Paper submitted for publication in the special issue in memory of

Professor Y.C. Chao of the Journal of Taiwan Institute of Chemical Engineers

META-MODELLING IN CHEMICAL PROCESS SYSTEM ENGINEERING

Olumayowa T. Kajero[1], Tao Chen[1], Yuan Yao[2], Yao Cheng Chuang[2], and

David Shan Hill Wong[2*]

[1] Department of Chemical and Process Engineering, University of Surrey, Guildford, GU2 7XH, United Kingdom

[2]Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan, R.O.C.

*corresponding author: dshwong@che.nthu.edu.tw

ABSTRACT

Use of computational fluid dynamics to model chemical process system has received much attention in recent years. However, even with state-of-the-art computing, it is still difficult to perform simulations with many physical factors taken into accounts. Hence, translation of such models into computationally easy surrogate models is necessary for successful applications of such high fidelity models to process design optimization, scale-up and model predictive control. In this work, the methodology, statistical background and past applications to chemical processes of meta-model development were reviewed. The objective is to help interested researchers be familiarized with the work that has been carried out and problems that remain to be investigated.

Keywords**:** *Metal-modelling*, *chemical process system engineering*

1. INTRODUCTION

Systematic accumulation of knowledge and drive towards optimal design is the key to intelligent and rapid development of chemical processes and products. Traditionally this is done in two distinct approaches: the first-principle approach and data-driven or black-box approach.

First principles, or physical approach requires scientific understandings of the workings of process and integrates them into deterministic input-output simulation models. Simulation models can be developed at different physical scales, e.g. steady state and dynamic process simulations model the operation performance of a plant, computer fluid dynamic (CFD) simulations model the momentum, material and heat transfer in an equipment, and molecular simulations model the relation between molecular structure as input and material property as output.

The black-box or data-driven approach rooted on the statistical theory of design of experiment (DOE) to direct experiments. DOE can be divided into two categories, the exploration of design space, e.g. screening designs and finding the optimum, e.g. response surface method. Traditional DOE theory were based on the assumptions that the input-output relations are relatively simple, consisting of linear, interaction, quadratic effects etc.

With the development of powerful computers, we can include more and more details into first-principle simulation models so s to improve the fidelity of the model. For example, we can model a continuous stirred tank reactor (CSTR) by assuming that it is a well-mix reactor. The mixing and heat transfer can be modelled using a CFD simulator and their effects can be integrated to the well-mix reactor through residence time distribution and heat transfer rate. Alternatively, one can take into account

reactions and change in physical properties with change in composition and temperature in a CFD simulation. Even we a given simulation model, the fidelity can increase by including more mesh into the solver. As the fidelity of the physical model increases, the number of parameters needed to be estimated, i.e. costs of calibrating the first-principle model increase. However, the computer time required for simulation also increase and the high cost the first-principle model becomes difficult to use.

This dilemma leads to a continuous effort to develop meta-models(models of model, or surrogate models) so that knowledge accumulated in such high fidelity models can be used efficiently in design, optimization and control. There have already been many useful reviews and books in the development and application of meta model and design of computer experiments, a brief list is provided here[1,2,3,4,5,6,7,8]. However, to the best of our knowledge, there is no such review attempt specifically from the perspective of a chemical process system engineer. Specifically, we shall attempt to address the following important issues:

(1) model representation

(2) model construction and evolution, and

(3) applications in chemical process system engineering.

2. META-MODELS REPRESENTATION

2.1 INPUT-OUTPUT RELATION

Consider an actual process with input $\boldsymbol{x} = \left[x_1 \cdots x_{K_x}\right]$ and output $\boldsymbol{y} = \left[y_1 \cdots y_{K_y}\right]$.

$$\boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{x}) \tag{1}$$

Let $\boldsymbol{\Psi}$ be a high-fidelity physical model with a set of parameters $\boldsymbol{\beta}$ that predict an output $\boldsymbol{y}^{\boldsymbol{\Psi}}$ at a given set of input with a set of physical meaning parameters $\boldsymbol{\vartheta}$

$$\boldsymbol{y}^{\boldsymbol{\Psi}} = \boldsymbol{\Psi}(\boldsymbol{x}, \boldsymbol{\vartheta})$$

(2)

A meta-model is model that approximate the high fidelity model

$$\boldsymbol{\Psi}(\boldsymbol{x}, \boldsymbol{\vartheta}) = \boldsymbol{\Omega}(\boldsymbol{x}, \boldsymbol{\beta}) + \boldsymbol{\Gamma}(\boldsymbol{x})$$

(3)

$\boldsymbol{\Omega}$ are functional approximators with good flexibility, ability to achieve sufficient accuracy, computational efficiency and simple implementation. $\boldsymbol{\Gamma}(\boldsymbol{x})$ is the error of the meta model at a specific input configuration. Common types of meta-models include polynomial, kriging, radial basis function and artificial neural network, etc. We should bear in mind that the definition of input $\boldsymbol{x}$ and output $\boldsymbol{y}$ may be different in different applications. For example, let us consider the CFD model of a heat exchanger with fixed geometry. We can try to construct a meta-model that only apply to hot and cold streams with specific physical properties. The input parameters $\boldsymbol{x}$ are the inlet flowrates and temperatures of the inlet hot and cold streams. However, if we want to construct a more general meta-model that can be applied to different fluids, then physical properties such as viscosities and thermo-conductivities will also be classified as inputs. Similarly we can define various sets of $\boldsymbol{y}$. A simple version of $\boldsymbol{y}$ will be the average temperature of outlet streams. A detailed version of $\boldsymbol{y}$ can be the temperatures and the velocities at different points inside the heat exchanger.

2.2 Types of Meta-Models

2.2.1 Polynomial

Polynomial meta-model is perhaps the simplest form of model presentation used in meta-modelling research. Some studies in the literature on this method are: Simpson et al[9], Palmer and Realff[10], Dutournie et al[11], Chen et al[12]. Simplicity implies ease in construction and application but also inability to describe complex input-output

relationships.

2.2.2 Kriging, Gaussian Process Model, and Radial Basis Function:

The work of Krige[13] was widely used in geostatistics[14] and spatial statistics[15]. Kriging assumes some form of correlation between points in the multi-dimensional input space, with the correlation being used to predict response values between observed points. A brief introduction to the formulation and construction of Kriging model[16,17] are described as follows.

Let $\widehat{\boldsymbol{X}} = [\widehat{\boldsymbol{x}}_1, \cdots \widehat{\boldsymbol{x}}_N]^T$ be a set of training data points (sites) and $\widehat{\boldsymbol{Y}} = [\widehat{\boldsymbol{y}}_1, \cdots \widehat{\boldsymbol{y}}_N]^T$ be the corresponding response variables for development of a Kriging model. The prediction for a new data point, $\boldsymbol{x}$ is given by

$$\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{f}^T(\boldsymbol{x})\boldsymbol{\beta} + \boldsymbol{r}^T(\boldsymbol{x})\boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1}(\widehat{\boldsymbol{Y}} - \boldsymbol{F}(\widehat{\boldsymbol{X}})\boldsymbol{\beta}),$$

where $\boldsymbol{f}(\boldsymbol{x})$ contains a set of regression functions of the input variables, and $\boldsymbol{\beta}$ is the corresponding regression coefficients to be estimated. $\boldsymbol{F}(\widehat{\boldsymbol{X}}) = [f(\hat{x}_1), \cdots, \boldsymbol{f}(\hat{x}_N))]^T$ is a matrix containing the regression functions calculated for all the training data points. $\boldsymbol{R}(\widehat{\boldsymbol{X}})$ is the correlation matrix which is obtained from correlation functions evaluated at each pair of the training points:

$$\boldsymbol{\Sigma}(\widehat{\boldsymbol{X}}) = \begin{bmatrix} \rho(\widehat{\boldsymbol{x}}_1, \widehat{\boldsymbol{x}}_1) & \cdots & \rho(\widehat{\boldsymbol{x}}_1, \widehat{\boldsymbol{x}}_N) \\ \vdots & \ddots & \vdots \\ \rho(\widehat{\boldsymbol{x}}_N, \widehat{\boldsymbol{x}}_1) & \cdots & \rho(\widehat{\boldsymbol{x}}_N, \widehat{\boldsymbol{x}}_N) \end{bmatrix}.$$

A widely used correlation function is the Gaussian function

$$\rho(\boldsymbol{x}, \boldsymbol{x}') = exp\left[-(\boldsymbol{x} - \boldsymbol{x}')^T diag\left[\theta_1 \cdots \theta_{K_x}\right](\boldsymbol{x} - \boldsymbol{x}')\right],$$

while

$$\boldsymbol{r}(\boldsymbol{x}) = [\rho(\boldsymbol{x}, \widehat{\boldsymbol{x}}_N), \cdots \rho(\boldsymbol{x}, \widehat{\boldsymbol{x}}_N)]$$

is vector of the correlation between a general point in the input space and the training sites. The parameters of the Kriging model are the parameters in the correlation function $\boldsymbol{\theta} = \left[\theta_1 \cdots \theta_{K_x}\right]$ and the regression coefficient $\boldsymbol{\beta}$. They can be estimated by

the following iterative procedure. First assume a value for $\boldsymbol{\theta}$, estimate the regression coefficient $\boldsymbol{\beta}$ by

$$\widetilde{\boldsymbol{\beta}} = \left(\boldsymbol{F}(\widehat{\boldsymbol{X}})^T \boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1} \boldsymbol{F}(\widehat{\boldsymbol{X}})\right)^{-1} \boldsymbol{F}(\widehat{\boldsymbol{X}})^T \boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1} \boldsymbol{Y}$$

The process variance can be calculated as

$$\sigma_p^2 = \frac{1}{N} (\boldsymbol{Y} - \boldsymbol{F}(\widehat{\boldsymbol{X}}))^T \boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1} \left(\boldsymbol{Y} - \boldsymbol{F}(\widehat{\boldsymbol{X}})\right)$$

A new set of correlation parameters $\boldsymbol{\theta}$ can be estimated by

$$\widetilde{\boldsymbol{\theta}} = \min_{\boldsymbol{\theta}} \left(\left|\boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})\right|^{1/N} \sigma_p^2\right)$$

The above procedure is repeated until values of $\widetilde{\boldsymbol{\theta}}$ and $\widetilde{\boldsymbol{\beta}}$ converge.

