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## Implementation of Sobol's Method of Global Sensitivity Analysis to a Compressor Simulation Model

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### ABSTRACT

Most simulation models are complex and nonlinear and so global sensitivity analysis is becoming a popular choice to predict the performance characteristics and behavior of the model. Global sensitivity analysis methods are generally variance-based methods that greatly rely on sampling methods and input parameter distribution. These methods don't rely on linearity or monotonicity of the model and can be applied to a diverse range of problem. Sobol's method—a variance based global sensitivity analysis method is applied to a nonlinear function to highlight and outline the implementation details of the method. It is used to calculate the sensitivities of the input parameter on the model output. The method is then applied to a reciprocating compressor model to determine the sensitivity of gas pulsation to suction manifold design parameters, namely radius, width and depth. The same method can be readily applied to any compressor simulation model.

### 1. INTRODUCTION

Compressor simulation models have inherent uncertainties associated with the input parameters and the output at times can be quite sensitive to the chosen set of input parameters. Most of the uncertainty and sensitivity analysis studies presented in literature assume an underlying model linearity and are focused on varying one parameter at a time. Local sensitivity analysis methods are usually focused on determining the behavior of the model around some local points (Saltelli et al., 2000). The most commonly used local sensitivity methods are screening design or one-at-a-time (OAT) techniques (Iman, 1986) and differential analysis (DA) (Iman, 1986). However, compressor models are generally nonlinear, and at times there could be interaction between the different parameters. In such situations, global sensitivity analysis methods, generally based on the decomposition of variance, are a better approach. Unlike local sensitivity analysis methods, global sensitivity analysis methods vary all variables simultaneously and each variable is varied through its entire range. The main motivation for applying the variance-based methods as opposed to regression based methods is that variance-based methods do not make any prior assumptions about the linearity or the monotonicity of the input-output relationship and, thus, these methods are applicable to models of any kind (Zheng and Rundell, 2006). Recently sensitivity analysis methods are also becoming increasingly popular in the area of compressor simulation models and many new sensitivity analysis techniques have been developed lately Bilal (2011) and (Bilal, et al., 2006). Bilal used Sobol's method of global sensitivity analysis to calculate the first order effects and total effects of the suction manifold parameters of a reciprocating compressor.

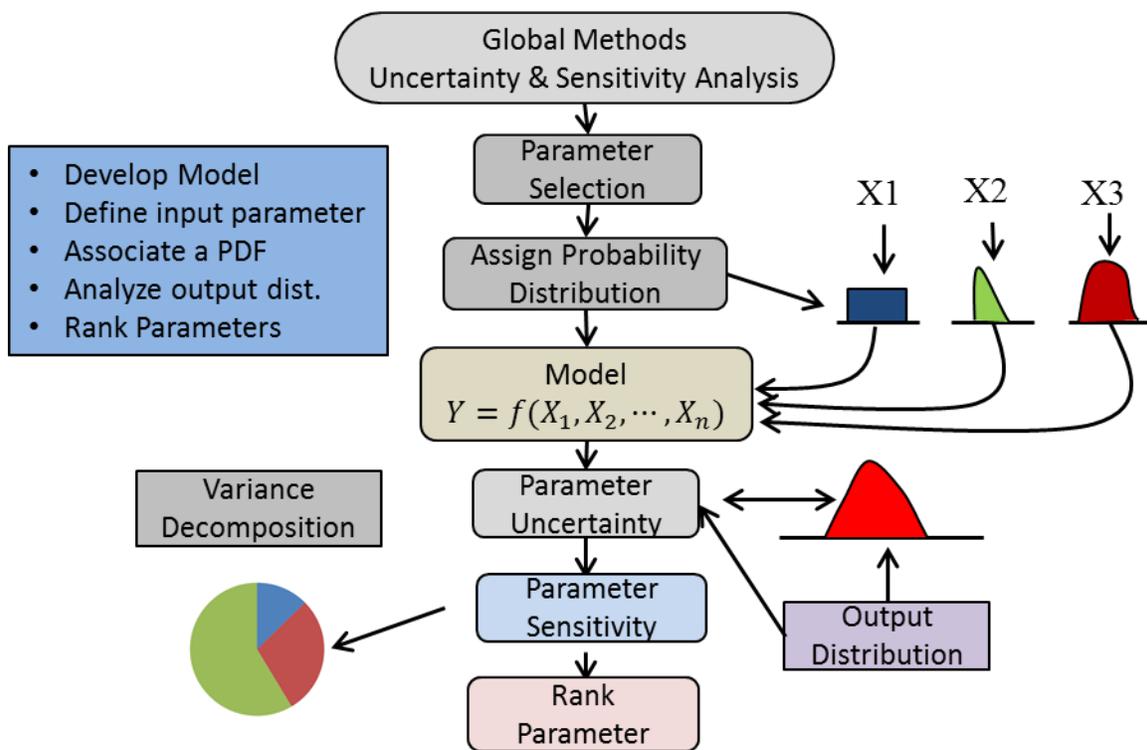
The focus of this paper is to highlight the importance of global sensitivity analysis methods, provide a clear and simple approach to implement it to any compressor simulation model for sensitivity analysis. In particular, Sobol's method of sensitivity analysis has been chosen to show the stepwise implementation details applied to a simple function and calculating its first order effect and total effects. The method is then applied to a simulation model of a multi-cylinder reciprocating compressor (Park et al., 2007) and (Park & et al., 2008), and the effects of sensitivities of the design parameter on gas pulsation are studied.

