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A Super-Convergent Stochastic Method Based on the Sobol Sequence for Multidimensional Sensitivity Analysis in Environmental Protection

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Abstract: Environmental security is among the top priorities worldwide, and there are many difficulties in this area. The reason for this is a painful subject for society and healthcare systems. Multidimensional sensitivity analysis is fundamental in the process of validating the accuracy and reliability of large-scale computational models of air pollution. In this paper, we present an improved version of the well-known Sobol sequence, which shows a significant improvement over the best available existing sequences in the measurement of the sensitivity indices of the digital ecosystem under consideration. We performed a complicated comparison with the best available low-discrepancy sequences for multidimensional sensitivity analysis to study the model's output with respect to variations in the input emissions of anthropogenic pollutants and to evaluate the rates of several chemical reactions. Our results, which are presented in this paper through a sensitivity analysis, will play an extremely important multi-sided role.

Keywords: air pollution modeling; sensitivity analysis; multidimensional integrals; Monte Carlo methods; digital sequences

MSC: 60J22; 62P12; 65C05; 68W20

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Citation: Dimov, I.; Todorov, V.; Georgiev, S. A Super-Convergent Stochastic Method Based on the Sobol Sequence for Multidimensional Sensitivity Analysis in Environmental Protection. *Axioms* **2023**, *12*, 146. https://doi.org/10.3390/axioms12020146

Academic Editor: Ilaria Cacciari

Received: 20 December 2022
Revised: 26 January 2023
Accepted: 27 January 2023
Published: 31 January 2023

1. Introduction

The purpose of our work is in the field of environmental security [1,2], since this is one of the key areas worldwide. By definition, a sensitivity analysis (SA) is an investigation of how much the uncertainty in the input data of a model is apportioned in the accuracy of the output results [3–7]; see Figure 1. Multidimensional SA [8–12] is a very challenging task when modeling, but it is often the key tool for studying a complex phenomenon [13–17].

The main problem in SA is the evaluation of the total sensitivity indices (SIs) [18–21]. The mathematical formulation for estimating the SIs is represented by a set of multidimensional integrals (MIs) [22–25]. The Monte Carlo (MC) and quasi-Monte Carlo (QMC) methods are the best tools for solving the MIs [22,26–31]. For a more clear explanation of the objectives in this paper, one should check [32–34].

The input data for SA were obtained with a large-scale model of the long-range transport of pollutants in the air—the **Uni**fied **D**anish **E**ulerian **M**odel **(UNI-DEM)** [35–39]. UNI-DEM is also a basic tool and important tool for the creation of a digital twin, namely, Digital Air (see [40]).

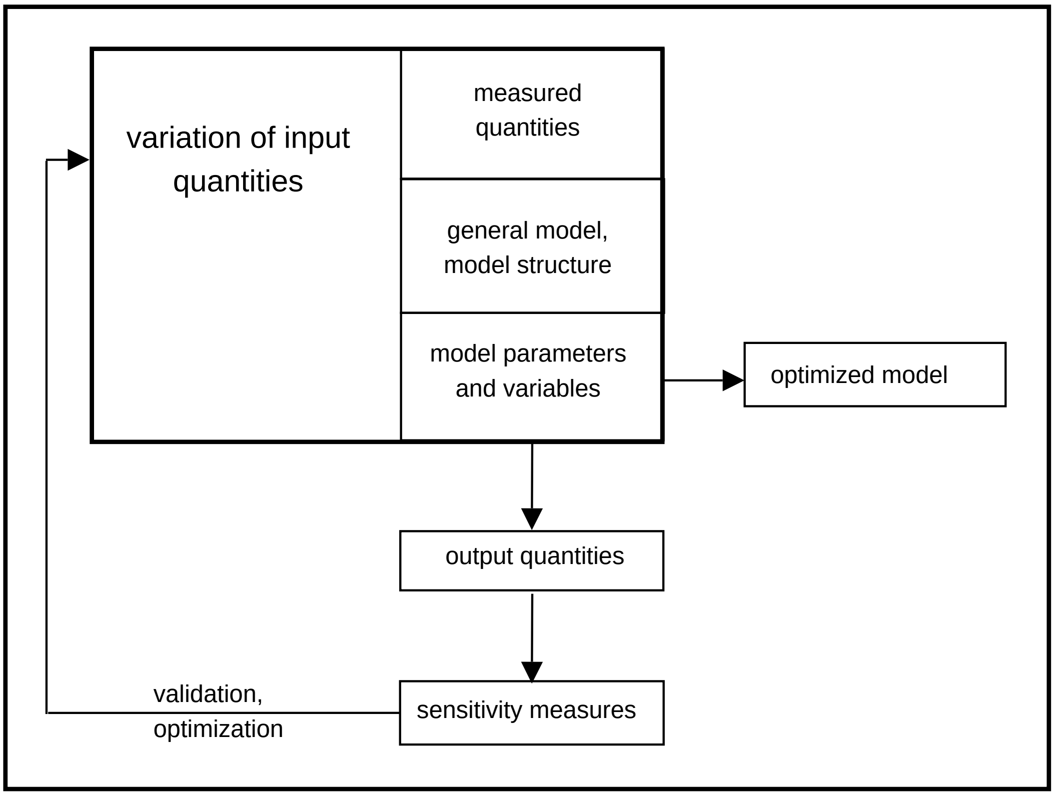

Figure 1. Methodology for performing sensitivity analysis.

