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Computer Experiment – a case study for Modelling and Simulation of Manufacturing Systems

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Abstract
Deterministic computer simulation of physical experiments is now a common technique in science and engineering. Often, physical experiments are too time consuming, expensive or impossible to conduct. Complex computer models or codes, rather than physical experiments lead to the study of computer experiments, which are used to investigate many scientific phenomena. A computer experiment consists of a number of runs of the computer code with different input choices. The Design and Analysis of Computer Experiments is a rapidly growing technique in statistical experimental design.

This paper aims to discuss some practical issues when designing a computer simulation and/or experiments for manufacturing systems. A case study approach is reviewed and presented.

Keywords*:*
Computer Experiments, Computer Simulation, Computer Code, Experimental Design, Modelling, Manufacturing Systems

1 INTRODUCTION

The motivation of this paper is to discuss impact of computer experiments in the manufacturing industry. In the real world the majority of processes are involved with a chance and uncertainty. In a deterministic world everything is assumed to be certain and as a result use of computer modeling and/or simulations are inevitable.

Deterministic computer modeling and/or simulations of physical experiments are now common techniques in science and engineering. Often, physical experiments are too time consuming, expensive or impossible to conduct. Complex computer models or codes, rather than physical experiments comprise computer experiments, which are used to investigate many scientific phenomena in the manufacturing industry. A computer experiment consists of a number of runs of the computer code with different input choices. The Design and Analysis of Computer Experiments (**DACE**) is a rapidly growing technique in statistical experimental design.

1.1 Computer Models in General

The advancement of high-speed computers has made experimentation via computer modelling common in many areas of science and technology. Computer modelling is having a significant impact on scientific research. Virtually every area of science and technology is affected. A computer model or simulator usually involves complicated or high dimensional mathematical functions. Based on the mathematical formulation, the computer model or code produces outputs, if the required values of the input variables are provided. Running the computer simulation can be expensive in different ways. It can be labour intensive and/or time consuming. If the computer simulator is expensive to run, a natural strategy is to build a predictor from relatively few runs to act as a computationally less expensive surrogate (Welch et al. 1992) which can be used in a variety of ways, for example during optimisation of the output.

In contrast, many complex processes that are conducted as physical experimentation are too time consuming and expensive (Sacks et al. 1989b). Moreover, for many systems such as global weather modelling, circuit simulations, environmental modelling and fire modelling, physical experimentation may simply be impossible. As a result, experimenters have increasingly moved to use mathematical models to simulate these complex systems. Enhancement of computer power has permitted both greater complexity and more extensive use of such models in scientific experimentation as well as in industrial and manufacturing processes. Computer simulation is invariably cheaper than physical experimentation although these codes can be computationally demanding (Welch and Sacks, 1991) and costly.

In general, computer models or codes consist of multivariate inputs, which can be scalars or functions (Sacks et al. 1989b) and the resulting output from the same code may also be univariate and/or multivariate. In addition, the output can be a time dependent function. The input dimension differs according to the purpose and basis of the original computer model. The technique of selecting a number of runs out of various input configurations of the computer model generates a Computer Experiment.

1.2 A Compartment Fire Model

Deterministic fire models attempt to represent mathematically the processes occurring in a compartment fire based on the laws of physics and chemistry. These models are also referred to as room fire models, computer fire models, or mathematical fire models. Ideally, they are such that discrete changes in any physical parameter can be evaluated in terms of the effect on fire hazard. While no such ideal exists in practice, a number of computer models are available that provide a reasonable amount of selected fire effects (Cooper and Forney, 1990).

Computer models have been used for some time in the design and analysis of fire protection hardware. The use of computer models, commonly known as design programs, has become the industry's standard method for designing water supply and automated sprinkler systems. These programs perform a large number of tedious and lengthy calculations and provide the user with accurate, cost optimised designs in a fraction of the time that would be required for manual procedures.

In addition to the design of fire protection hardware, computer models may also be used to help evaluate the effects of fire on both people and property. The models can provide a fast and more accurate estimate of the impact of a fire and help establish the measures needed to prevent or control it. While manual calculation methods provide good estimates of specific fire effects (e.g., prediction of time to flash over), they are not well suited for comprehensive analysis involving the time-dependent interactions of multiple physical and chemical processes present in developing fires.

