The role of sensitivity analysis in model improvement

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The paper will describe the role of global sensitivity and uncertainty analysis [1] in the evaluation and improvement of chemical and reactive flow models with applications from combustion kinetics [2-4] and atmospheric pollution dispersion [5]. The method of global sensitivity analysis via high dimensional model representations (HDMR) will be first introduced [1]. Its application will then be demonstrated firstly for models of fuel combustion including the oxidation of methanol and butane. The sensitivity analysis methods will then be illustrated for a model describing the reactive, turbulent dispersion of a plume of nitrogen oxides through a background atmosphere containing ozone [5]. This example serves to highlight the relative importance of chemical parameters and turbulence model parametrisations within such a reactive dispersion model. The applications illustrate the ability of the method to identify key input parameters which drive the uncertainty in the target predictions of the models. Improved quantification of these parameters would therefore reduce the overall uncertainty in the model predictions and therefore improve the robustness of the model over the test conditions. The feedback between key parameter identification and improved categorization via theoretical kinetic calculations will be highlighted.

[1] T. Ziehn, A.S. Tomlin, *Environmental Modelling and Software*, 2009, 24, 775-785.
[2] R.T. Skodje, A.S. Tomlin, S.J. Klippenstein, M.J. Davis, *Journal of Physical Chemistry*, 2010, 114(32), 8286-301.
[3] S.J. Klippenstein, L.B. Harding, M.J. Davis, A.S. Tomlin, R.T. Skodje, *Proceedings of the Combustion Institute*, 2011, 33, 351-357.
[4] M. Davis, R. Skodje, A.S. Tomlin, *Journal of Physical Chemistry A.*, 2011, 115, 1556-1578.
[5] T. Ziehn, N.S. Dixon, A.S. Tomlin, *Atmospheric Environment*, 2009, 43, 5978–5988.