By definition, the model can be introduced with a model function [41]:

$$u = f(x), \qquad x = (x_1, x_2, \ldots, x_d) \in U^d \equiv [0,1]^d.$$

The concept of the Sobol approach consists of the following representation of $f(x)$ and a constant f_0 [41]:

$$f(x) = f_0 + \sum_{\nu=1}^{d} \sum_{l_1 < \ldots < l_\nu} f_{l_1 \ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu}).$$

The above description is noted as the ANOVA representation of $f(x)$ if [41]:

$$\int_0^1 f_{l_1 \ldots l_\nu}(x_{l_1}, x_{l_2}, \ldots, x_{l_\nu}) \mathrm{d}x_{l_k} = 0, \quad 1 \le k \le \nu, \quad \nu = 1, \ldots, d.$$

The quantities

$$\mathbf{D} = \int_{U^d} f^2(x)\mathrm{d}x - f_0^2, \quad \mathbf{D}_{l_1 \ldots l_\nu} = \int f^2_{l_1 \ldots l_\nu} \mathrm{d}x_{l_1} \ldots \mathrm{d}x_{l_\nu}$$

are called total and partial variances [41]. The same is true for the total variance:

$$\mathbf{D} = \sum_{\nu=1}^{d} \sum_{l_1 < \ldots < l_\nu} \mathbf{D}_{l_1 \ldots l_\nu}.$$

The Sobol global SIs [6,41] are determined by:

$$S_{l_1 \ldots l_\nu} = \frac{\mathbf{D}_{l_1 \ldots l_\nu}}{\mathbf{D}}, \quad \nu \in \{1, \ldots, d\}.$$

Then, the **t**otal **s**ensitivity **i**ndex (TSI) of the input parameter $x_i, \ \ i \in \{1, \ldots, d\}$ is determined by [42]:

$$TSI(x_i) = S_i + \sum_{l_1 \neq i} S_{il_1} + \sum_{l_1, l_2 \neq i, l_1 < l_2} S_{il_1 l_2} + \ldots + S_{il_1 \ldots l_{d-1}},$$

where $S_{il_1 \ldots l_{j-1}}$ is the jth-order SI for x_i $(2 \leq j \leq d)$.

According to the definition in [43], when $j = 1$, the quantity S_i is called *the main effect* of x_i; if $j = 2$, S_{ij} are called *two-way interactions (second-order SIs)*; if $j = 3$, S_{ijk} are called *three-way interactions (third-order SIs)*, and so on. In this study, we are interested in the main effects and the two-way interactions.

The TSI of the output variance for an input parameter x_i, $i \in \{1, \ldots, d\}$ is represented as: $S_{T_i} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j < k} S_{ijk} + \ldots$; see [18]. With this, we show that multidimensional SA using Sobol's approach is turned into a problem of evaluating MIs [44].

In this paper, we aim to suggest implementations for the fast and accurate evaluation of the sensitivity indices. As mentioned earlier, the problem of SA is transformed into a multidimensional integration task that is approached by using novel quasi-Monte Carlo methods, which are compared with the best available algorithms in an application to large-scale modeling of atmospheric pollution. The methods are described in the next section, followed by a thorough analysis of the computational results.

2. Methods and Algorithms

Consider the following multidimensional problem:

$$S(f) := I = \int_{U^s} f(\mathrm{x}) \mathrm{dx},$$

where $\mathrm{x} \equiv (x_1, \ldots, x_s) \in U^s \subset \mathbb{R}^s$ and $f \in C(U^s)$.

In the simplest possible MC approach, "Crude", we introduce the random variable $\theta = f(\xi)$, for which

$$\mathbf{E}\theta = \int_{\Omega} f(\mathrm{x}) p(\mathrm{x}) \mathrm{dx},$$

and the random points $\xi_1, \xi_2, \ldots, \xi_N$ are independent realizations of the random point ξ with a probability density function $p(\mathrm{x})$ and $\theta_1 = f(\xi_1), \ldots, \theta_N = f(\xi_N)$. The **Crude MC** approach for the integral I is defined as [22]:

$$\overline{\theta}_N = \frac{1}{N} \sum_{i=1}^{N} \theta_i.$$

Let $\mathrm{x}_i = (x_i^{(1)}, x_i^{(2)}, \ldots, x_i^{(s)})$ for $i = 1, 2, \ldots$ and let $n = \ldots a_3(n), a_2(n), a_1(n)$ be the representation of n in base b.

Then, the discrepancy (star discrepancy) of the set is defined [22,24]:

$$D_N^* = D_N^*(\mathrm{x}_1, \ldots, \mathrm{x}_N) = \sup_{\Omega \subset E^s} \left| \frac{\#\{\mathrm{x}_n \in \Omega\}}{N} - V(\Omega) \right|,$$

where $E^s = [0, 1)^s$.

For the one-dimensional quasi-random number sequence, we introduce the radical inverse sequence [22,23]:

$$n = \sum_{i=0}^{\infty} a_{i+1}(n) b^i, \ \ \phi_b(n) = \sum_{i=0}^{\infty} a_{i+1}(n) b^{-(i+1)}.$$

The **van der Corput** sequence [45] is obtained when $b = 2$. Now, the multidimensional quasi-random number sequence is defined as: $X_n = (\phi_{b_1}(n), \phi_{b_2}(n), \ldots, \phi_{b_s}(n))$, where the bases b_i are all relatively prime: $(b_1, b_2, \ldots, b_s) \equiv (2, 3, 5, \ldots, p_s)$, where p_i denotes the i^{th} prime.

Now, the **Halton** sequence [46,47] is defined as:

$$s_n^{(k)} = \sum_{i=0}^{\infty} \sigma_{i+1}^{(k)} a_{i+1}^{(k)}(n) b_k^{-(i+1)},$$

where $(b_1, b_2, \ldots, b_s) \equiv (2, 3, 5, \ldots, p_s)$, p_i designates the i-th prime, and $\sigma_i^{(k)}$, $i \geq 1$ denotes the set of permutations on $(0, 1, 2, \ldots, p_k - 1)$.