Kriging is also termed Gaussian process in the literature with slightly different formulation[18,19,20].

Applications of Kriging, Gaussian process models in meta-model development have been extensively investigated by many authors. A chronological, but far from exhaustive, list is provided here[18,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47]. A review was provided by Kleijin[4] in 2009.

2.2.3 Support Vector Machine

Support vector machine (SVM)[48] was originally developed as a supervised learning classifier so that data in a (high dimensional) input space can be classified into groups according to their locations. The SVM can also be formulated into an input-output known as support vector regression (SVR)[49]. For a specific dimension in the output space, given a training data set $\widehat{\boldsymbol{X}} = [\widehat{\boldsymbol{x}}_1, \cdots \widehat{\boldsymbol{x}}_N]^T$ and $[\hat{y}_1, \cdots \hat{y}_N]^T$; a nonlinear SVR can be expressed as

$$y(\boldsymbol{x}) = \alpha_o + \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) K(x, \widehat{\boldsymbol{x}}_i)$$

where $\boldsymbol{\alpha}_i, \boldsymbol{\alpha}_i^*$ can be obtained by solving optimization problem

$$\max\left\{\begin{matrix}-\frac{1}{2}\sum_{n=1}^{N}\sum_{n\prime>n}^{N}[(\alpha_n-\alpha_n^*)(\alpha_{n\prime}-\alpha_{n\prime}^*)K(\widehat{\boldsymbol{x}}_n,\widehat{\boldsymbol{x}}_{n\prime})]\\ +\varepsilon\sum_{n=1}^{N}(\alpha_n+\alpha_n^*)+\sum_{n=1}^{m}\hat{y}_n(\alpha_n-\alpha_n^*)\end{matrix}\right\}$$

$$subject\ to:\begin{cases}\sum_{n=1}^{N}(\alpha_n-\alpha_n^*)=0\\ 0<\alpha_n,\alpha_n^*<C\end{cases}$$

The off-set parameter α_o, tolerance parameter ε and constraint parameter C are parameters to be chosen in training[50]. The solution of the above problem can be determined using a least square approach that uniquely determined by the input-output training data; the resulting model is known as known as least square support vector machine (LS-SVM)[51]. Several reports of using SVR in meta-modelling are given here[52,53,54,55,56].

2.2.4 *Multivariate Adaptive Regression Spline*

The multivariate adaptive regression spline (MARS) was introduced by Friedmann[57] attempts to fit a set of training data $\widehat{\boldsymbol{X}}=[\widehat{\boldsymbol{x}}_1,\cdots\widehat{\boldsymbol{x}}_N]^T$ and $\widehat{\boldsymbol{Y}}=[\widehat{\boldsymbol{y}}_1,\cdots\widehat{\boldsymbol{y}}_N]^T$ by selections from a set of basis functions

$$\boldsymbol{y}(\boldsymbol{x})=\sum_{\mathrm{m}=1}^{M}\beta_m\boldsymbol{B}_m(\boldsymbol{x})$$

The set of basis functions is given by:

$$\boldsymbol{B}_m(\boldsymbol{x})=\prod_{l=1}^{L_m}\left[s_{l,m}\left(x_{v(l,m)}-t_{l,m}\right)\right]_+^q$$

$s_{l,m}$ can take values of ±1. L_m is an interaction order of the m^{th} basis function. $[\cdot]_+^q$ is hinge function with the following form

$$\left[s_{k,m}\left(x_{v(k,m)}-t_{k,m}\right)\right]_+^q=\begin{cases}\left[s_{k,m}\left(x_{v(k,m)}-t_{k,m}\right)\right]^q & s_{k,m}\left(x_{v(k,m)}-t_{k,m}\right)>0\\ 0 & otherwise\end{cases}$$

$x_{v(k,m)}$ is value of one of the input variables, and $t_{k,m}$ is hinge point so that the basis function $\boldsymbol{B}_m(\boldsymbol{x})$ is cutoff either above or below the hinge point. The basis functions are selected using a forward-backward stepwise selection. MARS offers a flexible spline fit of an input and output relation that can be piecewise continuous. Use of MARS in meta-modelling have been discussed by many authors[58,59,10,60,61,62,63,64].

2.2.5 Radial Basis Function Network

A similar form of the above method is the radial basis function network (RBFN)[65]

$$\boldsymbol{y}(\boldsymbol{x}) = \omega_o + \sum_{i=1}^{n} \omega_i f(\|\boldsymbol{x} - \boldsymbol{c}_i\|).$$

The function f can take many forms such as linear, cubic, thin plate spline, Gaussian, mult-quadratic, and inverse multi-quadratic etc. The parameters of the function include the weighting coefficients $\boldsymbol{\omega}$ and the basis function centers $[\boldsymbol{c}_1 \cdots \boldsymbol{c}_n]$. They can be obtained by three step algorithm as follows. First a set of basis function centers were chosen by some clustering of training data in the input space (unsupervised learning). Secondly the weighting coefficients were determined by linear regressions. Then both the weighting coefficients and the basis function centers are updated by gradient search. Applications of radial basis function in meta-modelling have also been extensively investigated in the literature[66,67,58,60,68,69,70,71,72,73].

2.2.6 Artificial Neural Network (ANN)

Artificial neural network (ANN) has been built with the aim of modelling how the human brain functions. They were used in many fields of machine learning and artificial intelligence research such as speech recognition, image processing etc. It should be pointed out that RBFN and SVM are also forms of ANN interpreted in a general sense. However, in this manuscript, we used ANN to denote a common form known as the feed-forward multilayer perceptron (MLP). MLP can be expressed mathematically in the following form:

$$y^k{}_i = f\left(\sum_{j=1}^{K^{k-1}} w_{ij}^k f\left(y^{k-1}{}_j\right) + b_i^k\right)$$

$y^k{}_i$ is the output of the i^{th} neuron in the k^{th} layer. w_{ij} is a synaptic weight connecting the output of the j^{th} neuron in the $(\mathrm{k}-1)^{\text{th}}$ layer to the input of the the i^{th} neuron in the k^{th} layer. $b^k{}_i$ is the bias of the i^{th} neuron in the k^{th} layer. K^k is the number of neurons in the in the k^{th} layer. f is known as the activation function which can take many forms.

Sigmoids such as hyperbolic tangent and logistic functions are commonly used. It was proved that a single layer of such network is able to approximate and continuous function[74]. Applications of ANN in meta-modelling can also be found in wide variety of areas[75,58,76,77,78,79,80,81,82,83,84,85,86].

2.3 FEATURE SELECTION

In many high fidelity simulations, especially CFD, the output are not limited to a few variables but maps of spatial and temporal variations. While such maps can be discretized to generate a large number of variables, it is not clear how they should be incorporated into the meta-model. Using a dynamic system that has an input vector $\boldsymbol{x}$ and produces output in a period which can be discretized into $\boldsymbol{y} = [y_1, \cdots y_T]$, Conti et al[87] explained different possible ways of creating an emulator (meta-model). A multiple output (MO) emulator expressed the output at different time steps as a function of input

$$\boldsymbol{y} = \boldsymbol{\Omega}(\boldsymbol{x})$$

A multiple single output (MS) emulator expressed the output at each time instant as

$$y_i = \Omega_{\boldsymbol{i}}(\boldsymbol{x})$$

A time input (TI) emulator expressed

$$y = \Omega(\boldsymbol{x}, t)$$

Let us use Kriging model as an example, and n be the number of regression functions and m be the number of training data. The training of the MO emulator will required an inversion of $m \times m$ matrix $\boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})$ and $Tn \times Tn$ matrix $\boldsymbol{F}(\widehat{\boldsymbol{X}})^T \boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1} \boldsymbol{F}(\widehat{\boldsymbol{X}})$. Hence the size of matrix being inverted is dependent of T. The training of the MS emulator will required an inversion of $m \times m$ matrix in $\boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})$ and $n \times n$ matrix in $\boldsymbol{F}(\widehat{\boldsymbol{X}})^T \boldsymbol{\Sigma}(\widehat{\boldsymbol{X}})^{-1} \boldsymbol{F}(\widehat{\boldsymbol{X}})$. The size of the matrix inversion is always limited but the training time increases with T. In the TI emulator, the number of regression function

n has to be increased to account for variation due to time dependence. Similar conclusions can also be extended to spatially distributed output and spatial-temporal output.

One way of simplifying the meta-model representation is to reduce the dimension of the output in a MO emulator using feature extraction method such as principle component analysis (PCA)[88]. For example, Chen et al[20] used PCA to reduce the dimension of a two dimensional CFD simulation of dispersion dynamics of particulate aerosols and showed that output variations of 182250 spatial-temporal grid points can be reduced to scores of 8 principal components that can be efficiently modelled by a GPR. Similar works were reported by Jia et al[89] in real-time storm /hurricane risk assessment and Wang and Chen[90] in vapor cloud dispersion.

2.4 SUMMARY

In this section, we have examined several input and output relations commonly used for meta-modelling. However, other forms of input and output relations may be used depending on the nature of the problem. Meta-models used are often referred to being parametric or nonparametric. Parametric models (e.g. MARS/RBFN/ANN) usually assumed some forms of basis functions. The model coefficients are obtained from the training data using regression analysis. In principle, we can forget the training data set once the model is determined. The model complexity will increase as more basis functions were added to the systems. Since the number of parameters are not prefixed, therefore is always the danger of overfitting and the generalizability of the model is compromised. Cross validation is usually used to ensure that there is no overfitting[91]. Non-parametric models (e.g. Kriging/GPR/SVM) are basically interpolation models, the training data constitute the essential part of model parameters and must be memorized to make predictions. It should be noted that the need of data storage is not

really a disadvantage because data storage become less and less expensive with cloud technology and recall of old training data to train new model is also necessary even when a parametric model is used. As far as we know, there is no definitive conclusion that a specific form of input-output relation is superior in meta-modelling. It is generally assumed that input-output relation of a high fidelity first-principle model is inherently complex. Therefore the meta-model must be flexible enough to capture the complexity. Hence there must be an element in the meta model that ensure that it can serve as a universal function approximator.

3. META-MODEL CONSTRUCTION

3.1 DESIGN OF COMPUTER EXPERIMENT

The intuitive approach to meta-model construction may view each simulation run as an experiment and use traditional design of experiment (DOE) procedure to determine the locations of each simulation runs to be executed. This area is known as design of computer experiments[18,21].