1.3 Applications of Computer Model

One of the important application areas is the computer simulation of integrated circuits. Here **x** defines various circuit parameters, such as transistor characteristics, and **y** is a measurement of the circuit performance, such as output voltage. The literature shows some other applications in a wide variety of fields such as chemometrics (Ho et al., 1984), Heat combustion (Miller and Frenklach, 1983), VLSI-circuit design (Sharifzadeh et al., 1989), controlled-nuclear-fusion devices (Nassif et al., 1984), plant ecology (Bartell et al., 1981 and 1983), thermal-energy storage (Currin et al., 1988) and Biomechanical Engineering (Chang et al., 1999). Other application areas, as highlighted in Koehler (1990), were a mold filling process for manufacturing automobiles, chemical kinetic models, a thermal energy storage model and the transport of polycyclic aromatic hydrocarbon spills in streams using structured activity relationships model being of use in plant ecology. In fact, the widespread use of computer models and experiments for simulating real phenomena generates examples in virtually all areas of science and engineering.

1.4 The Approach Using a Simple Computer Model

We consider a simple computer model in this paper to initiate our approach and start from the basics. Fire is a complex phenomenon and a number of computer models have been developed that reflect this complexity, for use by scientists and engineers. One of the earliest models was the **ASET** (Available Safe Egress Time) mathematical model written in FORTRAN by Cooper (1980). Later, Walton (1985) implemented the model in Basic as **ASET-B** incorporating simpler numerical techniques to solve the differential equations involved.

ASET-B is a personal computer program for predicting the fire environment in a single room enclosure with all doors, windows and vents closed except for a small leak at floor level. This leak prevents the pressure from increasing in the room. A fire starts at some point below the ceiling and releases energy and the products of combustion. The rate at which these are released is likely to change with time. The hot products of combustion form a plume which, due to buoyancy, rises. As it does so, it draws in to the room cool air which decreases the plume's temperature and increases its volume flow rate. When the plume reaches the ceiling it spreads out and forms a hot gas layer which descends with time as the plume's gases continue to flow into it. There is a relatively sharp interface between the hot upper layer and the air in the lower part of the room which, in the **ASET-B** model, is considered to be at ambient temperature. The only interchange between the air in the lower part of the room and the hot upper layer is through the plume.

The computer model **ASET-B** solves several differential equations using a simpler numerical technique than in the original **ASET** program. **ASET-B** requires as inputs the height and area of the room, the elevation of the fire above the floor, a heat loss factor (the fraction of the heat released by the fire that is lost to the bounding surfaces of the enclosure) and a fire specified in terms of heat release rate which depends on the nature of the combustion material. For this study we have used the rate of release for a `*semi-universal fire*', corresponding to a ``*fuel package consisting of a polyurethane mattress with sheets, fuels similar to wood cribs and polyurethane on pallets, and commodities in paper cartons stacked on pallets*'' (Birk 1991, page 86). The program predicts the thickness and the temperature of the hot smoke layer as a function of time. A simple illustration of fire-in-enclosure flow dynamics for an ``*unvented*'' enclosure and the basic fire phenomena are presented in Figure 1.

The response **y** was taken as the time it takes for the height of the smoke layer to be at 5 ft (head height). This manipulation was carried out in order to make the output univariate.

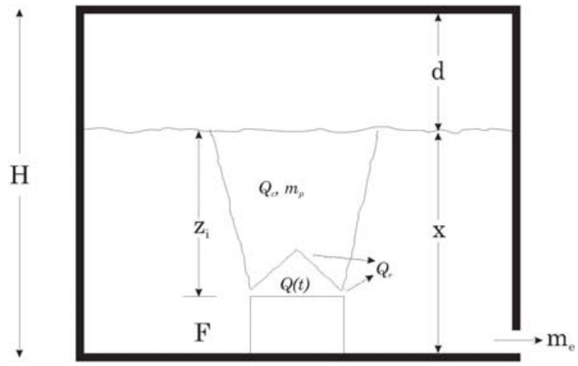

Figure 1: Simple Illustration of ASET-B enclosure fire

F – Height of base of fire

H – Height of room

m_e – Mass flow rate leaving crack like vent

m_p – Plume mass flow rate

Q_c – Convective energy release rate

Q_r – Radiative energy release rate

$Q_{(t)}$ – Heat release rate at time (**t**)

X – Height of interface above floor

Z_i – Interface height above fuel surface

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1.5 Modelling

The first stages of a computer experiment involve selecting the input variables and the range over which they will be explored. For the **ASET-B** model the inputs were taken to be the Heat Loss Fraction, the Fire Height, the Room Ceiling Height and the Room Floor Area giving a four dimensional configuration. The ranges of the variables are given in Table 1.

As indicated above the input variables $X_1,\ldots,X_4$, were coded as $x_1,\ldots,x_4$; where the x_i have a range of -1 to 1.

The number of runs (i.e.: sample size) required remains an open question for computer experiments [further details on sample size consideration are available in Sahama and Diamond, 2002]. Welch et al. (1996) suggest, as a guideline, that the number of runs in a computer experiment should be chosen to be 10 times the number of active inputs, which would lead to N=40 runs for this example if all four factors turn out to be active. To be conservative N=50 runs was used.