The standard M-dimensional **Hammersley** sequence [48], which is based on N samples, is simply composed of a first component of successive fractions $0/N, 1/N, \ldots, N/N$ paired with $M - 1$ one-dimensional van der Corput sequences by using the first $M - 1$ primes as bases. More precisely, if $p_1, p_2, \ldots, p_{s-1}$ are the first $s - 1$ prime numbers, then the Hammersley sequence $\{t_0, t_1, \ldots, t_{N-1}\}$ with N points in s dimensions is given by

$$t_i = \{i/n, \phi_{p_1}(i), \phi_{p_2}(i), \ldots, \phi_{p_{s-1}}(i)\},\ i = 0, 1, \ldots, N - 1.$$

The **Faure** sequence [49–51] is given by:

$$x_n^{(k)} = \begin{cases} \sum_{i=0}^{\infty} a_{i+1}(n) q^{-(i+1)}, & k = 1 \\ \sum_{j=0}^{\infty} c_{j+1} q^{-(j+1)}, & k \geq 2 \end{cases}, \quad \text{where} \quad j \geq 1,$$

$$c_j = \left[\sum_{i \geq j} (k-1)^{i-j} \frac{i!}{(i-j)!j!} a_i(n) \right] (\text{mod } q), \qquad q \text{ is a prime } (q \geq s \geq 2).$$

The **Sobol** sequence [52–54] is defined by:

$$\mathrm{x}_k \in \overline{\sigma}_i^{(k)}, k = 0, 1, 2, \ldots$$

where $\overline{\sigma}_i^{(k)}$, $i \geq 1$ are the set of permutations on every 2^k, $k = 0, 1, 2, \ldots$ subsequent points of the van der Corput sequence, defined by $n = \sum_{i=0}^{\infty} a_{i+1}(n) b^i$, $\phi_b(n) = \sum_{i=0}^{\infty} a_{i+1}(n) b^{-(i+1)}$ when $b = 2$.

In binary, for the Sobol sequence, we have that: $x_n^{(k)} = \bigoplus_{i \geq 0} a_{i+1}(n) v_i$, where v_i, $i = 1, \ldots, s$ is the set of directional numbers [55].

For the QMC algorithms, based on the **Halton**, **Faure** and **Sobol** sequences, it is known that the corresponding discrepancy is:

$$D_N^* = \mathcal{O}\left(\frac{\log^s N}{N} \right).$$

According to several important works [56–59], the convergence rate for the scrambling algorithms essentially improves the convergence rate for the unscrambled nets [56–59], which is $N^{-1}(\log\ N)^{s-1}$. The scrambling itself is based on the randomization of a single digit at each iteration. Let

$$x^{(i)} = (x_{i,1}, x_{i,2}, \ldots, x_{i,s}),\ i = 1, \ldots, n$$

be quasi-random numbers in $[0,1)^s$, and let

$$z^{(i)} = (z_{i,1}, z_{i,2}, \ldots, z_{i,s})$$

be the corresponding scrambled version of the point $x^{(i)}$. Let every $x_{i,j}$ be rewritten in base b as

$$x_{i,j} = (0.x_{i1,j}\ x_{i2,j} \ldots x_{iK,j} \ldots)_b,$$

with K being the number of digits for scrambling. For the scrambled Halton sequence **HaltonScr**, we apply a permutation of the radical inverse coefficients, which is obtained by applying a reverse-radix operation to each of the possible coefficient values [60]. For the scrambled Sobol sequence **SobolScr**, we use a random linear scramble blended with a random digital shift [61].

Now, we will introduce a super-convergent modified Sobol sequence **SobolBurkardt** based on the INSOBL and GOSOBL routines in ACM TOMS Algorithm 647 and ACM TOMS Algorithm 659, as well as a Burkardt modification [52–55,62–67]. The original code can only compute the next element of the sequence. Our modification allows the user to specify the index of the desired element. The novelty is that this is the first time that the SobolBurkardt algorithm has been applied for a multidimensional sensitivity analysis of this important digital ecosystem.

3. Results and Discussion

In this section, the advanced stochastic algorithms described above (**Crude, Sobol, Halton, SobolScr, HaltonScr, SobolBurkardt, Hammersley,** and **Faure**) are applied to sensitivity studies with respect to emission levels (**SSREL**) and with respect to some chemical reaction rates (**SSRCRR**) of varying concentrations of UNI-DEM pollutants [68,69]. We use the following notations: EQ refers to the estimated quantity, RV refers to the reference value, RE refers to the relative error, and AE refers to the approximate evaluation.

For **SSREL**, we will investigate an SA of the model output (in terms of the mean monthly concentrations of several important pollutants—in our case, the pollutant is ammonia in Milan) with respect to a variation in the input emissions from anthropogenic pollutants, which consist of four components, $\mathbf{E} = (\mathbf{E^A}, \mathbf{E^N}, \mathbf{E^S}, \mathbf{E^C})$:

$\mathbf{E^A}$—ammonia (NH_3);
$\mathbf{E^N}$—nitrogen oxides $(NO + NO_2)$;
$\mathbf{E^S}$—sulphur dioxide (SO_2);
$\mathbf{E^C}$—anthropogenic hydrocarbons.

The output of the model is the mean monthly concentration of the following three pollutants:

s_1—ozone (O_3);
s_2—ammonia (NH_3);
s_3—ammonium sulfate and ammonium nitrate ($NH_4SO_4 + NH_4NO_3$).

For **SSEL**, the results for the REs for the AE of the f_0, $\mathbf{D}$, S_i and S_i^{tot} when using **Crude, Sobol, Halton, SobolScr, HaltonScr, SobolBurkardt, Hammersley, Faure** are shown in Tables 1–6, respectively. The quantity f_0 is represented by a four-dimensional integral, whereas the rest are represented by eight-dimensional integrals.

Table 1. RE for the AE of $f_0 \approx 0.048$.

N	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
2^{10}	1.0203e-02	3.9357e-03	1.2390e-04	1.2705e-03	**3.2184e-05**	3.1204e-04	9.4069e-04	1.0719e-03
2^{12}	3.4246e-03	1.2987e-04	6.3427e-05	2.4660e-04	**3.8933e-05**	7.7941e-05	2.7420e-04	2.1904e-04
2^{14}	2.5052e-03	2.6150e-04	1.8131e-05	6.3003e-05	**2.2578e-06**	1.9536e-05	8.1670e-05	1.0380e-04
2^{16}	1.7268e-03	2.7494e-05	5.5507e-06	2.0393e-05	**1.3679e-06**	4.8674e-06	1.5065e-05	2.1263e-05
2^{18}	4.3151e-04	7.3643e-06	9.9981e-07	3.4937e-06	**2.9476e-07**	1.2169e-06	5.2156e-06	8.7604e-06
2^{20}	6.7226e-05	1.0424e-05	1.5965e-07	1.6832e-06	**1.0679e-07**	3.0421e-07	1.3526e-06	2.2097e-06
2^{22}	6.4635e-05	2.8139e-07	5.2930e-08	2.6354e-06	**2.9975e-08**	7.6057e-08	3.4984e-07	7.3248e-07
2^{24}	1.6251e-05	9.9372e-07	2.0211e-08	2.5353e-06	**6.3589e-09**	1.9014e-08	9.3610e-08	1.9655e-07

Table 2. RE for the AE of $\mathbf{D} \approx 0.0002$.