Traditional DOE methods can usually be classified as either one of the following two objectives, (i) screening experiments that try to identify factors (input variables or combination of input) that have statistically significant effects on the response (output); and response surface experiments that try to build a input-output relation which can predict the optimal input conditions[92,93].

Classical screening experiments include Factorial Design, Fractional Factorial Design, , etc. Another general class of screening are "optimal designs" that optimize some form of metric of the information matrix $\left|\left(\widehat{\boldsymbol{X}}^T\widehat{\boldsymbol{X}}\right)^{-1}\right|$ where $\widehat{\boldsymbol{X}}$ is matrix of the training data in a generalized parametric input space. For example the D-optimal design minimizes the determinant of Fischer information matrix.

Common experimental design for response surface experiments Central Composite

Design and Box-Behnken Design. Such designs usually possess the desirable property of having low prediction error.

In design of experiments, two kinds of errors are considered: (i) random errors that is measured by the variance of the predictions, (ii) systematic errors caused by mismatch of the model assumed and the actual response, i.e. bias. In design of computer experiments, the random error is expected to be small. Therefore designs that are based upon a preselected model and the assumption that bias is small compared to variance, such as the D-optimal design may not be appropriate.

Furthermore, even simulations are relative inexpensive compared to experiments, their execution takes time and effort. Therefore the number of runs a major concern. Relatively large number of runs are still required for some of these designs, especially when the dimensionality design space increases. Small response surface design can be used to reduce the number of runs Plackett-Burman Design[94], small composite design[95], saturated design[96] (see review by Draper and Lin[97] and Meyers and Montgomery[93]). However, as pointed out by Allen and Yu[98], the desirable properties of having prediction error may be compromised. Therefore design methods that sufficiently accounted for the effects of bias while without sacrificing variance, e.g. based on expected integral mean square error should be considered (Allen et al[99]).

Alternatively, another approach is to explore the design space so as to minimize un-sampled region. Examples of space filling design include: random or Monte Carlo sampling[100], orthogonal arrays[101], uniform design[102], Latin Hypercubes Sampling (LHS)[103,104], Hammersley Sampling (HSS)[105]. To measure the space filling nature of the design, a measure of the space filling nature should be defined, e.g. the modified L_2 discrepancy is often used for input variables scaled between [-1,1]

$$ML_2 = \left(\frac{4}{3}\right)^{K_x} - \frac{2^{1-K_x}}{N}\sum_{n=1}^{N}\prod_{k=1}^{K_x}(3-\hat{x}_{nk}^2) +$$

$$\frac{1}{N^2}\sum_{n=1}^{N}\sum_{n'=1}^{N}\prod_{k=1}^{K_x}\left(2-max(\hat{x}_{nk},\hat{x}_{n'k})\right)$$

The smaller the value, the better is the space filling properties. Another measure is the minimum Euclidean distance between the design points[106]

$$M_m = \min_{n,n'}\|\hat{\boldsymbol{x}}_n - \hat{\boldsymbol{x}}_{n'}\|$$

The larger the value is the better. To balance between space-filling properties and orthgonality, Cioppa and Lucas[107] proposed a design that created the best space filling properties, subject to constraints of orthogonality measures such as the maximum correlation between various dimensions $\rho_{max} = \max_{k,k'} cor(\hat{\boldsymbol{x}}_k, \hat{\boldsymbol{x}}_{k'})$ and conditional number of the information matrix of sampling points $cond(\hat{\boldsymbol{X}}^T\boldsymbol{X})$ in the design space.

3.2 ITERATIVE APPROACH

Despite the development of numerous sampling schemes, it is generally not realistic to expect a reliable meta-model can be build or the optimum of the actual model can be located using a single set of sampling data. It is necessary to balance between optimization and the fidelity of the approximate-model using iterative approach[108]. Early work in this area, reviewed by Wang and Shan[3] include reducing the dimension of design space by eliminating unimportant variables[109],[110]. An alternate approach is to survey a small design space and move limits towards the optimal region[111],[112],[113],[114]. Wang and Simpson[115] used a preliminary meta-model to generate a large number of points in the large design space and then cluster promising points. Meta-models for local region around cluster centers are then generated to refine the optimum. The above are optimization iterations designed for finding the optimum. Khu et al[60] also developed an evolutionary strategy using genetic algorithm for determination of the sample points. However, the objective function to be optimized is the sum square error between the actual model and predicted values of a validation data set. Thus the

iterative approach is designed to increase the fidelity of the model. Chen et al[116] argued that, even in optimization, with limited data, the initial meta-model cannot be completely trusted. Thus in early stages of the search, we need to focus on exploring under-sampled region. At later stages focus should be on finding the optimum since enough data has been accumulated for building an accurate enough model. An index, the predicted fitness of objective function at a sample point is defined as the information energy. An index of information content of sampling point was defined as the information entropy. New samples were generated based on Monte Carlo importance sampling of the free energy, with "temperature" which is related to the number of previously sampled points being a balancing parameter. Tang et al[117] and Chi et al[118] also used an evolutionary meta-model optimization in which the prediction uncertainty of the GPR was used in addition to the prediction mean to determine the future sampling points. An alternative method of preventing premature convergence is to use an index that took care of the uncertainty of the prediction, known as expected improvement (EI)[119]. EI recognizes that the predicted improvement is a random variable, because the meta-model gives prediction mean and variance. Therefore, the predicted improvement should be integrated with its probability density function to attain its expected value, i.e. EI, which should be the objective function to be optimized.

3.3 Model Migration

In many engineering applications, simulations were often called upon to solve problems with some degree of similarity. For example, CFD simulations were carried out and a "old" meta-model has been constructed for a given equipment with a set of geometrical design parameters with a fluid of given rheological properties. It would most desirable if we can construct "new" meta-model for another piece of

equipment that is similar in structure but with slightly different geometries and/or another fluid with different rheological properties, using the given "old" meta-model plus only a few simulation data . Another typical problem of in chemical engineering is scale-up of reactor. It is well known that optimal operating condition found for a reaction out in a lab size reactor may not work when a reactor is scaled to larger dimensions. Although kinetics and thermodynamics will not change as the equipment is scaled up. Mixing and heat transfer changes with dimension. CFD simulation were often used to solve scale-up problems, but CFD coupled with reaction is notoriously difficult to execute. Hence development of meta-models for design and optimization is necessary.

Gao and coworkers[120],[121],[122],[123] recognized the problem of how to efficiently modify an existing meta-process model to fit a different yet similar process. The existing model is denoted as the "base model", while the model to be developed for the new process is called as the "new model". At least one of the following two objectives are expected to be achieved.

(1) To attain similar prediction accuracy, fewer data are required for migrating from the base model to the new model than for developing an entirely new model without the migration step.

(2) The migrated new model is more accurate than the model developed without the aid of migration if nearly equal number of experimental data are used in model training.

Motivated by the standardization step in calibration model transfer [124], the migration can be conducted by a parametric scale and bias correction (SBC) of the base model[120],[123]:

$$\boldsymbol{y}(\boldsymbol{x}) = diag\left[s_{y,1} \cdots s_{y,K_y}\right] \boldsymbol{f}_o\left(diag\left[s_{x,1} \cdots s_{x,K_x}\right]\boldsymbol{x} + \boldsymbol{b_x}\right) + \boldsymbol{b}_y$$

where $\boldsymbol{f}_o$ denotes the base model; $s_{y,1} \cdots s_{y,K_y}$ and $s_{x,1} \cdots s_{x,K_x}$ are scaling parameters of different dimensions of the output and input space; $\boldsymbol{b}_y$ and $\boldsymbol{b}_x$ are bias vectors in the output and input space respectively. Data of the new process are used to determine the scale and bias transformation parameters. The SBC, being linear transformations in output and input space, is an arbitrary similarity condition that may not have sufficient flexibility to model the new process of interest. To overcome this limitation, Yan et al.[125] proposed a Bayesian migration method to update the scale-bias functions given experimental data from the new process. Their method is named as functional SBC, which is based on a GPR model framework. The input-output relation of the functional SBC is given by

$$\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{s}(x)\boldsymbol{f}_o(\boldsymbol{x}) + \boldsymbol{\delta}(\boldsymbol{x})$$

with $\boldsymbol{s}(x)$ being a linear scaling function

$$\boldsymbol{s}(\boldsymbol{x}) = \boldsymbol{s}_{yo} + diag\left[s_1 \cdots s_{K_y}\right]\boldsymbol{x}$$

and bias correction $\boldsymbol{\delta}(\boldsymbol{x})$ is chosen to be a Gaussian process with zero-mean. The underlying assumption that if the new process is similar to the old process, $\boldsymbol{\delta}(\boldsymbol{x})$ would be quite close to zero and its determination would require much less data points. Applicability of this method was recently demonstrated using sequential sampling and Bayesian techniques[126,127,128].

No physical reasoning has been given in developing SBC migration. However, it is well known that equations in transport phenomena can be reduced into universal form with dimensionless groups such as Reynolds number, Prandtl numbers and Nusselt numbers. Therefore, input-output relations of CFD may be scale-transformable through these dimensionless group. Recently Shen et al[129] demonstrated the advantages of performing experimental design using a dimensionless input space. Such advantages should be much more evident if applied to the design of computer

CFD experiments.

The functional SBC transformation can find its root from the work of Qian et al[38] where the same method was used to migrate between a model of low accuracy (LE) experiment and a high accuracy (HE) experiment. The concept is especially important for design of computer experiments, because complex computer codes can generate results with different levels of mesh densities. It is always desirable that a meta-model can be generated using more low fidelity runs and a small number of high fidelity runs. Kennedy and O'Hagan[130] first proposed using an auto regressive relation with a Gaussian process model bias term to connect meta-model of different levels of mesh fidelities. The problem of migrating between different levels of fidelity due to mesh densities has been well researched by many authors[131],[132],[133],[134],[135],[136],[137],[138].

It should be pointed out the complexity of a computer code can be increased not only increasing the mesh but increasing the physical processes being considered. Chuang et al[139] demonstrated by using a simple well-mixed CTSR model that contains only the kinetics of the reaction as the base model, new meta-models can be readily developed for full CFD simulations that take into account of mixing and heat transfer.