Table 1. Input Variables for **ASET-B** Fire Model

Variable	Variable Name	Minimum	Maximum
X_1	Heat Loss Fraction	0.6	0.9
X_2	Fire Height (ft)	1.0	3.0
X_3	Room Ceiling Height (ft)	8.0	12.0
X_4	Room Floor Area (sq. ft)	81.0	256.0

The actual input variables and response (Egress Time), generated from the ASET-B program, are given in Figure 2 as a pictorial representation of the design.

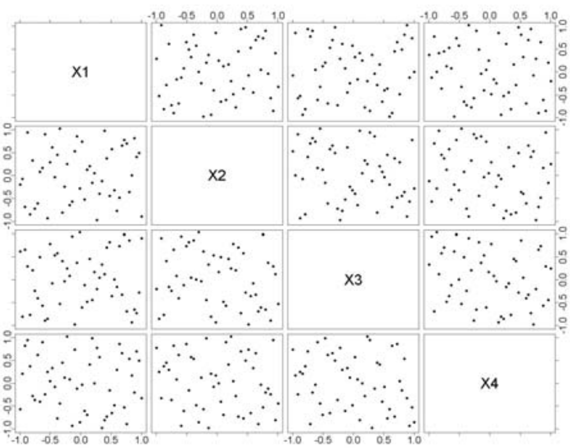

Figure 2: Projection Properties of a LHD with 50 runs

Modelling for the ASET-B responses were carried out as a realization of a stochastic process, following the methodology developed by Sacks et al. (1989b). A Latin Hypercube Design (LHD) is used to choose input factors for the ASET-B program. Based on this LHD, responses **y** from the model is generated to form a computer experiment. The egress time for each run of the LHD was calculated using linear interpolation by assuming that the height of the smoke layer is 5ft (head height). The responses are modelled as the realisation of a stochastic process, following the work of Sacks et al. (1989a). Maximum Likelihood Estimates (MLE) of the parameters are generated and these estimates used to make predictions at untried inputs. The prediction can be made using the Best Linear Unbiased Predictor (BLUP), a methodology introduced by Henderson (1975b) and Goldberger (1962). A graphical interpretation of the results is presented.

The response was modeled as:

Response = Linear Model + Departure

$$y_x = \sum_{j=1}^{k} \beta_j f_j(x) + z(x) \qquad (1)$$

The systematic departure z as a realization of stochastic process in which the covariance functions of z relates to the smoothness of the response. The covariance of the response to two d-dimensional inputs $t = (t_1.....t_d)$ and $u = (u_1....u_d)$ is given by,

$$Cov(z(t),z(u)) = \sigma_z^2 \prod_{j=1}^{d} R_j(t_j,u_j) \qquad (2)$$

where

$$R_j(t_j,u_j) = \exp(-\theta(t_j - u_j)^2) \qquad (3)$$

Here the $\theta > 0$ defines the correlation structures of z and σ_z^2 is a scale factor.

1.6 Prediction

Given the estimated parameters, prediction at untried inputs can be made using Best Liner Unbiased Predictor (BLUP). The prediction at **x** is given by:

$$\hat{y}(x) = \hat{\beta} + r^T(x) R_D^{-1}(y - 1\hat{\beta}) \qquad (4)$$

where

$$r(x) = [R(x_1,x),....., R(x_n,x)]^T \qquad (5)$$

For a prediction to be useful it should be supplemented by a measure of its precision. A number of different measures have been introduced for computer experiments and their utilities have been reviewed. To keep his paper simple and less complicated we choose one of the most important measures of Empirical Root Mean Square Error (ERMSE). The ERMSE is calculated as below:

$$ERMSE = \left\{ \frac{1}{N} \sum_{N} [\hat{y}(x) - y(x)]^2 \right\}^{\frac{1}{2}} \qquad (6)$$

where **x** is a set of N randomly selected points over the experimental region R.

Mean Square Error at a point **x** given by

$$MSE[\hat{y}(x)] = \sigma^2 \left[1 - (1 \quad r^T(x)) \begin{pmatrix} 0 & 1^T \\ 1 & R_D \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ r(x) \end{pmatrix} \right] \qquad (7)$$

1.7 Interpretation of the Results

To see the usefulness of the predictions the **ASET-B** model was run for 100 random points over the design range and predictions made based on the fitted computer model. Figure 3 show that the predictions match the actual responses from **ASET-B** quite closely.