N	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
2^{10}	1.1512e-01	4.9749e-02	7.1268e-03	**2.3682e-05**	6.7011e-03	4.8069e-05	9.5574e-03	1.6311e-02
2^{12}	2.8713e-02	2.0956e-02	1.9934e-04	4.1419e-02	6.3515e-04	**3.4443e-05**	5.4084e-03	8.9236e-03
2^{14}	4.3025e-02	1.2616e-02	4.4340e-04	3.0360e-02	3.9327e-04	**1.1423e-05**	8.7477e-04	2.1762e-03
2^{16}	1.7631e-02	2.5870e-03	3.5633e-05	9.2840e-03	7.0199e-05	**2.1854e-06**	1.8611e-04	7.4398e-04
2^{18}	1.1619e-02	4.8769e-03	**2.9050e-07**	1.2815e-03	2.3876e-05	4.8831e-07	1.1921e-04	1.0464e-04
2^{20}	5.7971e-03	4.1506e-03	2.5912e-06	3.1609e-03	8.2241e-07	**1.4083e-07**	1.7133e-05	4.5200e-06
2^{22}	7.3641e-04	2.7822e-04	**6.2903e-09**	1.1248e-04	6.6268e-07	3.5174e-08	5.3706e-06	1.2021e-05
2^{24}	1.9965e-03	9.7523e-05	1.0005e-07	2.5393e-04	4.7561e-07	**8.3121e-09**	1.2264e-06	3.5571e-06

Table 3. RV for the SIs.

EQ	S_1	S_2	S_3	S_4	S_1^{tot}	S_2^{tot}	S_3^{tot}	S_4^{tot}
RV	9e-01	2e-04	1e-01	4e-05	9e-01	2e-04	1e-01	5e-05

Table 4. RE for the SIs for $N = 2^{16}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
S_1	8.2327e-03	1.1349e-03	9.4160e-05	5.0373e-04	8.8491e-06	**3.5897e-07**	2.2607e-04	8.4508e-05
S_2	2.2865e+00	2.2951e-01	1.3709e-02	4.5285e-01	9.8766e-03	**1.2305e-06**	4.4931e-02	1.5962e-03
S_3	5.3236e-02	8.1938e-03	7.7523e-04	5.5827e-04	5.5051e-05	**2.7527e-06**	1.5531e-03	7.1000e-04
S_4	3.0153e+00	2.8075e-01	1.5219e-02	1.5771e+00	2.0713e-02	**4.9246e-04**	5.3609e-02	1.9105e-01
S_1^{tot}	6.9713e-03	1.0656e-03	9.9495e-05	1.0465e-04	1.1359e-05	**3.7471e-07**	2.0379e-04	9.7769e-05
S_2^{tot}	1.6677e+00	3.6735e-01	1.3941e-02	6.4351e-02	2.2279e-02	**4.2315e-06**	5.4409e-02	2.3218e-02
S_3^{tot}	6.2479e-02	8.2600e-03	7.4348e-04	3.5816e-03	1.0982e-04	**2.9046e-06**	1.6943e-03	6.7067e-04
S_4^{tot}	1.1430e+00	6.1265e-02	2.6594e-02	7.4372e-01	3.5606e-02	**2.5552e-04**	2.2248e-02	1.8200e-01

Table 5. RE for the SIs for $N = 2^{20}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
S_1	7.8667e-04	2.1597e-04	2.6599e-06	5.1404e-05	1.2762e-06	**2.1825e-08**	1.5146e-05	1.8801e-06
S_2	5.5512e-01	9.4219e-02	3.2670e-04	7.0608e-02	6.0694e-04	**8.1926e-07**	4.3471e-03	1.0155e-05
S_3	3.4181e-03	2.3580e-03	2.5627e-05	1.3056e-03	5.5697e-06	**1.8444e-07**	1.2672e-04	3.0339e-05
S_4	2.1558e-01	1.2257e-01	2.7219e-03	1.1810e-01	1.4168e-04	**8.2138e-07**	3.1331e-03	1.4615e-03
S_1^{tot}	5.2742e-04	2.4774e-04	3.0506e-06	1.1877e-04	5.5864e-07	**2.2577e-08**	1.6584e-05	3.7084e-06
S_2^{tot}	4.4329e-01	1.3121e-01	5.4168e-04	1.4930e-01	4.0881e-04	**2.1735e-06**	3.5704e-03	3.5910e-04
S_3^{tot}	5.3285e-03	2.0721e-03	2.1735e-05	7.8154e-04	9.8251e-06	**1.7849e-07**	1.1337e-04	1.4981e-05
S_4^{tot}	1.4729e-01	3.5556e-01	5.6925e-04	4.4828e-01	5.4686e-04	**9.7585e-07**	4.8967e-04	5.0071e-04

Table 6. RE for the SIs for $N = 2^{24}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.
S_1	2.0736e-04	1.3934e-05	3.4925e-07	2.3960e-05	2.3188e-08	**1.0992e-09**	1.4617e-06	4.4858e-07
S_2	3.3428e-03	1.8492e-02	4.4499e-05	1.5117e-03	3.1834e-05	**3.4635e-07**	2.4492e-04	1.3112e-04
S_3	1.3562e-03	2.6740e-04	2.2549e-06	2.4102e-04	8.3994e-07	**1.2762e-08**	1.1318e-05	2.9601e-06
S_4	1.6781e-01	8.3326e-02	6.1322e-05	3.7933e-02	1.8936e-05	**1.6676e-07**	2.1226e-05	1.0984e-04
S_1^{tot}	1.6667e-04	2.2386e-05	2.8847e-07	2.8570e-05	1.1619e-07	**1.6654e-09**	1.4402e-06	4.2689e-07
S_2^{tot}	6.3335e-02	3.2626e-02	9.5529e-05	1.6607e-03	1.8561e-05	**1.6473e-06**	1.8253e-04	3.5099e-04
S_3^{tot}	1.7633e-03	2.0139e-04	2.6217e-06	1.7782e-04	1.7446e-07	**1.2317e-08**	1.1402e-05	3.0813e-06
S_4^{tot}	1.5280e-02	8.2177e-02	6.5367e-05	1.3593e-02	2.3192e-05	**5.2088e-07**	1.8787e-04	2.5714e-05