## 2. GLOBAL SENSITIVITY ANALYSIS

Sensitivity analysis has been defined (Saltelli et al., 2000) as “the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variations, and of how the given model depends upon the information fed into it.”

A schematic of the global methods of sensitivity analysis process is shown in Figure 1. To perform global sensitivity analysis the following steps are implemented:

1. Parameters are selected and probabilities and distributions are assigned to all parameters.
2. A set of random input vectors is generated from the associated probability distribution for each parameter.
3. The model is evaluated for each set of input vectors.
4. The uncertainty of the output distribution is determined.
5. Sensitivity analysis is used to rank the input parameters according to their influence on the output.



**Figure 1:** Schematic for global sensitivity analysis

## 3. VARIANCE BASED SENSITIVITY ANALYSIS METHODS

Global sensitivity analysis methods are variance-based methods and rely heavily on sampling methods and input parameter distribution. The concept of using variance as an indicator of the importance of an input parameter is the basis for many variance-based sensitivity analysis methods. The importance of the given input factor can be measured by a term defined as the sensitivity index, which is the fractional contribution to the output variance due to uncertainties in the inputs. While there are many methods available for analyzing the decomposition of variance as a sensitivity measure, the Method of Sobol (Sobol, 2001) is used to show the steps involved in implementing the

equations. This method is one of the most established and widely used methods and is capable of computing the ‘Total Sensitivity Indices’ (TSI), which measures the main effects of a given parameter and all the interactions (of any order) involving that parameter (Sobol, 1993). For example, if there are three input parameters, A, B, and C, then the total effect of parameter A on the output is,

$$TS(A) = S(A) + S(AB) + S(AC) + S(ABC) \quad (1)$$

where  $TS(i)$  is the total sensitivity index of parameter  $i$ , and  $S(A)$  denotes the first order sensitivity index for parameter A,  $S(A_j)$  denotes the second-order sensitivity index for the parameter A and j (*for j* ( $\neq A$ )), i.e. the interaction between parameters A and  $j(\neq A)$ , and so on.

### 3.1 Variance Based Sensitivity Analysis

Before explaining Sobol’s method, a general method capable of measuring only the first-order effects is explained below. Most of the variance-based methods depend on the estimation of the following quantity

$$\frac{Var_X[E(Y|X)]}{Var(Y)}$$

Where  $Y$  denotes the output variable,  $X$  denotes an input variable,  $E(Y|X)$  denotes the expectation of  $Y$  conditional on a fixed value of  $X$ , and the variance is taken over all possible values of  $X$ , and  $V(Y)$  is total output variance of the output  $Y$ .

## 4. SOBOL’S METHOD OF SENSITIVITY ANALYSIS

Sobol’s method uses the decomposition of variance to calculate the Sobol’s sensitivity indexes (Sobol, 1993). The basis of the method is the decomposition of the model output function  $y = f(x)$  into summands of variance using combinations of input parameters in increasing dimensionality. This method was used to perform the sensitivity analysis of the suction manifold of a compressor (Bilal, 2011). The Sobol’s method is explained below following the procedure outlined in (Sobol, 1993) .