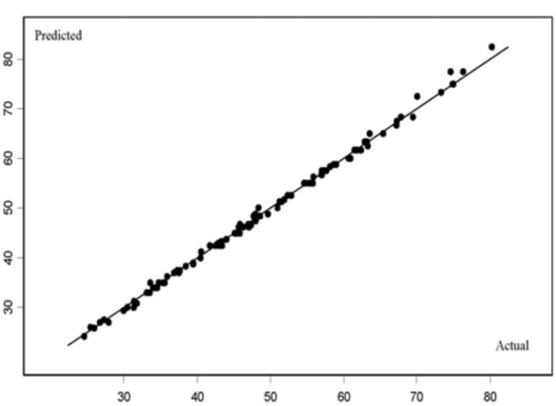

Figure 3: Accuracy of Prediction for Egress Time

Figures 4 and 5 depict the main effects and interaction effects estimated over the experimental region using the results above. The main effect given in Figure 4 shows that the Egress Time increases as each of the input factors increases, with the most important factors over the ranges studied being Room Floor Area (D) and Fire Height (B). Heat Loss Fraction (A) and Room Ceiling Height (C) are less important in this model. Similarly, the estimated interaction effects given in Figure 5 contours prove that the deviations from additivity are quite small since the interactions are small relative to the main effect. This is the case for the joint effect presented in Figure 6.

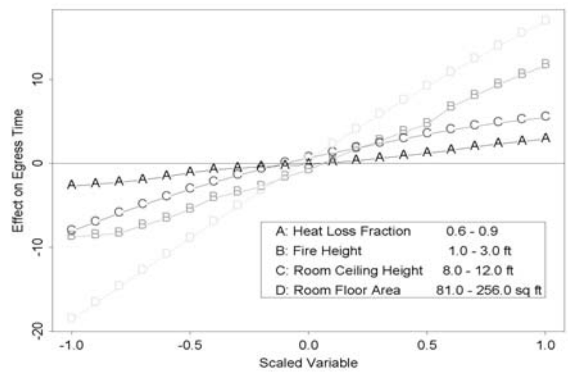

Figure 4: Main Effect plot for the ASET-B Computer Model

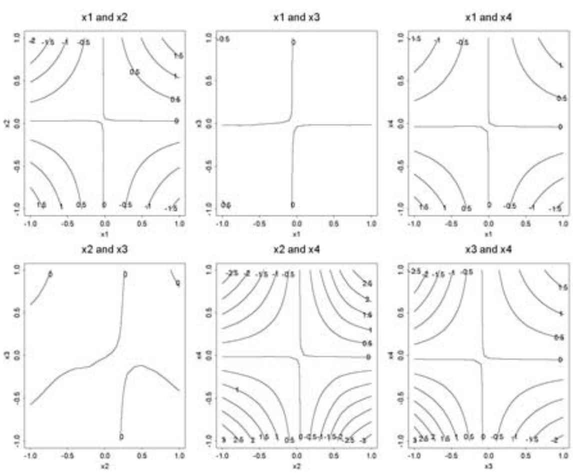

Figure 5: Interaction Plot for the ASET-B Computer Model

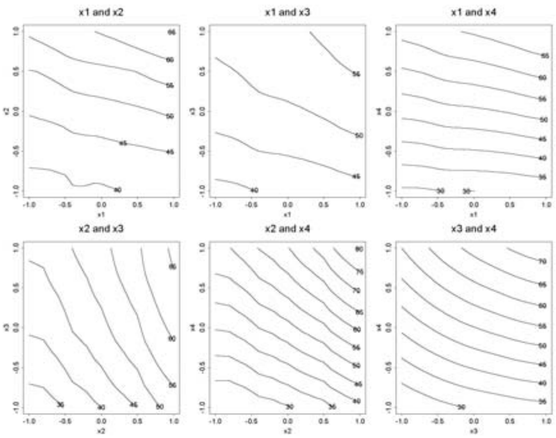

Figure 6: Joint Effect Plot for the ASET-B Computer Model

2 CONCLUSIONS

ASET-B has been successfully modeled using the methodology introduced in DACE. The model gives prediction at untried inputs that are very close to the actual response.

The main effect diagram shows that over the range studied, the egress time increase almost linearly as the input variables increase. The two-factor interaction diagrams show that non-additivity is quite small for this model. This is supported by the Functional Analysis of Variance.

As presented in Figures 3, 4, 5, and 6, the Room Floor Area (D) and Fire Height (B) are more significant factors than the other factors. Also, in the two-way interaction effects, the factors involving (D) and (B) are much higher compared to the other two variables, (C) and (A), however, as can be seen, the two-way interaction effects are small when compared to the large main effects.

The results show that, as far as DACE is concerned, using the Computer Experiment approach can minimise the unnecessary re-running of complex computer code with several input.

Practical issues and challenges remain in the selection of the sample size (i.e. number of runs) and determination of the active main effects in order to quantify the number of runs for the computer experiment.

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