## Accelerate global sensitivity analysis using Artificial Neural Network algorithm

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Global sensitivity and uncertainty analysis has attracted more and more attentions in combustion chemistry study recently. High computational cost is one of the key factors restricting its application in complex combustion chemical models. In this work, Artificial Neural Network (ANN) [4] has been used to accelerate convergent speed of two widely used quantitative global sensitivity analysis methods - Sobol' sensitivity estimation [1] and Random Sampling – High Dimensional Model Representations (RS-HDMR) [2, 3]. The ANN was constructed using original model samples firstly, and then a well-trained ANN was used to generate numerous samples for global sensitivity analysis with Sobol' sensitivity estimation or RS-HDMR. With the help of ANN, the computational cost of Sobol' sensitivity estimation can be reduced greatly and the model output can be obtained at any point in the parameter space, thus this method can be easily applied into practical models. Compared with the traditional optimization methods of RS-HDMR, the proposed ANN optimized RS-HDMR method (ANN-HDMR) has better acceleration of convergence, as well as better stability. An important analytical function — Sobol' g-function and two practical models in combustion — master equation kinetic model and reaction kinetic model were taken as examples to reveal the instability of the traditional optimization methods for RS-HDMR and tested the performances of ANN-HDMR. The results show that only a few tenths (even a few percent) of original samples are needed in some conditions for ANN-HDMR method, and no important parameters were ignored. In addition, the "residual effect" was introduced to determine the important terms and to reduce the calculation. With this method, only a small portion of the second or higher order terms will be calculated. Based on the above methods, a user friendly program for global sensitivity analysis was developed by MATLAB, and will be provided to potential users.

- [1] I. M. Sobol', Matem. Modelirovanie 2 (1990) 112-118.
- [2] Ö. Alış, H. Rabitz, J. Math. Chem. 29 (2001) 127-142.
- [3] G. Li, S.W. Wang, H. Rabitz, J. Phys. Chem. A 106 (2002) 8721-8733.
- [4] D.E. Rumelhart, G.E. Hinton, R.J. Williams, Nature 323 (1986) 533-536.