To determine the sensitivity of the output  $Y$  to the variation of an input parameter, an input factor space,  $\Omega^k = (x|0 \leq x_i \leq 1; i = 1, \dots, k)$ , is defined. The main idea behind Sobol’s approach for computation of sensitivity indices is the decomposition of the function  $f(x)$  into summands of increasing dimensionality, namely

$$f(x_1, \dots, x_k) = f_0 + \sum_{i=1}^k f_i(x_i) + \sum_{1 \leq i < j \leq k} f_{ij}(x_i, x_j) + \dots + f_{1,2,\dots,k}(x_1, \dots, x_k). \quad (2)$$

For (2) to hold,  $f_0$  must be a constant, and the integrals of every summand over any of its own variables must be zero, i.e.,

$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_k} = 0, \text{ if } 1 \leq k \leq s \quad (3)$$

A consequence of (2) and (3) is that all summands in (1) are orthogonal, i.e. *if*  $(i_1, \dots, i_s) \neq (j_1, \dots, j_l)$ , then

$$\int_{\Omega^k} f_{i_1, \dots, i_s} f_{j_1, \dots, j_l} dx = 0 \quad (4)$$

Since at least one of the indices will not be repeated, the corresponding integral will vanish due to (3). Another consequence is that

$$f_0 = \int_{\Omega^k} f(x) dx \quad (5)$$

It was showed in (Sobol, 1993) that the decomposition was unique and that all the elements in (1) can be calculated through multidimensional integrals, namely

$$f_i(x_i) = -f_0 + \int_0^1 \cdots \int_0^1 f(x) dx_{\sim i}, \quad (6)$$

$$f_{ij}(x_i, x_j) = -f_0 - f_i(x_j) - f_j(x_i) + \int_0^1 \cdots \int_0^1 f(x) dx_{\sim (ij)}, \quad (7)$$

where the convention is used that  $dx_{\sim i}, dx_{\sim (ij)}$  denotes the integration over all variables except  $x_i$ , and  $x_i$  and  $x_j$ , respectively. Similar formulae can be obtained for higher-order terms.

The total variance  $D$  of  $f(x)$  is defined to be

$$D = \int_{\Omega^k} f^2(x) - f_0^2, \quad (8)$$

The partial variances for each of the terms in (1) can be computed

$$D_{i_1, \dots, i_s} = \int_0^1 \cdots \int_0^1 f_{i_1, \dots, i_s}^2(x_{i_1}, \dots, x_{i_s}) dx_{i_1}, \dots, dx_{i_s} \quad (9)$$

where  $1 \leq i_1 < \dots < i_s \leq k$  and  $s = 1, \dots, k$ . By squaring and integrating (2) over  $k$ , and by (4), the following is obtained:

$$D = \sum_{i=1}^k D_i + \sum_{1 \leq i < j \leq k} D_{ij} + \cdots + D_{1,2,\dots,k}. \quad (10)$$

Hence, the sensitivity measures  $S(i_1, \dots, i_s)$  are defined as

$$S_{i_1, \dots, i_s} = \frac{D_{i_1, \dots, i_s}}{D}, \text{ for } 1 \leq i_1 < \dots < i_s \leq k, \quad (11)$$

where  $S_i$  is called the first-order sensitivity index for factor  $x_i$ , which measures the main effects of  $x_i$  on the output, i.e. the partial contribution of  $x_i$  to the variance of  $f(x)$ . Similarly,  $S_{ij}$ , for  $i \neq j$ , is called the second-order sensitivity index, which measures the effects of interactions between  $x_i$  and  $x_j$ , and so on. The decomposition in (9) has the useful property that all the terms in (10) sum to 1; that is,

$$\sum_{i=1}^k S_i + \sum_{1 \leq i < j \leq k} S_{ij} + \cdots + S_{1,2,\dots,k} = 1. \quad (12)$$

In practice, Sobol's method is relatively easy to implement using Monte Carlo based integration. Sobol's first order and total effect sensitivity indices can be implemented relatively easily if equation (5), (8), and (9) are expressed in a discrete form as shown below by equations (13), (14), and (15) and detailed in (Zheng & Rundell, 2006). Similarly, the equation (15) to compute the total effect is also taken from (Zheng & Rundell, 2006).