In theory, using the Gaussian process model for a bias term allows us to include any differences between the "new" and "old" processes. It should be noted that the migration is feasible even if new variables were added to the "new process". The success of migration depends on the functional similarity between the input-out relations of "new" and "old" processes in the old input-space. In other words, as the computational model become more complex, less and less significant variations will be left out. The bias term approaches a zero function.

3.4 SUMMARY

In this section, various sampling method for constructing meta-models were

reviewed. The general consensus up to now is that space filling design should be the most appropriate for building meta-models. However, when a meta-model was used for optimization, a balance of importance sampling and space-filling needs should be considered, especially in evolutionary procedures. Migration of meta-models is also an important research area. Migration between different meshing densities has been extensively studied. Dimensional analysis is the underlying assumption of scaling transformation. The bias term in the functional scale and bias correction incorporate enough flexibility to allow for migration between models of different complexities due to inclusion of additional physical considerations.

4. APPLICATIONS

4.1 PROCESS DESIGN AND OPTIMIZATION

The most straightforward application of meta-modelling is process design and optimization. Meta-model optimization has already been extensively used in design and optimization of many different processes. A wide variety of applications include flowsheeting[10,140,141,142,143,144]; boiler and combustion processes[145,146,147]; separation processes such as simulated moving bed chromatography[148], pressure swing adsorption[149] heated integrated column[144], divided wall column[150], CO2 capture process[151]; reactor operation such as iron oxide reduction[152], nano-particle synthesis[153], bacteria cultivation[154]; polymer processing[155]; chemical processes in semiconductor industry[156,157,158]; etc. In should be pointed out that in some of these work, actual experiments instead of higher fidelity simulations were used. Using data-driven models as response surface model and iterative evolutionary strategy to direct additional experiments and finding the optimum process condition can be classified in general as “meta-model assisted optimization”.

A notable development is the use of surrogate model in superstructure optimization, in which a surrogate model with categorical variables is required[141]. However, the construction of a meta-model with categorical variables has not been thoroughly investigated. The intuitive approach is to create samples at every possible combination of categorical variables. However, such an approach would not work if the number and levels of categorical variables are large. Qian and Wu[159] have discussed the use of GPR with quantitative and qualitative input as a surrogate model for computer experiments. The covariance structure between category variables were estimated using data sampled so that one does not have to perform experiments at every possible combination of categorical variables. However, the parameter estimation, or training, involved a complex semidefinite optimization problem that is difficult to solve. Experimental design methods have been proposed[160]. The potential of such models, sampling and optimization strategy in flowsheet and equipment design for chemical engineers is enormous. Unfortunately, there seems to be no research on this subject in the chemical engineering literature.

4.2 PROCESS CONTROL

It should be pointed out that there are numerous studies data-driven models such as ANN[161], RBFN[162], SVM[163], GPR[164] can be used to represent nonlinear time series. Such models have been used in soft-sensors development to predictive important quality variables online[165,166,167,168,169,170]. They can of course be used in nonlinear model predictive control (NMPC)[171,172,173]. However, such data-driven models cannot be considered as meta-model discussed in this work, because they are not surrogates of a more complex model. Moreover, they are usually obtained from online data, thus experimental design to construct these models received much less interest to adaptive

or just-in-time strategies. Tsen et al[174] proposed a hybrid approach in which first-principle simulation data were trained together with experimental data to obtain an ANN model for use in control. Such hybrid models[175],[176] were developed because of the need of using prior first-principle knowledge to avoid unreasonable extrapolations and the necessity to accommodate with experimental information, i.e. migration to a more accurate and realistic model for control purposes.

Conceivably, a surrogate dynamic model for control can be generated using complex high fidelity dynamic simulation. However, many researchers prefer to use another technique known as the "reduced-order-model" (ROM) in which the surrogate was developed by reducing the original differential algebraic equations (DAE) system into lower order models by collocation or other mathematically rigorous simplification techniques. Such methods have been developed for distillation columns[177], bio-reactors[178], air separation[179,180] etc. Since the reduced models is still an equation based modles, ROMs are not meta-model as we have discussed.

Perhaps the closest form of meta-model in process control is under the banner of "approximate dynamic programming" for optimal control[181,182]. The objective of optimal control (and dynamic programming) is to minimize a certain "cost-to-go" function, which is usually a time-discounted sum of costs of individual time points. The major challenge under this framework is that the computation needed to evaluate the cost-to-go is often very high, and thus on-line control is almost infeasible. Here the idea of meta-modelling can help: a large number of simulations can be conducted off-line to generate simulation data, and a meta-model (termed "approximate cost-to-go function") can be developed to approximate the relationship between state/manipulated variables and the cost-to-go function. This approximate function is then used for on-line control, and also subsequently improved.

4.3 Model Calibration

The advantage of using meta-model as a surrogate of high fidelity model so that design space can be efficiently explored for process improvement is intuitive and straightforward. However, meta-model can also be used to improve predictions of high fidelity model. Typically, a high fidelity model requires a set of physical meaningful parameters $\boldsymbol{\vartheta}$ to make predictions (see equation 1). For example, in CFD simulations of reactors, $\boldsymbol{\vartheta}$ may consists of transport properties such as viscosity, thermoconductivity, diffusion coefficient, surface tension, thermodynamic properties such as heat capacities, model parameters for vapor-liquid equilibrium calculations, as well as kinetic parameters such as rate constants and activation energies. Theoretically, these parameters can be measured by independent experiments. In practice, they have to be calibrated by fitting simulation results with experimental data. To do so the high fidelity simulations has to be carried out at different parameter settings for each of the experiment conditions. This is of course computationally laborious and often impossible when the number of parameters to be determined is large.

Alternatively, we can construct a meta-model that includes the parameter $\boldsymbol{\vartheta}$ as our input and characteristic experimental observations as our output. Meta-model can be constructed with selected simulations at certain experiment conditions and parameter settings. Iterative sampling can be carried to minimize a fitness-function of sum-square-errors (SSE) of meta-model predictions of all experimental data.

The calibration of computer models dates back as far as 1978 (O'Hagan, 1978[183]), where the Bayesian calibration approach was used. This involves fitting the posterior distribution of best input parameter. The application of Bayesian calibration approach to univariate computer models was demonstrated by Kennedy and O'Hagan[184]. Similar

application in multivariate, temporal and spatial computer models have been demonstrated in several papers[185,186,187,87, 188,189]. Other calibration methods have been mentioned in the literature different from the Bayesian approach. Some of them can be found in the book by Kleijnen[46] where calibration was referred to as simulation optimization.

Examples of model calibration applications include: (1) energy simulation model of buildings, using a Gaussian process regression technique with a radial basis function kernel[190], (2) water distribution systems, involving an evolutionary-based meta-model with an innovative hybridization of Genetic Algorithm and Radial Basis Function[60] (Khu et al, 2004); an Artificial Neural Network linked to Genetic Algorithm[191],[192],[193] (3) mechanical and aerospace systems which utilizes Radial Basis Function with non-dominated Sorting Genetic Algorithm (NSGA-II) (Khalfallah and Ghenaiet, 2015).

4.4 SENSITIVITY ANALYSIS

A computer model can help us to locate the optimal operation of a process, it can also help us to evaluate the sensitivity of the response to a certain input. Sensitivity analysis can also be applied uncertain parameters of a model. Sensitivity can be characterized locally by carrying out one-at-time changes to each input and examine the effect on output. Chang et al provided an example of such approach biochemical network[194] was analyzed and simplified. Alternatively global variance based index such as the Sobol indices[195], fast amplitude sensitivity test (FAST)[196,197], high dimensional model representation (HDMR)[198], polynomial chaos expansion (PCE)[199],[200]etc. can be calculated. Calculation of these global sensitivity indices is of course time-consuming using the high fidelity model. However these indices can be relatively easy using meta-models.[30,40,201,202.]. Applications of sensitivity analysis

(and the closely related uncertainty analysis), with or without a meta-model to chemical engineering related problems include reaction kinetics[203],[204], biological system modelling[205], process design[206], enhanced oil recovery simulation[207], vapour cloud dispersion90, etc.

4.5 SUMMARY

In this section, we have examined some applications of meta-modelling in the field of chemical process system engineering. As we have seen, the most common application is process optimization and design. However, meta-model development with categorical variables is only in its early stage. Thus applications of meta-model optimization to design problems involving flowsheet structure and non-linear integer programing have been limited. While there are many applications in using data-driven soft-sensor and reduced order models in nonlinear model predictive control, these models are not meta-model as defined in this study. The closest form of meta-model application is approximate dynamic programming. We have also pointed out that meta-model can be used for model calibration and sensitivity analysis. Application of sensitivity analysis to chemical engineering related problems, especially analysis of kinetics reaction network has been well researched, partly because the need of a meta model is much less due to relative ease of ODE simulations.

5. CONCLUSIONS

The objective of this review is to provide chemical process system engineers with the statistical background that has been developed for design of computer experiment and use of meta-models for optimization. We have introduced various forms of meta-model representation. Interpolation model such as Kriging/GPR seems a useful model in many cases. Methods of sampling in meta-model construction and optimization

has also been surveyed. In general we found that space filling design is the suitable choice of initial experimental design and some form of balance between exploring uncertain region and confirmation of optimal prediction must be struck in evolutionary optimization. Examination of applications of chemical engineering related problems found that most applications of meta-modelling emphasize on optimization. However, optimization with categorical variables is still under-researched because meta-model theory and sampling techniques for this kind of problems have not been fully understood. With such knowledge, our ability to use complex, high fidelity, time consuming simulation tools more efficiently in understanding process behavior, optimize process design, and improve process control, can be enhanced.

ACKNOWLEDGEMENT

O. Kajero's PhD is funded by the Tertiary Education Trust Fund (TETFUND), Nigeria in collaboration with University of Lagos, Nigeria. This work was also partially supported

by an International Exchange grant co-funded by the Taiwan Ministry of Science & Technology (Grant number: MOST 104-2911-I-007-516) and the UK Royal Society (Grant number: IE140859).