In the case of **SSRCRR**, we will investigate the ozone concentrations in Genova according to the rates of variation of these chemical reactions, which are ## $1, 3, 7, 22$ (time-dependent) and $27, 28$ (time-independent) in the CBM-IV scheme [36]:

$$
\begin{array}{llll}
[\#\mathbf{1}] & NO_2 + h\nu \Longrightarrow NO + O; & [\#\mathbf{22}] & HO_2 + NO \Longrightarrow OH + NO_2; \\
[\#\mathbf{3}] & O_3 + NO \Longrightarrow NO_2; & [\#\mathbf{27}] & HO_2 + HO_2 \Longrightarrow H_2O_2; \\
[\#\mathbf{7}] & NO_2 + O_3 \Longrightarrow NO_3; & [\#\mathbf{28}] & OH + CO \Longrightarrow HO_2.
\end{array}
$$

In the case of **SSRCRR**, the results for the REs for the AE of $f_0, \mathbf{D}, S_i, S_{ij}$ and S_i^{tot} when using **Crude, Sobol, Halton, SobolScr, HaltonScr, SobolBurkardt, Hammersley,** and **Faure** are shown in Tables 7–12, respectively. As in the first case study, the quantity f_0 is represented by a six-dimensional integral, whereas the rest are represented by twelve-dimensional integrals.

Table 7. RE for the AE of $f_0 \approx 0.27$.

N	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.
2^{10}	6.9655e-04	5.4667e-03	2.3082e-04	3.4210e-03	**5.6900e-05**	7.4862e-05	4.1854e-04	7.1609e-04
2^{12}	8.0553e-04	1.2813e-03	5.2018e-05	4.7690e-04	2.6389e-05	1.9276e-05	**9.5472e-06**	2.1299e-04
2^{14}	2.8035e-03	6.2099e-04	7.3376e-06	6.2799e-04	**3.0524e-06**	5.1234e-06	2.9530e-05	8.1662e-05
2^{16}	5.9493e-04	2.8573e-04	3.7954e-06	1.9229e-04	2.3340e-06	1.1163e-06	**2.3321e-08**	2.1019e-05
2^{18}	7.6591e-04	6.6531e-05	1.1971e-06	1.1310e-04	**8.7046e-08**	2.7827e-07	1.6929e-07	2.2650e-06
2^{20}	3.4494e-04	8.7911e-05	1.6779e-07	8.7082e-06	**6.7087e-08**	6.9884e-08	3.4223e-07	1.4563e-06
2^{22}	4.6980e-05	7.0708e-06	5.3112e-08	3.7792e-06	1.7722e-08	**1.7505e-08**	2.0582e-08	2.8503e-07
2^{24}	8.6192e-06	1.7612e-06	1.7067e-08	5.0282e-06	**2.8300e-09**	4.4216e-09	4.0232e-08	1.3888e-07

Table 8. RE for the AE of $\mathbf{D} \approx 0.0025$.

N	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.	Rel.
2^{10}	7.2185e-02	3.2247e-01	2.7457e-02	5.4393e-02	1.4921e-02	**1.2142e-03**	3.2650e-03	5.5993e-02
2^{12}	9.5413e-02	3.7489e-02	3.9106e-04	6.3568e-02	2.6089e-04	**1.7948e-04**	2.7657e-03	9.8882e-03
2^{14}	6.3987e-02	5.3502e-03	5.6572e-04	1.2435e-02	8.6275e-04	**7.9574e-05**	4.1922e-04	2.5751e-03
2^{16}	2.9741e-02	7.3035e-03	9.8183e-05	3.1588e-03	**4.9265e-06**	5.9331e-05	3.0149e-04	1.4318e-04
2^{18}	7.4173e-03	8.5445e-04	1.3087e-04	8.3308e-03	5.3107e-06	**2.3567e-06**	3.8389e-05	8.6347e-05
2^{20}	8.9182e-03	2.9016e-03	2.0972e-05	2.5124e-03	1.5891e-05	**6.3664e-07**	8.8067e-06	1.0199e-04
2^{22}	2.2089e-03	2.8472e-04	1.3319e-06	3.8414e-04	3.1070e-06	**1.4675e-07**	6.1293e-06	4.2886e-06
2^{24}	1.2915e-03	6.0220e-04	1.2283e-06	8.8956e-04	2.9419e-07	**2.9072e-08**	1.0318e-06	1.1132e-05

Table 9. RV for the SIs.

EQ	S_1	S_2	S_3	S_4	S_5	S_6	S_1^{tot}	S_2^{tot}	S_3^{tot}	S_4^{tot}	S_5^{tot}	S_6^{tot}	S_{12}	S_{14}	S_{24}	S_{45}
RV	4e-1	3e-1	5e-2	3e-1	4e-7	2e-2	4e-1	3e-1	5e-2	3e-1	2e-4	2e-2	6e-3	5e-3	3e-3	1e-5