$$f_0 = \int f(x) dx \approx \frac{1}{N} \sum_{k=1}^N f(x_k), \quad (13)$$

$$D = \int f^2(x)dx - f_0^2 \approx \frac{1}{N} \sum_{k=1}^N f^2(x_k) - f_0^2 \quad (14)$$

$$D_i = D - \frac{1}{2} [f(x) - f(x_i, x'_{-i})]^2 dx dx'_{-i} \approx D - \frac{1}{2N} \sum_{k=1}^N [f(x_k) - f(x_{ik} - x'_{-ik})]^2 \quad (15)$$

$$D_i^{tot} = \frac{1}{2} \int [f(x) - f(x'_i, x_i)]^2 dx dx'_i \approx \frac{1}{2N} \sum_{k=1}^N [f(x_k) - f(x'_{ik}, x_{-ik})]^2 \quad (16)$$

where  $N$  is the sampling size for Monte Carlo discretization, and  $x_{-1} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_m)$  is the parameter combination complementary to  $x_i$ .

## 5. IMPLEMENTATION OF SOBOL'S METHODS OF SENSITIVITY ANALYSIS APPLIED TO A SIMPLE MODEL

To elaborate the procedure to implement the Sobol's method of sensitivity analysis, a trial function is chosen and step outline above the explained stepwise.

Let the trial function be

$$f(x) = x_1 + x_2 x_3^2 \quad (17)$$

### 5.1 Steps for implementation

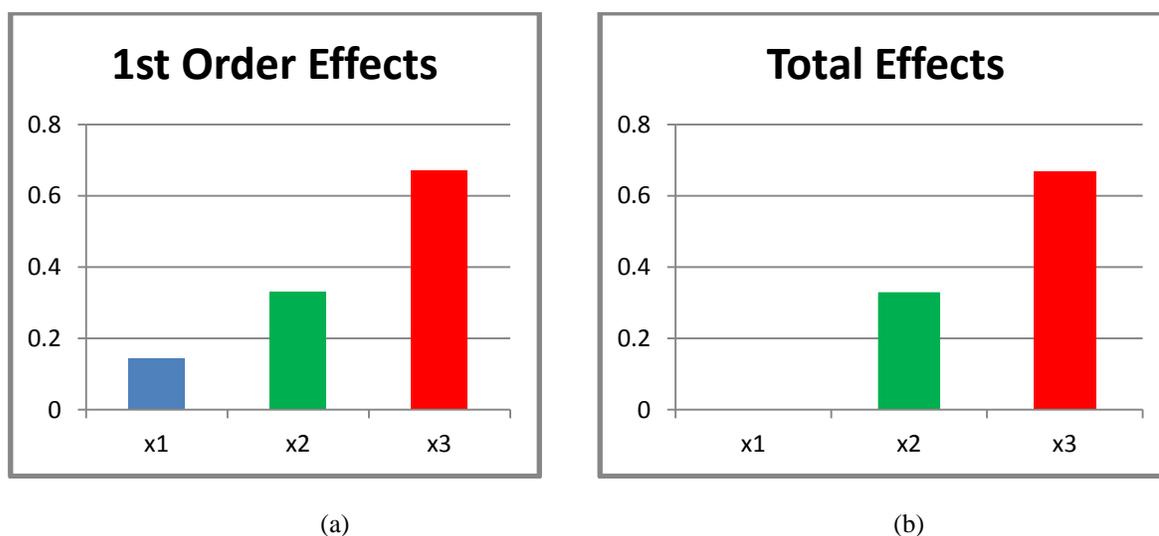
1. Select the total number of simulations to be performed.
2. Select the parameters for sensitivity analysis. In this case these are  $x_1$ ,  $x_2$ , and  $x_3$ .
3. Assume ranges for test variables:  $x_1 = [1, 1000]$ ;  $x_2 = [1, 100]$ ; and  $x_3 = [1, 10]$ ;
4. Choose a distribution for each of the parameters. In this case a uniform distribution is chosen for all three parameters.
5. Calculate the mean and variance of the parameters using equations (13) and (14).
6. Compute the partial variance or first order effects for each parameter by fixing the values of that parameter and varying the remaining parameters. Note that two parameter spaces i.e. primary and complementary parameter spaces are needed to implement equations (15)
7. Compute total sensitivity effects for the three parameters using (16).
8. Sort the parameter according to their sensitivities. The complete simulation code written in Matlab<sup>®</sup> is attached in the appendix.