REFERENCES

1. Simpson, T. W.; Peplinski, J. D.; Koch, P. N.; Allen, J. K., Metamodels for computer-based engineering design: survey and recommendations. *Engineering with Computers* **2001,** *17* (2), 129-150.
2. Chen, V. C. P.; Tsui, K. L.; Barton, R. R.; Meckesheimer, M., A review on design, modeling and applications of computer experiments. *Iie Transactions* **2006,** *38* (4), 273-291.
3. Wang, G. G.; Shan, S., Review of metamodeling techniques in support of engineering design optimization. *Journal of Mechanical Design* **2007,** *129* (4), 370-380.
4. Kleijnen, J. P. C., Kriging metamodeling in simulation: A review. *Eur. J. Oper. Res.* **2009,** *192* (3), 707-716.
5. Levy, S.; Steinberg, D. M., Computer experiments: a review. *AStA-Adv. Stat. Anal.* **2010,** *94* (4), 311-324.

6. Shan, S.; Wang, G. G., Survey of modeling and optimization strategies to solve high-dimensional design problems with computationally-expensive black-box functions. *Structural and Multidisciplinary Optimization* **2010,** *41* (2), 219-241.
7. Blondet, G.; Le Duigou, J.; Boudaoud, N.; Eynard, B., Simulation data management for adaptive design of experiments: A litterature review. *Mechanics & Industry* **2015,** *16* (6).
8. Santner, T. J.; Williams, B. J.; Notz, W. I., *The design and analysis of computer experiments*. Springer Science & Business Media: 2013.
9. Simpson, T. W.; Lin, D. K.; Chen, W., Sampling strategies for computer experiments: design and analysis. *International Journal of Reliability and Applications* **2001,** *2* (3), 209-240.
10. Palmer, K.; Realff, M., Metamodeling approach to optimization of steady-state flowsheet simulations - Model generation. *Chemical Engineering Research & Design* **2002,** *80* (A7), 760-772.
11. Dutournie, P.; Salagnac, P.; Glouannec, P., Optimization of radiant-convective drying of a porous medium by design of experiment methodology. *Dry. Technol.* **2006,** *24* (8), 953-963.
12. Chen, V. C.; Tsui, K.-L.; Barton, R. R.; Meckesheimer, M., A review on design, modeling and applications of computer experiments. *IIE transactions* **2006,** *38* (4), 273-291.
13. Krige, D., A statistical approach to some mine valuations and allied problems at the Witwatersrand, University of Witwatersrand. Masters: 1951.
14. Matheron, G., Principles of geostatistics. *Economic geology* **1963,** *58* (8), 1246-1266.
15. Cressie, N., Statistics for spatial data: Wiley series in probability and statistics. *Wiley-Interscience New York* **1993,** *15*, 16.
16. Chang, K.-t., *Introduction to geographic information systems*. McGraw-Hill Higher Education Boston: 2006.
17. Lophaven, S. N.; Nielsen, H. B.; Søndergaard, J. *DACE-A Matlab Kriging toolbox, version 2.0*; 2002.
18. Sacks, J.; Welch, W. J.; Mitchell, T. J.; Wynn, H. P., Design and analysis of computer experiments. *Statistical science* **1989**, 409-423.
19. Jones, D. R., A taxonomy of global optimization methods based on response surfaces. *Journal of global optimization* **2001,** *21* (4), 345-383.
20. Chen, T.; Hadinoto, K.; Yan, W.; Ma, Y., Efficient meta-modelling of complex process simulations with time–space-dependent outputs. *Computers & chemical engineering* **2011,** *35* (3), 502-509.
21. Sacks, J.; Schiller, S. B.; Welch, W. J., Designs for computer experiments. *Technometrics* **1989,** *31* (1), 41-47.
22. Barton, R. R. In *Simulation metamodels*, Proceedings of the 30th conference on Winter simulation, IEEE Computer Society Press: 1998; pp 167-176.
23. Simpson, T. W.; Mistree, F., Kriging models for global approximation in simulation-based multidisciplinary design optimization. *Aiaa Journal* **2001,** *39* (12), 2233-2241.
24. Meckesheimer, M.; Booker, A. J.; Barton, R. R.; Simpson, T. W., Computationally inexpensive metamodel assessment strategies. *AIAA journal* **2002,** *40* (10), 2053-2060.
25. Shin, M.; Sargent, R. G.; Goel, A. L. In *Optimization and response surfaces: Gaussian radial basis functions for simulation metamodeling*, Proceedings of the 34th conference on Winter simulation: exploring new frontiers, Winter Simulation Conference: 2002; pp 483-488.

26. Allen, T. T.; Bernshteyn, M. A.; Kabiri-Bamoradian, K., Constructing meta-models for computer experiments. *J. Qual. Technol.* **2003,** *35* (3), 264-274.
27. Ong, Y. S.; Nair, P. B.; Keane, A. J., Evolutionary optimization of computationally expensive problems via surrogate modeling. *Aiaa Journal* **2003,** *41* (4), 687-696.
28. Kleijnen, J. P. C., An overview of the design and analysis of simulation experiments for sensitivity analysis. *Eur. J. Oper. Res.* **2005,** *164* (2), 287-300.
29. Li, R. Z.; Sudjianto, A., Analysis of computer experiments using penalized likelihood in Gaussian kriging models. *Technometrics* **2005,** *47* (2), 111-120.
30. Martin, J. D.; Simpson, T. W., Use of kriging models to approximate deterministic computer models. *AIAA journal* **2005,** *43* (4), 853-863.
31. Wang, L.; Beeson, D.; Akkaram, S.; Wiggs, G. In *Gaussian process meta-models for efficient probabilistic design in complex engineering design spaces*, ASME 2005 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, American Society of Mechanical Engineers: 2005; pp 785-798.
32. Barton, R. R.; Meckesheimer, M., Metamodel-based simulation optimization. *Handbooks in operations research and management science* **2006,** *13*, 535-574.
33. Joseph, V. R., Limit kriging. *Technometrics* **2006,** *48* (4), 458-466.
34. Zhou, Z.; Ong, Y. S.; Nair, P. B.; Keane, A. J.; Lum, K. Y., Combining global and local surrogate models to accelerate evolutionary optimization. *Systems, Man, and Cybernetics, Part C: Applications and Reviews, IEEE Transactions on* **2007,** *37* (1), 66-76.
35. Joseph, V. R.; Hung, Y.; Sudjianto, A., Blind kriging: a new method for developing metamodels. *Journal of Mechanical Design* **2008,** *130* (3).
36. Knowles, J.; Nakayama, H., Meta-modeling in multiobjective optimization. In *Multiobjective optimization*, Springer: 2008; pp 245-284.
37. Marrel, A.; Iooss, B.; Van Dorpe, F.; Volkova, E., An efficient methodology for modeling complex computer codes with Gaussian processes. *Computational Statistics & Data Analysis* **2008,** *52* (10), 4731-4744.
38. Qian, P. Z. G.; Wu, H. Q.; Wu, C. F. J., Gaussian Process Models for Computer Experiments With Qualitative and Quantitative Factors. *Technometrics* **2008,** *50* (3), 383-396.
39. Drignei, D., A Kriging Approach to the Analysis of Climate Model Experiments. *Journal of Agricultural Biological and Environmental Statistics* **2009,** *14* (1), 99-114.
40. Marrel, A.; Iooss, B.; Laurent, B.; Roustant, O., Calculations of sobol indices for the gaussian process metamodel. *Reliability Engineering & System Safety* **2009,** *94* (3), 742-751.
41. Antognini, A. B.; Zagoraiou, M., Exact optimal designs for computer experiments via Kriging metamodelling. *Journal of Statistical Planning and Inference* **2010,** *140* (9), 2607-2617.
42. Yin, J.; Ng, S. H.; Ng, K. M., Kriging metamodel with modified nugget-effect: The heteroscedastic variance case. *Computers & Industrial Engineering* **2011,** *61* (3), 760-777.
43. Zhou, Q.; Qian, P. Z. G.; Zhou, S. Y., A Simple Approach to Emulation for Computer Models With Qualitative and Quantitative Factors. *Technometrics* **2011,** *53* (3), 266-273.
44. Gramacy, R. B.; Lee, H. K., Bayesian treed Gaussian process models with an application to computer modeling. *Journal of the American Statistical Association* **2012**.
45. Roustant, O.; Ginsbourger, D.; Deville, Y., DiceKriging, DiceOptim: Two R Packages for the Analysis of Computer Experiments by Kriging-Based Metamodeling

and Optimization. *Journal of Statistical Software* **2012,** *51* (1), 1-55.
46. Kleijnen, J. P. C.; Mehdad, E., Multivariate versus univariate Kriging metamodels for multi-response simulation models. *Eur. J. Oper. Res.* **2014,** *236* (2), 573-582.
47. Peng, C. Y.; Wu, C. F. J., On the Choice of Nugget in Kriging Modeling for Deterministic Computer Experiments. *Journal of Computational and Graphical Statistics* **2014,** *23* (1), 151-168.
48. Cortes, C.; Vapnik, V., Support-vector networks. *Machine learning* **1995,** *20* (3), 273-297.
49. Smola, A. J.; Schölkopf, B., A tutorial on support vector regression. *Statistics and computing* **2004,** *14* (3), 199-222.
50. Keerthi, S. S.; Shevade, S. K.; Bhattacharyya, C.; Murthy, K. R. K., Improvements to Platt's SMO algorithm for SVM classifier design. *Neural Computation* **2001,** *13* (3), 637-649.
51. Suykens, J. A.; Vandewalle, J., Least squares support vector machine classifiers. *Neural processing letters* **1999,** *9* (3), 293-300.
52. Clarke, S. M.; Griebsch, J. H.; Simpson, T. W., Analysis of support vector regression for approximation of complex engineering analyses. *Journal of mechanical design* **2005,** *127* (6), 1077-1087.
53. Pan, F.; Zhu, P.; Zhang, Y., Metamodel-based lightweight design of B-pillar with TWB structure via support vector regression. *Computers & structures* **2010,** *88* (1), 36-44.
54. Eisenhower, B.; O'Neill, Z.; Narayanan, S.; Fonoberov, V. A.; Mezić, I., A methodology for meta-model based optimization in building energy models. *Energy and Buildings* **2012,** *47*, 292-301.
55. Liu, Y.; Pender, G., A flood inundation modelling using v-support vector machine regression model. *Engineering Applications of Artificial Intelligence* **2015,** *46*, 223-231.
56. Mirfenderesgi, G.; Mousavi, S. J., Adaptive meta-modeling-based simulation optimization in basin-scale optimum water allocation: a comparative analysis of meta-models. *Journal of Hydroinformatics* **2015**, jh2015157.
57. Friedman, J. H., Multivariate adaptive regression splines. *The annals of statistics* **1991**, 1-67.
58. Jin, R.; Chen, W.; Simpson, T. W., Comparative studies of metamodelling techniques under multiple modelling criteria. *Structural and Multidisciplinary Optimization* **2001,** *23* (1), 1-13.
59. Simpson, T. W.; Poplinski, J.; Koch, P. N.; Allen, J. K., Metamodels for computer-based engineering design: survey and recommendations. *Engineering with computers* **2001,** *17* (2), 129-150.
60. Khu, S.; Savic, D.; Liu, Y.; Madsen, H. In *A fast evolutionary-based metamodelling approach for the calibration of a rainfall-runoff model*, Trans. 2nd Biennial Meeting of the International Environmental Modelling and Software Society, iEMSs: Manno, Switzerland, Citeseer: 2004.
61. Schueremans, L.; Van Gemert, D., Benefit of splines and neural networks in simulation based structural reliability analysis. *Structural safety* **2005,** *27* (3), 246-261.
62. De Wilde, P.; Tian, W., Predicting the performance of an office under climate change: a study of metrics, sensitivity and zonal resolution. *Energy and Buildings* **2010,** *42* (10), 1674-1684.
63. Shahsavani, D.; Tarantola, S.; Ratto, M., Evaluation of MARS modeling technique for sensitivity analysis of model output. *Procedia-Social and Behavioral Sciences* **2010,** *2* (6), 7737-7738.
64. Costas, M.; Díaz, J.; Romera, L.; Hernández, S., A multi-objective surrogate-based