Table 10. RE for the SIs for $N = 2^{16}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
S_1	5.6096e-03	2.2562e-02	2.6780e-04	1.0569e-02	4.0640e-04	**5.0479e-05**	1.4076e-03	1.5499e-03
S_2	4.7347e-02	4.4525e-03	7.4595e-04	3.2242e-02	3.5900e-04	**5.2674e-05**	2.6596e-03	8.0331e-04
S_3	1.3830e-01	1.3689e-02	1.1337e-03	2.8586e-02	2.9528e-04	**9.0627e-05**	9.2017e-03	1.6311e-03
S_4	1.0483e-02	1.4615e-02	**5.2549e-05**	1.5857e-02	5.7186e-05	1.3944e-04	2.5660e-03	2.4591e-04
S_5	8.7257e+02	1.2792e+02	2.5051e+01	8.3791e+02	6.0590e+01	**1.0815e-01**	1.1486e+02	1.7275e+01
S_6	2.6892e-01	1.3325e-02	**1.4048e-03**	5.3342e-02	5.7510e-03	2.8293e-03	5.3261e-03	3.4148e-03
S_1^{tot}	2.8312e-02	2.0949e-02	6.1051e-04	1.5397e-02	**2.5768e-05**	5.0376e-05	1.5374e-03	1.0829e-03
S_2^{tot}	3.6260e-02	1.1178e-02	7.5957e-04	1.2953e-02	**7.6079e-06**	5.2434e-05	2.1988e-03	1.1931e-03
S_3^{tot}	1.6244e-01	9.9579e-03	1.9693e-04	4.1651e-02	5.8182e-04	**4.4610e-05**	9.4855e-03	2.7481e-03
S_4^{tot}	2.4677e-02	2.4355e-02	3.3704e-04	1.8186e-02	**8.1095e-05**	3.3843e-04	2.7377e-03	1.9728e-04
S_5^{tot}	2.4371e+00	5.3034e-01	7.9725e-02	2.3535e+00	4.5454e-02	**5.7438e-04**	1.0409e-01	8.9565e-03
S_6^{tot}	2.7228e-01	2.0409e-02	3.1290e-03	4.2927e-02	6.8957e-03	**5.8755e-05**	1.4960e-03	4.3337e-03
S_{12}	6.3125e-01	6.4533e-02	6.6778e-03	5.4471e-01	1.5688e-02	**2.0980e-04**	1.1473e-02	2.5217e-02
S_{14}	8.2786e-01	2.4557e-01	1.8711e-02	4.4225e-02	2.5486e-03	**1.6580e-04**	2.9238e-03	1.7521e-02
S_{24}	2.2332e-01	5.7049e-01	1.8916e-02	4.7501e-01	9.5940e-03	**9.3286e-05**	2.1281e-02	1.7537e-02
S_{45}	1.8853e+01	1.1031e+00	2.8122e-01	3.0144e+00	5.8655e-01	**3.4207e-03**	2.5773e-01	3.6417e-01

Table 11. RE for the SIs for $N = 2^{20}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
S_1	2.5476e-03	3.6651e-03	4.0993e-06	5.3088e-03	1.0701e-05	**2.3960e-07**	1.3095e-04	4.0799e-05
S_2	1.9128e-02	4.2272e-03	2.8757e-05	1.9508e-03	1.1891e-05	**2.5158e-07**	2.1987e-04	8.1976e-05
S_3	3.4996e-03	2.3071e-03	6.0559e-05	1.2243e-02	9.9222e-05	**4.2361e-07**	2.5731e-04	1.3818e-04
S_4	1.7948e-02	5.9751e-03	6.0523e-06	2.6551e-04	1.5029e-05	**1.1424e-08**	1.1228e-04	6.7408e-05
S_5	1.8681e+02	7.2157e+01	3.4310e+00	1.0230e+01	2.5657e+00	**2.4081e-02**	2.9289e+00	2.0537e-01
S_6	5.3782e-02	8.7395e-03	2.3861e-05	3.4768e-05	5.2251e-05	**5.1582e-06**	1.2032e-04	9.9070e-05
S_1^{tot}	7.9477e-03	2.9054e-03	9.1197e-06	1.3012e-03	6.3677e-06	**5.3664e-08**	1.2711e-04	2.9498e-06
S_2^{tot}	1.9734e-02	8.5173e-03	1.9271e-05	3.8451e-03	2.6525e-06	**2.0871e-07**	1.9914e-04	6.5812e-05
S_3^{tot}	3.0996e-03	5.9973e-03	1.4852e-05	1.4544e-02	1.1736e-04	**1.5835e-07**	2.3601e-04	1.1388e-04
S_4^{tot}	2.0145e-02	1.2986e-03	5.1517e-05	1.7639e-03	2.3539e-05	**5.6942e-08**	8.9964e-05	8.9036e-05
S_5^{tot}	5.8023e-01	4.4475e-03	2.4738e-03	2.5033e-01	6.3792e-04	**4.0769e-06**	7.2792e-03	9.9166e-03
S_6^{tot}	7.2660e-02	5.5229e-03	2.0946e-05	3.5088e-03	1.7813e-04	**1.2202e-06**	1.4599e-04	2.7537e-04
S_{12}	1.3345e-01	2.6400e-02	3.6606e-04	4.0445e-01	7.8494e-04	**2.5191e-06**	4.2430e-04	6.8564e-04
S_{14}	2.7148e-01	8.8282e-03	1.2694e-03	2.6693e-03	6.4115e-04	**7.2053e-08**	1.8270e-03	1.2351e-03
S_{24}	3.0686e-01	3.0429e-01	7.1327e-04	1.7343e-01	3.1628e-05	**3.6191e-07**	1.3293e-03	2.5331e-04
S_{45}	3.1523e+00	6.1996e-01	6.5205e-02	7.4406e-01	2.3682e-02	**2.3323e-06**	7.5214e-03	3.6786e-02

Table 12. RE for the SIs for $N = 2^{24}$.

