors, namely, system and deviation variables, system constraints, system goals, bounds, and the deviation function are described in detail in (Mistree, et al., 1993). The mathematical formulation for a compromise DSP is as follows:

Given *An alternative to be improved. Assumptions used to model the domain of interest.*

The system parameters:

n	number of system variables, q inequality constraints
$p + q$	number of system constraints,
m	number of system goals
$g_i(X)$	system constraint function
$f_k(d_i)$	function of deviation variables minimized at priority level k for the preemptive case.

Find: *control variables and deviation variables*

$X_i \quad i = 1, \ldots, n; \qquad d_i^-, d_i^+ \quad i = 1, \ldots, m$

Satisfy

System constraints (linear, nonlinear)

$g_i(\mathbf{X}) = 0 \; ; i = 1, .., p$

$g_i(\mathbf{X}) \geq 0 \; ; i = p+1, .., p+q$

System goals (linear, nonlinear)

$A_i(\mathbf{X}) + d_i^- - d_i^+ = G_i \; ; i = 1, \ldots, m$

Bounds

$X_i^{min} \leq X_i \leq X_i^{max} ; i = 1, \ldots, n$

$d_i^-, d_i^+ \geq 0 \; ; i = 1, \ldots, m$

$d_i^- \cdot d_i^+ = 0 \; ; i = 1, \ldots, m$

Minimize: *deviation function*

$\mathbf{Z} = [\, f_1(d_i^-, d_i^+), ..., f_k(d_i^-, d_i^+) \,]$

The responses surfaces are used in formulating the goals in the compromise formulation. The particularization of the compromise DSP for the step change in steam usage is presented in (Bailey, 1997; Bailey, et al., 1998 (in press)).

5.3 Solution Exploration

Following the procedure outlined in Section 4, solution exploration points are identified that surround the compromise DSP solution. At each of these points, the four deviation variables are calculated using the simulation model of Kalundborg (not the response surfaces). These deviation variable values are then compared to the deviation variable values for the compromise DSP solution. In Table I, the solution exploration points and associated deviation values are shown for three of the ten control variables to illustrate this process.

Table I Solution Exploration Step

RUN	CONTROL VARIABLES (mnths)				DEVIATION VARIABLES			
	STMCT	**STMDEL**	**…**	**ATUSE**	**d_1**	**d_2**	**d_3**	**d_4**
cDSP	3.25	0.5	…	12	0.250	1.85e-3	0.0326	0.945
1	3	0.5	…	12	0.219	1.85e-3	0.0337	0.948
	percent difference from cDSP solution				-12.4	0	+3.37	+0.317
2	3.5	0.5	…	12	0.283	1.85e-3	0.0317	0.942
	percent difference from cDSP solution				***+13.2***	0	-2.76	-0.317
3	3.25	0.75	…	12	0.263	1.85e-3	0.0341	0.944
	percent difference from cDSP solution				+5.2	0	+4.6	-0.106
4	3.25	1.0	…	12	0.276	1.85e-3	0.0356	0.944
	percent difference from cDSP solution				***+10.4***	0	+9.20	-0.106
5	3.25	0.5	…	10	0.272	1.90e-3	0.0351	0.952
	percent difference from cDSP solution				+8.8	+2.70	+7.67	+0.741
6	3.25	0.5	…	11	0.261	1.87e-3	0.0338	0.948
	percent difference from cDSP solution				+4.4	+1.08	+3.68	+0.317
* control variables not shown are set to cDSP solution variables for the runs shown **STMCT**: steam correction time; **STMDEL**: steam delay; **ATUSE**: steam usage averaging time								

A solution exploration point is accepted into the final range of specifications only if none of the four deviation variable values increase to more than ten percent of the deviation variable values from the compromise DSP. In Table II, all but two deviation variables for the solution exploration points are in an acceptable range. The two unacceptable points (the steam correction time, STMCT, at 3.5 months, and the steam delay, STMDEL at 1.0 months) are those associated with runs two and four. All exploration points that have deviation variable values within ten percent of the compromise DSP values (runs 1, 3, 5, and 6) are included in the final solution ranges.

The range of solutions obtained for the case study, developed using the solution exploration process, are shown in Table II. The solutions uniformly encourage the use of short delay times and long averaging times, while correction times display no general trend. Shorter delays times are representative of situations in which decisions are made with more current information. Interesting to note is that the solution exploration process has provided a range of solutions that are satisficing (the delay times do not have to be as short as possible to achieve desirable responses). Long averaging times are characteristic of systems that react to disturbances gradually (not abruptly). Therefore, a long term approach to handling disturbances in the Kalundborg model results in better performance.

The verification of these results is not shown here, however, it may be found in its entirety in (Bailey, 1997) and in an abbreviated form in (Bailey, et al., 1998 (in press)). Through the verification process, the solution ranges are shown to produce the desired robust behaviors in the model.

TABLE II Ranged Set Of Solutions

CONTROL VARIABLE	SOLUTION VALUES (in months)
steam correction time	3.0 - 3.25
steam delay time	0.5 - 0.75
steam generation averaging time	5.0 - 6.0
steam usage averaging time	10.0 - 12.0
gas correction time	0.5
gas delay time	0.5 - 1.0
gas purification averaging time	9.25 - 11.25
wallboard correction time	4.0 - 6.0
wallboard delay time	0.5 - 1.0
wallboard production averaging time	10.0 - 12.0

6 Closure

The opportunity for using design of experiments and response surfaces in the improvement process of a model certainly exists. The transferal of these tools from other disciplines, however, must be done with care -- assumptions concerning their use must be examined. In the case where a model is a large approximation of reality, the use of response surfaces to determine the final solution is questionable since these response surfaces are also approximations. Nevertheless, response surfaces are powerful and have potential for increasing the efficiency and effectiveness of system dynamics studies. Our approach is to use response surfaces to direct attention to a particular location in the design space and then, returning to the simulation model, develop a range of solutions that will lead to the desired behaviors. The particular implementation of this approach, based on the Robust Concept Exploration Method, is outlined in this paper and explored through an example.

One potential drawback to this approach is that the added step -- returning to the simulation model -- will decrease the efficiency of the process. While some efficiency is lost, the total number of simulation runs added is only twice the number of control parameters -- in our example, twenty runs. Including all of the data entry and analysis, the added step required roughly two hours to perform for the Kalundborg example. The reduction in approximation accomplished and the range of solutions developed during the added solution exploration step are determined to outweigh this slight loss in efficiency.

Approaches such as the one presented here, in which heuristics and mathematical tools are combined in a system dynamics study, are developing as important tools in the improvement of model behavior. For an experienced person, the emphasis might lean towards heuristics, while, for a novice, the mathematical tools can help that person gain experience while reducing the number of major mistakes made along the way. Each component, the heuristic and the mathematical, is an important element to a successful study.

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