## 6. RESULTS

The trial function was calculated for 1000 iterations and the first order effects and the total effects of the parameters are shown in Table 1. It was found that parameter  $x_1$  was the least sensitive parameter and  $x_3$  was found to be the most sensitive parameter. In terms of total effects, the similar behavior was seen and also plotted in Figure 2. It is also seen from Figure 2 that the total effects of  $x_1$  are quite close to zero, i.e. there is not much interaction going on between  $x_1$  and other parameters.

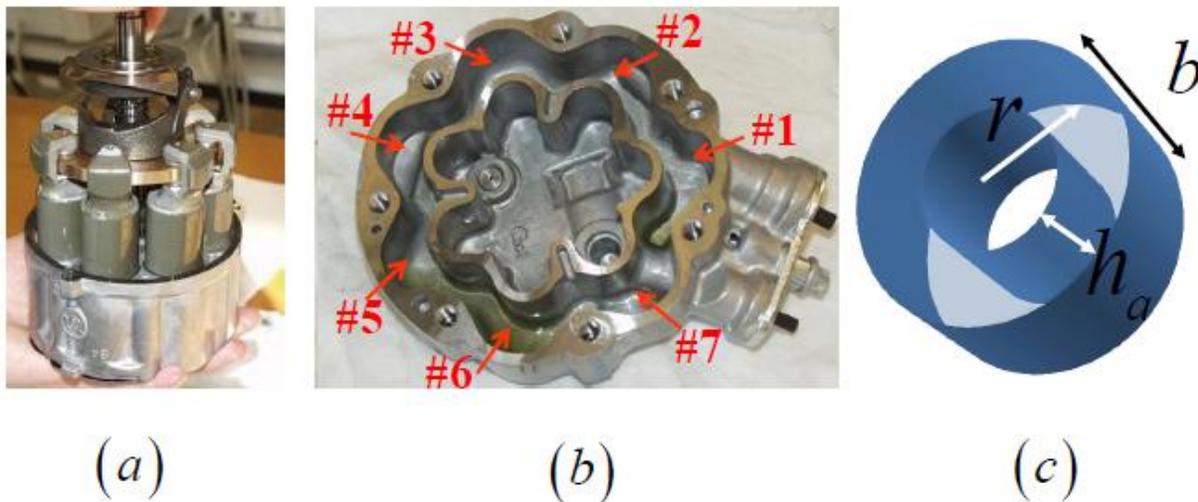
**Table 1:** First order effects and the total effect

Parameters	1st Order Effects	Total Effects
x1	0.1446	0.0004
x2	0.33	0.3297
x3	0.6713	0.6694

**Figure 2:** First order effects (a) and total effects (b) of the three parameters using Sobol's method of Sensitivity Analysis.

## 7. APPLICATION OF SOBEL'S METHOD TO A COMPRESSOR MODEL

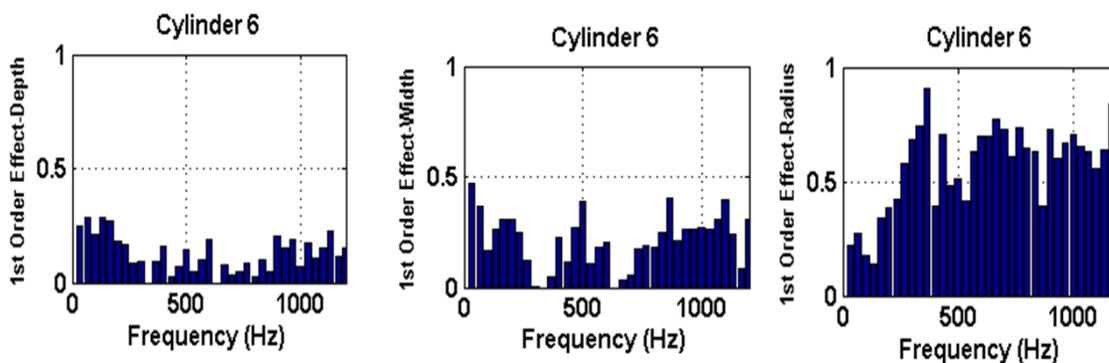
Sobel's method of sensitivity analysis was applied to a compressor simulation model, the details of which can be found in (Bilal, 2011) and (Park, 2004). The objective was to determine the sensitivity of gas pulsations to the design parameters of the suction manifold. The actual suction manifold is shown in Figure 3. The design parameters that were varied are shown in Table 2. Sobol's method of sensitivity analysis as described above was applied to the model of the simplified suction manifold. First order effects and total effects of the gas pulsation due to changes in the suction manifold radius, width and depth were calculated. It was shown that the suction manifold pressure response was most sensitive to changes in manifold radius, followed by manifold width and depth. Figure 4 shows the first order effect of parameter variation on the gas pulsation in the suction manifold at valve location 6. It shows the effects of gas pulsation in the frequency range of 0-1200 Hz by varying the parameters within the limits specified in Table 2. It is seen in Figure 4 that the effect of depth on gas pulsation is the least, followed by width and manifold radius. Also, it can be seen that at low frequencies, manifold depth and width have more effect on gas pulsations, whereas at high frequency radius is the more significant parameter. Figure 5 shows the Total effect of the gas pulsation due changes in the suction manifold radius, width and depth.