EQ	Crude	Sobol	Halton	SobolScr	HaltonScr	SobolBurkardt	Hammersley	Faure
	Rel.	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**	**Rel.**
S_1	2.4330e-03	5.4855e-05	4.3425e-07	1.8394e-04	2.1469e-06	**4.7652e-09**	1.3630e-05	3.8605e-07
S_2	1.8600e-03	8.6539e-04	3.2927e-06	6.3174e-05	1.1980e-06	**1.4631e-08**	1.0881e-05	3.5242e-06
S_3	3.9300e-03	5.6418e-06	3.5322e-06	7.4251e-04	2.2399e-06	**2.1141e-08**	2.4177e-05	9.2757e-06
S_4	1.7259e-03	4.5923e-04	1.7289e-06	6.7281e-05	1.1772e-06	**4.6307e-09**	2.5453e-06	1.0124e-07
S_5	6.2991e+01	4.5863e+01	1.9926e-01	3.4058e+01	3.0171e-01	**8.9687e-06**	1.0382e-01	3.4176e-01
S_6	1.3933e-02	1.0439e-03	6.1108e-06	5.4044e-04	7.0985e-06	**4.4536e-08**	4.1129e-05	2.9285e-05
S_1^{tot}	1.9688e-03	7.3326e-04	1.8221e-06	3.4036e-04	1.3386e-07	**1.7085e-08**	1.2335e-05	3.6610e-06
S_2^{tot}	2.6026e-03	6.2024e-04	3.6497e-06	3.8882e-04	2.3226e-08	**8.5909e-09**	9.5810e-06	7.6348e-07
S_3^{tot}	2.0711e-03	7.2188e-04	4.3511e-06	4.1485e-04	2.6316e-06	**1.9892e-08**	2.2909e-05	1.2053e-05
S_4^{tot}	1.7469e-03	3.0923e-04	3.2059e-06	2.0661e-04	1.8443e-06	**7.0485e-09**	1.3456e-06	2.3401e-07
S_5^{tot}	4.2987e-02	8.4511e-02	2.4261e-04	4.7671e-02	1.8005e-04	**4.6423e-06**	4.0002e-04	6.5404e-04
S_6^{tot}	5.3593e-03	2.4417e-03	1.1304e-05	1.4773e-04	1.5546e-05	**1.1218e-07**	3.6764e-05	4.4269e-05
S_{12}	2.4931e-02	3.3850e-02	4.9860e-06	8.1074e-04	1.0919e-04	**4.3575e-07**	5.9259e-05	2.6114e-04
S_{14}	1.2130e-02	1.8289e-02	1.0087e-04	1.0448e-02	3.1657e-05	**6.5546e-07**	2.2484e-04	2.8465e-05
S_{24}	2.6639e-02	3.3815e-02	4.2851e-05	2.8599e-02	8.4836e-06	**1.2394e-07**	2.7452e-05	6.0399e-05
S_{45}	1.5179e-01	1.2626e-01	3.2937e-03	2.1289e-01	4.5098e-04	**2.2539e-08**	2.2560e-03	2.8349e-03

In the case of **SSREL**, one may observe the following. In Table 1, for the model function f_0, the best algorithm for all numbers of samples is HaltonScr, followed by SobolBurkardt. For $N = 2^{24}$, for the total variance **D**, the best algorithm is SobolBurkardt, followed by the Halton sequence—see the results in Table 2. However, for $N = 2^{18}$ and $N = 2^{22}$, the Halton sequence produces slightly better results—see Table 2. The behavior of the algorithm can also be seen in Figure 2. The RVs for the first and total SIs are presented in Table 3. From Tables 4–6, one can conclude that for all first-order SIs and TSIs, the best algorithm is SobolBurkardt, followed by HaltonScr and the Halton sequence. It is important that the scrambling procedure improves the results of the Sobol and Halton sequences by at least one order for most of the cases—see the values for S_2^{tot} and S_3^{tot} in Table 6. In [42], it was pointed out that having the smallest possible SIs is the most important aspect of a model. In our case, these are S_4 and S_4^{tot}—see Table 3. For them, SobolBurkardt significantly improved upon the results of the other sequences, and one can also see that the Hammersley and Faure sequences performed better than the Crude algorithm, as expected.

The performance of the algorithms in the case of SSREL can be generalized in this way: The algorithm that we implemented, SobolBurkardt, held the smallest relative errors for all SIs; the scrambled Halton and original Halton sequences were the next, followed by the Hammersley, Faure, scrambled Sobol, and Sobol algorithms; the worst was the plain algorithm.

In the case of **SSRCRR**, the following observations could be made. In Table 7, for the model function f_0, the best algorithm for all numbers of samples except $N = 2^{12}$, $N = 2^{16}$, and $N = 2^{22}$ was HaltonScr; for $N = 2^{22}$, the best algorithm was SobolBurkardt, and in the other two cases, the best algorithm was the Hammersley sequence. The RVs of the first- and second-order SIs and TSIs are given in Table 9. For all numbers of samples except $N = 2^{16}$, for the total variance D, the best algorithm was SobolBurkardt—see the results in Table 8. However, for $N = 2^{16}$, the scrambled Halton sequence produced results that was one order better than our SobolBurkardt algorithm. The behavior of the algorithm can also be seen in Figure 3. For a low number of samples, $N = 2^{16}$, as shown in Table 10, the Halton sequence was better than our SobolBurkardt algorithm for S_4 and S_6, and the scrambled Halton sequence was better than our algorithm for the total SIs S_1^{tot}, S_2^{tot}, and S_4^{tot}. As previously mentioned, having the smallest possible SIs is the most important aspect of a model. Here, these were S_5, S_{45}, and S_5^{tot}—see Table 9. For them, our SobolBurkardt implementation performed better than the other algorithms. However, for larger numbers of samples, as shown in Tables 11 and 12, one can conclude that for all first-order SIs, second-order SIs, and TSIs, the best algorithm was SobolBurkardt, followed by the HaltonScr and scrambled Sobol sequence algorithms. It is important that the scrambling procedure significantly improved the results of the Sobol and Halton sequences for some of the cases—see the values for S_4 and S_6 in Table 12. For all of the cases, the Hammersley and Faure sequences performed better than the Crude algorithm, as expected.

The performance of the algorithms in the case of SSREL can be generalized in such a way: The SobolBurkardt algorithm that we implemented held the smallest REs for all SIs; the scrambled Halton and the original Halton sequence are the next, followed by the Hammersley, Faure, scrambled Sobol, and Sobol algorithms, and the worst was the Crude algorithm.

The overall conclusion is that the implemented SobolBurkardt algorithm was the best approach among the benchmarked algorithms, and the values of the relative errors showed its supremacy over the majority of the existing methods when applied to multidimensional air pollution sensitivity analysis.

