Atmos. Chem. Phys. Discuss., 4, S2045–S2047, 2004
www.atmos-chem-phys.org/acpd/4/S2045/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Parametric sensitivity and uncertainty analysis of dimethylsulfide oxidation in the remote marine boundary layer" *by* D. D. Lucas and R. G. Prinn

A. Saltelli (Referee)

ANDREA.SALTELLI@JRC.IT

Received and published: 11 October 2004

This is an interesting paper and my comment concerns primarily the methodology for sensitivity analysis.

Practitioners often differ on the meaning of sensitivity analysis, but a widespread opinion (Rabitz et al., 2000) is that you can have two alternative broad objectives for doing it. One is mapping the input output relationship, and another assessing the relative importance of input factors in determining the uncertainty in the output.

The sensitivity analysis run in this paper is somehow old fashioned, in what it misses much of the recent methodological work on the topic (see sources at http://sensitivity-

analysis.jrc.cec.eu.int/; note that there was an international conference on the topic this year in New Mexico, US), yet it covers reasonably well the first objective, which is often of interest in chemistry, but does rather poorly on the second. In particular, after having clearly demonstrated that the model is rich in structure and interactions, the authors fail to provide any of the summary measure that would assess the global importance of factors. Take for instance figure 6. It is instructive, but it only maps the total sensitivity of a factor against itself. Where is the effect of the other factors? And where is the synthesis of all that as a measure of ranking the input factors?

The authors have estimated their model over a large set of Monte Carlo runs. Could they produce the model coefficient of determination for the set as a function of time for selected output variables? A suggestion would also be to compute on these the input - output standardised regression coefficients, a measure that provides for multidimensional averaging (the effect of X(I) on Y(K) is averaged over the space of X(I) as well as over the space of all X(J), J different from I.

The are a variety of decomposition used for model representations, such as projection pursuits, radial functions, ANOVA high dimension model representation (ANOVA-HDMR, often used in sensitivity analysis) and cut-HDMR, often used in SA for chemical systems (Saltelli et al., 2000, a multi author book, covers most of this material. Alternatively see Rabitz et al., 1997). The present paper presents a rather novel representation (from the 1997 paper from Tatang et al.).. The reader might be interested in a mention of the specificity (advantage disadvantage) of this method versus others.

The author make clearly the point of the inability of the local methods to estimate moment (section 6.3.2). PCM and DIM-M agree with one another, which is good given the resources spent in building PCM, but DIM-S cannot give the same result. Yet in the rest of the paper the authors try to make the point that after all DIM-S sensitivities and DIM-M give the same message. Looking at the results, I would rather say the opposite. If the system were linear, which we agreed it is not, DIM-M should be proportional to dY/dX(I) times sigma(X (I))/sigma(Y), and there is no way that the result can be

ACPD

4, S2045–S2047, 2004

Interactive Comment

independent from sigma(X(I)). Furthermore the system is non linear and hence dY/dX changes both with X(I) and with X(˜I) (the complementary set).

End of page 10 the importance of CH3SO2 dissociation in Saltelli and Hjorth 1995 versus the present paper. It is only natural that the results using different models differ, yet this conclusion should not be arrived at by comparing local derivatives output with global measures output.

At the bottomline I would like the authors to try at least a global sensitivity analysis measure, such as e.g. the Morris method (Morris 1991) or other.

Morris, M.D., 1991, Factorial Sampling Plans for Preliminary Computational Experiments, Technometrics, 33(2), 161-174.

Rabitz, H., Ö. F. Aliş, 2000, Managing the Tyranny of Parameters in Mathematical Modelling of Physical Systems [HDMR], in Saltelli et al., 2000.

Rabitz, H., Ö. F. Aliş, J. Shorter, and K. Shim, 1999, Efficient input-output model representations, Computer Physics Communications, 117, 11-20.

Saltelli, A., K. Chan and M. Scott, Eds., 2000, Sensitivity Analysis, John Wiley & Sons.

Interactive comment on Atmos. Chem. Phys. Discuss., 4, 6379, 2004.