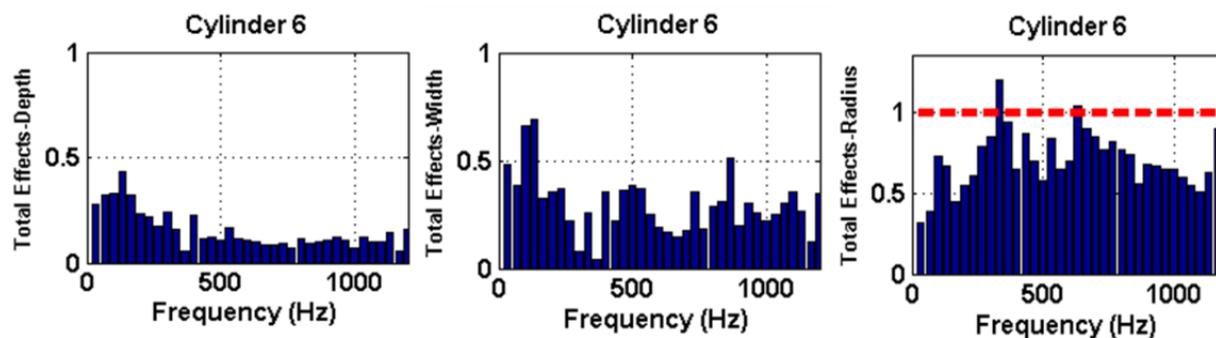
**Figure 3:** (a) A multi-cylinder reciprocating compressor and; (b) the suction manifold of the compressor with suction valves marked; (c) simplified mathematical representation of the suction manifold, where  $r$ ,  $b$ , and  $h_a$  respectively represent radius, depth and width of the suction manifold.

**Table 2:** Numerical values of parameters used in the simulation

Variables	Mean (mm)	Minimum Value (mm)	Maximum Value (mm)
Manifold radius, $r$	50	30	70
Manifold depth, $b$	27	20	40
Manifold width, $h_a$	14	8	20



**Figure 4:** First order indices of manifold depth, width and radius, using Sobol's method.



**Figure 5:** Total effect indices manifold depth, width and radius, using Sobol's method.

## 8. CONCLUSION

Sensitivity Analysis has become a standard part of any simulation routine that is used to predict the performance characteristics and behavior of a simulation model. Sobol's Methods—a global sensitivity analysis method—was presented and applied to a simple trial function to highlight the implementation details of the simulation model. A stepwise detail was provided to implement each equation described in the method. A Matlab® code with implementation details of the simulation for the trial function is also provided in the appendix. First order effects and total effects were computed and parameters were ranked according to their contribution to the overall variance of the function. The main advantage of this method is that it does not assume any prior condition of model being linear or monotonicity between input and output. Subsequently, the same method was applied to a compressor simulation model and the sensitivity of the suction manifold design parameters on the gas pulsations was determined. The same method of sensitivity analysis can be applied to all type of compressor simulation models.