optimization of the crashworthiness of a hybrid impact absorber. *International Journal of Mechanical Sciences* **2014,** *88*, 46-54.
65. Mason, J.; Cox, M. In *Algorithms for approximation: based on the proceedings of the IMA Conference on Algorithms for the Approximation of Functions and Data, held at the Royal Military College of Science, Shrivenham, July 1985, volume 10 of The Institute of Mathematics and Its Applications conference, new series*, The Institute of Mathematics and Its Applications conference series, new series, 1987.
66. Kadirkamanathan, V.; Niranjan, M., A function estimation approach to sequential learning with neural networks. *Neural Computation* **1993,** *5* (6), 954-975.
67. Yingwei, L.; Sundararajan, N.; Saratchandran, P., A sequential learning scheme for function approximation using minimal radial basis function neural networks. *Neural computation* **1997,** *9* (2), 461-478.
68. Garcet, J. P.; Ordonez, A.; Roosen, J.; Vanclooster, M., Metamodelling: Theory, concepts and application to nitrate leaching modelling. *Ecological modelling* **2006,** *193* (3), 629-644.
69. Mullur, A. A.; Messac, A., Metamodeling using extended radial basis functions: a comparative approach. *Engineering with Computers* **2006,** *21* (3), 203-217.
70. Regis, R. G.; Shoemaker, C. A., A stochastic radial basis function method for the global optimization of expensive functions. *INFORMS Journal on Computing* **2007,** *19* (4), 497-509.
71. Kitayama, S.; Arakawa, M.; Yamazaki, K., Sequential approximate optimization using radial basis function network for engineering optimization. *Optimization and Engineering* **2011,** *12* (4), 535-557.
72. Gu, J.; Li, G.; Dong, Z., Hybrid and adaptive meta-model-based global optimization. *Engineering Optimization* **2012,** *44* (1), 87-104.
73. Farshidi, A.; Rakai, L.; Samimi, B.; Behjat, L.; Westwick, D., A new a priori net length estimation technique for integrated circuits using radial basis functions. *Computers & Electrical Engineering* **2013,** *39* (4), 1204-1218.
74. Cybenko, G., Approximation by superpositions of a sigmoidal function. *Mathematics of control, signals and systems* **1989,** *2* (4), 303-314.
75. Badiru, A. B.; Sieger, D. B., Neural network as a simulation metamodel in economic analysis of risky projects. *Eur. J. Oper. Res.* **1998,** *105* (1), 130-142.
76. Fonseca, D.; Navaresse, D.; Moynihan, G., Simulation metamodeling through artificial neural networks. *Engineering Applications of Artificial Intelligence* **2003,** *16* (3), 177-183.
77. El Tabach, E.; Lancelot, L.; Shahrour, I.; Najjar, Y., Use of artificial neural network simulation metamodelling to assess groundwater contamination in a road project. *Mathematical and computer modelling* **2007,** *45* (7), 766-776.
78. Gorissen, D.; Hendrickx, W.; Dhaene, T. In *Adaptive Global Metamodeling with Neural Networks*, ESANN, Citeseer: 2007; pp 187-192.
79. Kuo, Y.; Yang, T.; Peters, B. A.; Chang, I., Simulation metamodel development using uniform design and neural networks for automated material handling systems in semiconductor wafer fabrication. *Simulation Modelling Practice and Theory* **2007,** *15* (8), 1002-1015.
80. Chan, W.; Fu, M.; Lu, J., An integrated FEM and ANN methodology for metal-formed product design. *Engineering Applications of Artificial Intelligence* **2008,** *21* (8), 1170-1181.
81. Khosravi, A.; Nahavandi, S.; Creighton, D. In *Constructing prediction intervals for neural network metamodels of complex systems*, Neural Networks, 2009. IJCNN 2009. International Joint Conference on, IEEE: 2009; pp 1576-1582.

82. Li, Y.; Ng, S. H.; Xie, M.; Goh, T., A systematic comparison of metamodeling techniques for simulation optimization in decision support systems. *Applied Soft Computing* **2010,** *10* (4), 1257-1273.
83. Lönn, D.; Fyllingen, Ø.; Nilssona, L., An approach to robust optimization of impact problems using random samples and meta-modelling. *International Journal of Impact Engineering* **2010,** *37* (6), 723-734.
84. Hanspal, N. S.; Allison, B. A.; Deka, L.; Das, D. B., Artificial neural network (ANN) modeling of dynamic effects on two-phase flow in homogenous porous media. *Journal of Hydroinformatics* **2013,** *15* (2), 540-554.
85. Tøndel, K.; Vik, J. O.; Martens, H.; Indahl, U. G.; Smith, N.; Omholt, S. W., Hierarchical multivariate regression-based sensitivity analysis reveals complex parameter interaction patterns in dynamic models. *Chemometrics and Intelligent Laboratory Systems* **2013,** *120*, 25-41.
86. Behandish, M.; Wu, Z., Concurrent pump scheduling and storage level optimization using meta-models and evolutionary algorithms. *Procedia Engineering* **2014,** *70*, 103-112.
87. Conti, S.; O'Hagan, A., Bayesian emulation of complex multi-output and dynamic computer models. *Journal of statistical planning and inference* **2010,** *140* (3), 640-651.
88. Jolliffe, I., *Principal component analysis*. Wiley Online Library: 2002.
89. Jia, G.; Taflanidis, A. A., Kriging metamodeling for approximation of high-dimensional wave and surge responses in real-time storm/hurricane risk assessment. *Computer Methods in Applied Mechanics and Engineering* **2013,** *261*, 24-38.
90. Wang, K.; Chen, T.; Kwa, S. T.; Ma, Y.; Lau, R., Meta-modelling for fast analysis of CFD-simulated vapour cloud dispersion processes. *Computers & Chemical Engineering* **2014,** *69*, 89-97.
91. Arlot, S.; Celisse, A., A survey of cross-validation procedures for model selection. *Statistics surveys* **2010,** *4*, 40-79.
92. Goos, P.; Jones, B., *Optimal design of experiments: a case study approach*. John Wiley & Sons: 2011.
93. Myers, R. H.; Montgomery, D. C.; Anderson-Cook, C. M., *Response surface methodology: process and product optimization using designed experiments*. John Wiley & Sons: 2016.
94. Plackett, R. L.; Burman, J. P., The design of optimum multifactorial experiments. *Biometrika* **1946,** *33* (4), 305-325.
95. Hartley, H. O., Smallest composite designs for quadratic response surfaces. *Biometrics* **1959,** *15* (4), 611-624.
96. Lin, D. K., A new class of supersaturated designs. *Technometrics* **1993,** *35* (1), 28-31.
97. Draper, N. R.; Lin, D. K., Small response-surface designs. *Technometrics* **1990,** *32* (2), 187-194.
98. Allen, T. T.; Yu, L., Low - cost response surface methods from simulation optimization. *Quality and Reliability Engineering International* **2002,** *18* (1), 5-17.
99. Allen, T. T.; Yu, L.; Schmitz, J., An experimental design criterion for minimizing meta-model prediction errors applied to die casting process design. *Journal of the Royal Statistical Society: Series C (Applied Statistics)* **2003,** *52* (1), 103-117.
100. Echard, B.; Gayton, N.; Lemaire, M., AK-MCS: an active learning reliability method combining Kriging and Monte Carlo simulation. *Structural Safety* **2011,** *33* (2), 145-154.
101. Taguchi, G., Taguchi methods: design of experiments. American Supplier Institute. *Inc., MI* **1993**.