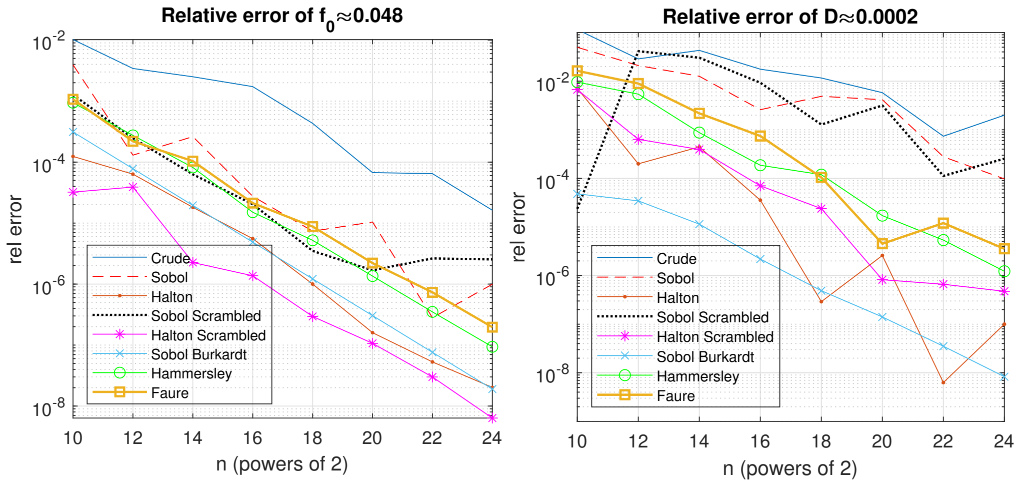

Figure 2. RE for the AE of $f_0 \approx 0.048$ and **D** ≈ 0.0002.

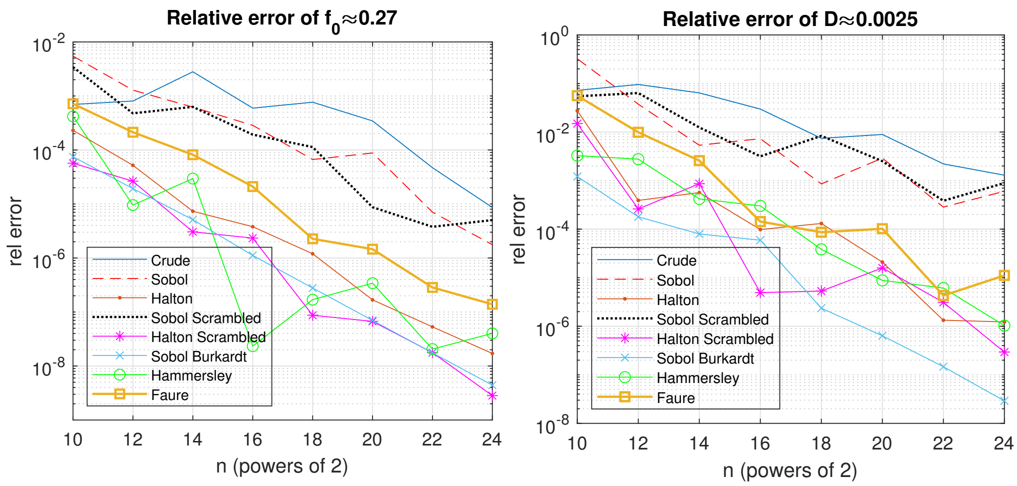

Figure 3. RE for the AE of $f_0 \approx 0.27$ and **D** ≈ 0.0025.

4. Conclusions

Our paper treats a very important area of environmental safety. The computational accuracy and numerical efficiency in terms of the relative error for one of the best available stochastic methods for multidimensional integration were studied for the sensitivity of the Unified Danish Eulerian model's output to find the variations in the rate constants of chosen chemical reactions and the variations in selected input emissions of anthropogenic pollutants. We implemented an improved Sobol sequence based on a Burkardt modification, which dramatically improved upon the results produced by other low-discrepancy sequences that have been used until now to perform multidimensional sensitivity analyses of this model. In addition, for the first time, we included the Faure and Hammersley sequences in our comparison; they have never before been compared with the Sobol and Halton sequences for this particular and very important large-scale air pollution model.

When compared with the results reported in recent studies, our results show significant improvements in terms of the accuracy and lower computational costs of the suggested algorithm. Our improvements when calculating the sensitivity indices of the model will significantly help provide a more accurate evaluation of agricultural losses. The most important effect of our results will be our contribution to the estimation of harmful emissions' effects on human health.

There are many ways in which this investigation could be extended. Some of the straightforward ones include exploring other quasi-sequences with possibly better properties, scrambling and shifting the existing sequences, and creating new ones from suitable generation vectors or generation matrices.

Author Contributions: Conceptualization, V.T.; methodology, V.T.; software, V.T. and S.G.; validation, V.T. and S.G.; formal analysis, V.T.; investigation, V.T.; resources, V.T.; data curation, V.T. and S.G.; writing—original draft preparation, V.T. and S.G.; writing—review and editing, I.D., V.T. and S.G.; visualization, V.T. and S.G.; supervision, I.D. and V.T.; project administration, I.D. and V.T.; funding acquisition, I.D. All authors have read and agreed to the published version of the manuscript.

Funding: The development of stochastic methods was supported by the Bulgarian National Science Fund under Bilateral Project KP-06-Russia/17 "New Highly Efficient Stochastic Simulation Methods and Applications". The Sobol global approach estimation was supported by the Bulgarian National Science Fund under Project KP-06-M32/2—17.12.2019 "Advanced Stochastic and Deterministic Approaches for Large-Scale Problems of Computational Mathematics". The multidimensional sensitivity analysis was supported by the Bulgarian National Science Fund under Project KP-06-N52/5 "Efficient methods for modeling, optimization and decision making". The optimization of the Sobol algorithm was supported by the Bulgarian National Science Fund under Project KP-06-N62/6 "Machine learning through physics-informed neural networks". The experimental study was supported by the National Program "Young Scientists and Postdoctoral Researchers-2"—Bulgarian Academy of Sciences.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

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