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## APPENDIX

Matlab Code for Implementation of the Sobols Methods of Sensitivity Analysis

```

% Sobol Sensitivity Analysis program (trial)
% Author: Nasir Bilal, Purdue University
% 23 March 14
% We choose a trial function: fx=x1+5*x2*x3^2; to test the values
clear all; close all; clc;
N=1000; % total no. of simulated model output to quantify sensitivity
kp=[1 1 1];
n_p=size(kp,2) % number of model parameters to perform sensitivity analysis
on
PS=[]; % parameter space
comp_PS=[]; % complementary parameter space-- need to be defined for Monte
Carlo Simulation
n_base= ceil(N/n_p); % base no. of simulations so total no. of model eval ~ N
%-----
% determine parameter space for computations
% random sampling of parameter space using uniform distribution
%R=ceil(random('unif',1,5,n_base,2*n_p)) % 0,1 = range of dist., n_base=rows,
2*n_p=cols
%-----
% Assume some ranges for test variable: x1=1~1000; x2=10~100; x3=10~10;
% r_x1=ceil(random('unif',1,1000,n_base,2*n_p));
% r_x2=ceil(random('unif',10,100,n_base,2*n_p));
% r_x3=ceil(random('unif',50,200,n_base,2*n_p));
PS=[ceil((1 + 1000.*rand(n_base,1))) ceil((10 + 90.*rand(n_base,1))) ceil((1
+ 10.*rand(n_base,1)))]];
comp_PS=[ceil((1 + 1000.*rand(n_base,1))) ceil((10 + 90.*rand(n_base,1)))
ceil((1 + 10.*rand(n_base,1)))]];
output=[];
c_out_1=[];
c_out_t=[];
for i=1:n_base
    kp=PS(i,:);
    output(i,:)=Sobol_obj(kp);
    for j=1:n_p
        kp=[comp_PS(i,1:j-1),PS(i,j),comp_PS(i,j+1:n_p)];
        c_out_1(i,:,j)=Sobol_obj(kp);
        kp = [PS(i,1:j-1),comp_PS(i,j),PS(i,j+1:n_p)];
        c_out_t(i,:,j)=Sobol_obj(kp);
    end
end
end
%compute variances
n_out = size(output,2); %size of output of objective function
f0 = zeros(1,n_out); % integral of model output
D=zeros(1,n_out); % total variance
%monte carlo integrations to estimate integral functions
for i = 1:n_base
    f0 = f0+output(i,:)/n_base; % estimate integral of model output
    D = D+output(i,:).^2/n_base; % start computation of total variance of
model output
end
D=D-f0.^2
Dj=ones(n_p,1)*D% partial variances associated with parameter j
Dtotj=zeros(n_p,n_out); % total partial variance associated with parameter j

```

```

for i = 1:n_base
    for j = 1:n_p
        Dj(j,:)=Dj(j,:)-(output(i,:)-c_out_1(i,:,j)).^2/(2*n_base); %start
        computation of partial variances
        Dtotj(j,:)=Dtotj(j,:)+(output(i,:)-c_out_t(i,:,j)).^2/(2*n_base);
        %total variance due to pj
    end
end
%compute sensitivity indices from variances
Sob_1 = Dj./(ones(n_p,1)*D); %first order
Sob_t = Dtotj./(ones(n_p,1)*D); % total effect

%sort sensitivity rankings
%rank_Sob_1j: sorted Sobol first order rankings in terms of ascending
magnitude
%rank_Sob_1jp: parameters ranked in ascending order via Sobol first order
values
[rank_Sob_1 rank_Sob_1p] = sort(Sob_1);
%rank_Sob_tj: sorted Sobol total effect rankings in terms of ascending
magnitude
%rank_Sob_tjp: parameters ranked in ascending order via Sobol total effect
values
[rank_Sob_t rank_Sob_tp] = sort(Sob_t);

%immediately report back
sens_ind = Sob_1 %report back first order effect sensitivity indices
rank_sens = rank_Sob_1 %report back ranked sensitivity indices
rank_sens_p = rank_Sob_1p %report back ranked parameters

save Sobol_result PS comp_PS output c_out_1 c_out_t Sob_1 Sob_t rank_Sob_1
rank_Sob_1p rank_Sob_t rank_Sob_tp
'Sobol first order Results' % display on MATLAB command window

```

---



---

Matlab function used with the main program

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---

```

function out=Sobol_obj(kp)
% a function that works with the trial Sobol Method program
% the trial function is fx: x1+5*x2*x3^2;
x1=kp(1);
x2=kp(2);
x3=kp(3);
out= x1+5*x2*x3^2;
end

```