102. Fang, K.-T.; Lin, D. K.; Winker, P.; Zhang, Y., Uniform design: theory and application. *Technometrics* **2000,** *42* (3), 237-248.
103. McKay, M. D.; Beckman, R. J.; Conover, W. J., A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* **2000,** *42* (1), 55-61.
104. Ye, K. Q., Orthogonal column Latin hypercubes and their application in computer experiments. *Journal of the American Statistical Association* **1998,** *93* (444), 1430-1439.
105. Diwekar, U. M.; Kalagnanam, J. R., Efficient sampling technique for optimization under uncertainty. *AIChE Journal* **1997,** *43* (2), 440-447.
106. Morris, M. D.; Mitchell, T. J., Exploratory designs for computational experiments. *Journal of statistical planning and inference* **1995,** *43* (3), 381-402.
107. Cioppa, T. M.; Lucas, T. W., Efficient nearly orthogonal and space-filling Latin hypercubes. *Technometrics* **2012**.
108. Dennis, J.; Torczon, T. In *Approximation model management for optimization*, Proceedings of the Sixth AIAA/NASA/USAF Multidisciplinary Analysis & Optimization Symposium, 1996; pp 4-6.
109. Welch, W. J.; Buck, R. J.; Sacks, J.; Wynn, H. P.; Mitchell, T. J.; Morris, M. D., Screening, predicting, and computer experiments. *Technometrics* **1992,** *34* (1), 15-25.
110. Balabanov, V. O.; Giunta, A. A.; Golovidov, O.; Grossman, B.; Mason, W. H.; Watson, L. T.; Haftka, R. T., Reasonable design space approach to response surface approximation. *Journal of Aircraft* **1999,** *36* (1), 308-315.
111. Alexandrov, N. M.; Dennis Jr, J. E.; Lewis, R. M.; Torczon, V., A trust-region framework for managing the use of approximation models in optimization. *Structural optimization* **1998,** *15* (1), 16-23.
112. Wujek, B.; Renaud, J., New adaptive move-limit management strategy for approximate optimization, part 1. *AIAA journal* **1998,** *36* (10), 1911-1921.
113. Wujek, B.; Renaud, J., New adaptive move-limit management strategy for approximate optimization, part 2. *AIAA journal* **1998,** *36* (10), 1922-1934.
114. Wang, G. G., Adaptive response surface method using inherited latin hypercube design points. *Transactions-American Society of Mechanical Engineers Journal of Mechanical Design* **2003,** *125* (2), 210-220.
115. Wang, G. G.; Simpson, T., Fuzzy clustering based hierarchical metamodeling for design space reduction and optimization. *Engineering Optimization* **2004,** *36* (3), 313-335.
116. Chen, J.; Wong, D. S. H.; Jang, S. S.; Yang, S. L., Product and process development using artificial neural-network model and information analysis. *AIChE journal* **1998,** *44* (4), 876-887.
117. Tang, Q.; Lau, Y. B.; Hu, S.; Yan, W.; Yang, Y.; Chen, T., Response surface methodology using Gaussian processes: towards optimizing the trans-stilbene epoxidation over Co 2+–NaX catalysts. *Chemical Engineering Journal* **2010,** *156* (2), 423-431.
118. Chi, G.; Hu, S.; Yang, Y.; Chen, T., Response surface methodology with prediction uncertainty: A multi-objective optimisation approach. *Chemical engineering research and design* **2012,** *90* (9), 1235-1244.
119. Jones, D. R.; Schonlau, M.; Welch, W. J., Efficient global optimization of expensive black-box functions. *Journal of Global optimization* **1998,** *13* (4), 455-492.
120. Lu, J.; Gao, F., Process modeling based on process similarity. *Industrial & Engineering Chemistry Research* **2008,** *47* (6), 1967-1974.
121. Lu, J.; Gao, F., Model migration with inclusive similarity for development of a

new process model. *Industrial & Engineering Chemistry Research* **2008,** *47* (23), 9508-9516.
122. Lu, J.; Yao, Y.; Gao, F., Model migration for development of a new process model. *Industrial & Engineering Chemistry Research* **2008,** *48* (21), 9603-9610.
123. Lu, J.; Yao, K.; Gao, F., Process similarity and developing new process models through migration. *AIChE journal* **2009,** *55* (9), 2318-2328.
124. Feudale, R. N.; Woody, N. A.; Tan, H.; Myles, A. J.; Brown, S. D.; Ferré, J., Transfer of multivariate calibration models: a review. *Chemometrics and Intelligent Laboratory Systems* **2002,** *64* (2), 181-192.
125. Yan, W.; Hu, S.; Yang, Y.; Gao, F.; Chen, T., Bayesian migration of Gaussian process regression for rapid process modeling and optimization. *Chemical engineering journal* **2011,** *166* (3), 1095-1103.
126. Luo, L.; Yao, Y.; Gao, F., Bayesian improved model migration methodology for fast process modeling by incorporating prior information. *Chemical Engineering Science* **2015,** *134*, 23-35.
127. Luo, L.; Yao, Y.; Gao, F., Iterative improvement of parameter estimation for model migration by means of sequential experiments. *Computers & Chemical Engineering* **2015,** *73*, 128-140.
128. Luo, L.; Yao, Y.; Gao, F., Cost-effective process modeling and optimization methodology assisted by robust migration techniques. *Industrial & Engineering Chemistry Research* **2015,** *54* (21), 5736-5748.
129. Shen, W. J.; Davis, T.; Lin, D. K. J.; Nachtsheim, C. J., Dimensional Analysis and Its Applications in Statistics. *J. Qual. Technol.* **2014,** *46* (3), 185-198.
130. Kennedy, M. C.; O'Hagan, A., Predicting the output from a complex computer code when fast approximations are available. *Biometrika* **2000,** *87* (1), 1-13.
131. Cumming, J. A.; Goldstein, M., Bayes linear uncertainty analysis for oil reservoirs based on multiscale computer experiments. *O'Hagan, West, AM (eds.) The Oxford Handbook of Applied Bayesian Analysis* **2009**, 241-270.
132. Han, Z.-H.; Zimmermann, R.; Görtz, S., A new cokriging method for variable-fidelity surrogate modeling of aerodynamic data. *AIAA Paper* **2010,** *1225*, 2010.
133. Joshi, Y., Reduced order thermal models of multiscale microsystems. *Journal of Heat Transfer* **2012,** *134* (3), 031008.
134. Goh, J.; Bingham, D.; Holloway, J. P.; Grosskopf, M. J.; Kuranz, C. C.; Rutter, E., Prediction and computer model calibration using outputs from multifidelity simulators. *Technometrics* **2013,** *55* (4), 501-512.
135. Xiong, S.; Qian, P. Z.; Wu, C. J., Sequential design and analysis of high-accuracy and low-accuracy computer codes. *Technometrics* **2013,** *55* (1), 37-46.
136. Tuo, R.; Wu, C. J.; Yu, D., Surrogate modeling of computer experiments with different mesh densities. *Technometrics* **2014,** *56* (3), 372-380.
137. Yang, J.; Liu, M.-Q.; Lin, D. K., Construction of nested orthogonal Latin hypercube designs. *Statistica Sinica* **2014,** *24* (1).
138. He, X.; Tuo, R.; Wu, C. J., Optimization of multi-fidelity computer experiments via the EQIE criterion. *Technometrics* **2016,** (just-accepted), 1-34.
139. Chuang, Y.-C.; Chan, C.-H.; Chen, T.; Yao, Y.; Wong, D. S. H., Surrogate model calibration for computational fluid dynamics (CFD) using Bayesian migration. In *The 7th International Symposium on Design, Operation & Control of Chemical Processes (PSE Asia 2016)*, Tokyo, Japan, 2016; p No. 78.
140. Palmer, K.; Realff, M., Optimization and validation of steady-state flowsheet simulation metamodels. *Chemical Engineering Research & Design* **2002,** *80* (A7), 773-782.

141. Henao, C. A.; Maravelias, C. T., Surrogate-based superstructure optimization framework. *AIChE Journal* **2011,** *57* (5), 1216-1232.
142. Wright, M. M.; Román-Leshkov, Y.; Green, W. H., Investigating the techno-economic trade-offs of hydrogen source using a response surface model of drop-in biofuel production via bio-oil upgrading. *Biofuels, Bioproducts and Biorefining* **2012,** *6* (5), 503-520.
143. Fahmi, I.; Cremaschi, S., Process synthesis of biodiesel production plant using artificial neural networks as the surrogate models. *Computers & Chemical Engineering* **2012,** *46*, 105-123.
144. Ochoa-Estopier, L. M.; Jobson, M.; Smith, R., The use of reduced models for design and optimisation of heat-integrated crude oil distillation systems. *Energy* **2014,** *75*, 5-13.
145. Chu, J.-Z.; Shieh, S.-S.; Jang, S.-S.; Chien, C.-I.; Wan, H.-P.; Ko, H.-H., Constrained optimization of combustion in a simulated coal-fired boiler using artificial neural network model and information analysis☆. *Fuel* **2003,** *82* (6), 693-703.
146. Kusiak, A.; Song, Z., Combustion efficiency optimization and virtual testing: A data-mining approach. *Industrial Informatics, IEEE Transactions on* **2006,** *2* (3), 176-184.
147. Zheng, L.; Zhou, H.; Wang, C.; Cen, K., Combining support vector regression and ant colony optimization to reduce NOx emissions in coal-fired utility boilers. *Energy & Fuels* **2008,** *22* (2), 1034-1040.
148. Li, S.; Feng, L.; Benner, P.; Seidel-Morgenstern, A., Using surrogate models for efficient optimization of simulated moving bed chromatography. *Computers & Chemical Engineering* **2014,** *67*, 121-132.
149. Beck, J.; Friedrich, D.; Brandani, S.; Fraga, E. S., Multi-objective optimisation using surrogate models for the design of VPSA systems. *Computers & Chemical Engineering* **2015,** *82*, 318-329.
150. Gutiérrez-Antonio, C.; Briones-Ramírez, A., Multiobjective Stochastic Optimization of Dividing-wall Distillation Columns Using a Surrogate Model Based on Neural Networks. *Chemical and Biochemical Engineering Quarterly* **2016,** *29* (4), 491-504.
151. Nuchitprasittichai, A.; Cremaschi, S., An algorithm to determine sample sizes for optimization with artificial neural networks. *AIChE Journal* **2013,** *59* (3), 805-812.
152. Wiltowski, T.; Piotrowski, K.; Lorethova, H.; Stonawski, L.; Mondal, K.; Lalvani, S., Neural network approximation of iron oxide reduction process. *Chemical Engineering and Processing: Process Intensification* **2005,** *44* (7), 775-783.
153. Chang, J.-S.; Lee, Y.-P.; Wang, R.-C., Optimization of nanosized silver particle synthesis via experimental design. *Industrial & engineering chemistry research* **2007,** *46* (17), 5591-5599.
154. Chang, J.-S.; Lee, J.-T.; Chang, A.-C., Neural-network rate-function modeling of submerged cultivation of Monascus anka. *Biochemical Engineering Journal* **2006,** *32* (2), 119-126.
155. Chen, J.; Jang, S.-S.; Wong, D. S. H.; Ma, C.-C. M.; Lin, J.-M., Optimal design of filament winding using neural network experimental design scheme. *Journal of Composite Materials* **1999,** *33* (24), 2281-2300.
156. Chen, J.; Chu, P. P.-T.; Wong, D. S. H.; Jang, S.-S., Optimal design using neural network and information analysis in plasma etching. *Journal of Vacuum Science & Technology B* **1999,** *17* (1), 145-153.
157. Liau, L.-K.; Huang, C.-J.; Chen, C.-C.; Huang, C.-S.; Chen, C.-T.; Lin, S.-C.; Kuo,

L.-C., Process modeling and optimization of PECVD silicon nitride coated on silicon solar cell using neural networks. *Solar energy materials and solar cells* **2002,** *71* (2), 169-179.
158. Chuang, Y.-C.; Chen, C.-T., Mathematical modeling and optimal design of an MOCVD reactor for GaAs film growth. *Journal of the Taiwan Institute of Chemical Engineers* **2014,** *45* (1), 254-267.
159. Qian, P. Z.; Wu, H.; Wu, C. J., Gaussian process models for computer experiments with qualitative and quantitative factors. *Technometrics* **2012**.
160. Qian, P. Z.; Wu, C. J., Sliced space-filling designs. *Biometrika* **2009,** *96* (4), 945-956.
161. Zhang, G. P., Time series forecasting using a hybrid ARIMA and neural network model. *Neurocomputing* **2003,** *50*, 159-175.
162. Chen, S., Nonlinear time series modelling and prediction using Gaussian RBF networks with enhanced cllustering and RLS learning. *Electronics letters* **1995,** *31* (2), 117-118.
163. Sapankevych, N. I.; Sankar, R., Time series prediction using support vector machines: a survey. *Computational Intelligence Magazine, IEEE* **2009,** *4* (2), 24-38.
164. Wang, J.; Hertzmann, A.; Blei, D. M. In *Gaussian process dynamical models*, Advances in neural information processing systems, 2005; pp 1441-1448.
165. Joseph, B.; Hanratty, F. W., Predictive control of quality in a batch manufacturing process using artificial neural network models. *Industrial & engineering chemistry research* **1993,** *32* (9), 1951-1961.
166. Desai, K.; Badhe, Y.; Tambe, S. S.; Kulkarni, B. D., Soft-sensor development for fed-batch bioreactors using support vector regression. *Biochemical Engineering Journal* **2006,** *27* (3), 225-239.
167. Gonzaga, J.; Meleiro, L.; Kiang, C.; Maciel Filho, R., ANN-based soft-sensor for real-time process monitoring and control of an industrial polymerization process. *Computers & Chemical Engineering* **2009,** *33* (1), 43-49.
168. Liu, G.; Zhou, D.; Xu, H.; Mei, C., Model optimization of SVM for a fermentation soft sensor. *Expert Systems with Applications* **2010,** *37* (4), 2708-2713.
169. Ge, Z.; Chen, T.; Song, Z., Quality prediction for polypropylene production process based on CLGPR model. *Control Engineering Practice* **2011,** *19* (5), 423-432.
170. Yu, J., Online quality prediction of nonlinear and non-Gaussian chemical processes with shifting dynamics using finite mixture model based Gaussian process regression approach. *Chemical engineering science* **2012,** *82*, 22-30.
171. Nahas, E.; Henson, M.; Seborg, D., Nonlinear internal model control strategy for neural network models. *Computers & Chemical Engineering* **1992,** *16* (12), 1039-1057.
172. Willis, M. J.; Montague, G. A.; Di Massimo, C.; Tham, M. T.; Morris, A., Artificial neural networks in process estimation and control. *Automatica* **1992,** *28* (6), 1181-1187.
173. Kocijan, J.; Murray-Smith, R.; Rasmussen, C. E.; Girard, A. In *Gaussian process model based predictive control*, American Control Conference, 2004. Proceedings of the 2004, IEEE: 2004; pp 2214-2219.
174. Tsen, A. Y. D.; Jang, S. S.; Wong, D. S. H.; Joseph, B., Predictive control of quality in batch polymerization using hybrid ANN models. *AIChE Journal* **1996,** *42* (2), 455-465.
175. Ng, C.; Hussain, M., Hybrid neural network—prior knowledge model in temperature control of a semi-batch polymerization process. *Chemical Engineering and Processing: Process Intensification* **2004,** *43* (4), 559-570.
176. Fullana, M.; Trabelsi, F.; Recasens, F., Use of neural net computing for statistical

and kinetic modelling and simulation of supercritical fluid extractors. *Chemical engineering science* **1999,** *54* (24), 5845-5862.
177. Cho, Y.; Joseph, B., Reduced - order steady - state and dynamic models for separation processes. Part I. Development of the model reduction procedure. *AIChE journal* **1983,** *29* (2), 261-269.
178. Dochain, D.; Babary, J.-P.; Tali-Maamar, N., Modelling and adaptive control of nonlinear distributed parameter bioreactors via orthogonal collocation. *Automatica* **1992,** *28* (5), 873-883.
179. Huang, R.; Zavala, V. M.; Biegler, L. T., Advanced step nonlinear model predictive control for air separation units. *Journal of Process Control* **2009,** *19* (4), 678-685.
180. Chen, Z.; Henson, M. A.; Belanger, P.; Megan, L., Nonlinear model predictive control of high purity distillation columns for cryogenic air separation. *Control Systems Technology, IEEE Transactions on* **2010,** *18* (4), 811-821.
181. Lee, J. M.; Lee, J. H., Approximate dynamic programming-based approaches for input–output data-driven control of nonlinear processes. *Automatica* **2005,** *41* (7), 1281-1288.
182. Lee, J. M.; Kaisare, N. S.; Lee, J. H., Choice of approximator and design of penalty function for an approximate dynamic programming based control approach. *Journal of process control* **2006,** *16* (2), 135-156.
183. O'Hagan, A.; Kingman, J., Curve fitting and optimal design for prediction. *Journal of the Royal Statistical Society. Series B (Methodological)* **1978**, 1-42.
184. Kennedy, M. C.; O'Hagan, A., Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **2001,** *63* (3), 425-464.
185. Wilkinson, R. D., Bayesian calibration of expensive multivariate computer experiments. *Large-Scale Inverse Problems and Quantification of Uncertainty* **2010**, 195-215.
186. Rougier, J., Efficient emulators for multivariate deterministic functions. *Journal of Computational and Graphical Statistics* **2008,** *17* (4), 827-843.
187. McFarland, J.; Mahadevan, S.; Romero, V.; Swiler, L., Calibration and uncertainty analysis for computer simulations with multivariate output. *AIAA journal* **2008,** *46* (5), 1253-1265.
188. Bhat, K. S.; Haran, M.; Goes, M., Computer model calibration with multivariate spatial output: A case study. *Frontiers of Statistical Decision Making and Bayesian Analysis* **2010**, 168-184.
189. Paulo, R.; García-Donato, G.; Palomo, J., Calibration of computer models with multivariate output. *Computational Statistics & Data Analysis* **2012,** *56* (12), 3959-3974.
190. Manfren, M.; Aste, N.; Moshksar, R., Calibration and uncertainty analysis for computer models–a meta-model based approach for integrated building energy simulation. *Applied energy* **2013,** *103*, 627-641.
191. Broad, D.; Dandy, G. C.; Maier, H. R., Water distribution system optimization using metamodels. *Journal of Water Resources Planning and Management* **2005,** *131* (3), 172-180.
192. Yazdi, J.; Neyshabouri, S. S., Adaptive surrogate modeling for optimization of flood control detention dams. *Environmental Modelling & Software* **2014,** *61*, 106-120.
193. Broad, D. R.; Dandy, G. C.; Maier, H. R., A systematic approach to determining metamodel scope for risk-based optimization and its application to water distribution system design. *Environmental Modelling & Software* **2015,** *69*, 382-395.
194. Yu, C. J.; Chen, Y. Y.; Peng, S. C.; Wong, D. S. H.; Chuang, Y. J., Core network

identification using parametric sensitivity and multi-way principal component analysis in NFkB signaling network. *Journal of the Taiwan Institute of Chemical Engineers* **2013,** *44* (5), 724-733.
195. Sobol, I. M., Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Mathematics and computers in simulation* **2001,** *55* (1), 271-280.
196. Cukier, R.; Fortuin, C.; Shuler, K. E.; Petschek, A.; Schaibly, J., Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I Theory. *The Journal of chemical physics* **1973,** *59* (8), 3873-3878.
197. McRae, G. J.; Tilden, J. W.; Seinfeld, J. H., Global sensitivity analysis—a computational implementation of the Fourier amplitude sensitivity test (FAST). *Computers & Chemical Engineering* **1982,** *6* (1), 15-25.
198. Sobol, I. M., Theorems and examples on high dimensional model representation. *Reliability Engineering & System Safety* **2003,** *79* (2), 187-193.
199. Xiu, D.; Karniadakis, G. E., Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of computational physics* **2003,** *187* (1), 137-167.
200. Crestaux, T.; Le Maıˆtre, O.; Martinez, J.-M., Polynomial chaos expansion for sensitivity analysis. *Reliability Engineering & System Safety* **2009,** *94* (7), 1161-1172.
201. Saltelli, A.; Annoni, P.; Azzini, I.; Campolongo, F.; Ratto, M.; Tarantola, S., Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. *Computer Physics Communications* **2010,** *181* (2), 259-270.
202. Janon, A.; Klein, T.; Lagnoux, A.; Nodet, M.; Prieur, C., Asymptotic normality and efficiency of two Sobol index estimators. *ESAIM: Probability and Statistics* **2014,** *18*, 342-364.
203. Koda, M.; Mcrae, G. J.; Seinfeld, J. H., Automatic sensitivity analysis of kinetic mechanisms. *International Journal of Chemical Kinetics* **1979,** *11* (4), 427-444.
204. Saltelli, A.; Ratto, M.; Tarantola, S.; Campolongo, F., Sensitivity analysis for chemical models. *Chemical reviews* **2005,** *105* (7), 2811-2828.
205. Kiparissides, A.; Kucherenko, S.; Mantalaris, A.; Pistikopoulos, E., Global sensitivity analysis challenges in biological systems modeling. *Industrial & Engineering Chemistry Research* **2009,** *48* (15), 7168-7180.
206. Lucay, F.; Cisternas, L.; Gálvez, E., Global sensitivity analysis for identifying critical process design decisions. *Chemical Engineering Research and Design* **2015,** *103*, 74-83.
207. Carrero, E.; Queipo, N. V.; Pintos, S.; Zerpa, L. E., Global sensitivity analysis of Alkali–Surfactant–Polymer enhanced oil recovery processes. *Journal of Petroleum Science and Engineering* **2007,** *58* (1), 30-42.