Sensitivity Analysis and Optimization of a Numerical Model of Helium APPJ Afterglow Using the Elementary Effects Method

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Abstract: We illustrate the applicability of the elementary effects method for sensitivity analysis and optimization of models in plasma physics. In the first part of this contribution, we will illustrate how the method is used for assessing in what way individual experimental inputs influence the solution. In the second part, we used the method to reduce an already optimized reaction scheme from 125 to 63 reactions.

Keywords: helium, plasma jet, sensitivity analysis, elementary effects

1. Introduction

Numerical simulations clearly play an important role in the field of plasma physics because they help to grasp the strongly non-linear behaviour of the fourth state of matter. Within typical laboratory plasmas, the models often have to account for the interplay of coupled physical phenomena. Firstly, electromagnetic fields, electron kinetics, neutral gas chemistry, transport and mixing influence each other on a wide range of spatial and temporal time scales, and secondly, the non-equilibrium nature of the plasma allows for a very large number of new kinetic pathways which are thermodynamically unfavourable.

Taking this into account, it is inevitable that every plasma model will depend on a number of input parameters with large uncertainty intervals, be it reaction cross-sections, material properties or experimental inputs to the model. The number of these model inputs is usually very high – up to thousands of reactions can be included in a plasma model – and sometimes, the uncertainties of the input parameters can be relatively large – even when they are obtained from an experimental input.

In case the model does not agree well with the experimental validation, we are often facing the challenge of identifying the cause of such discrepancy. Additionally, the behaviour of the model with regard to the input parameters is often counter-intuitive, for example a 30% error in one parameter (e.g. wall sticking coefficient) may have a much larger influence on the result than a 30% error in another parameter (e.g. ionization rate). Furthermore, there might be non-linear interactions coming to play (e.g. the model is only sensitive to the wall sticking coefficient if the ionization rate is high enough).

It is not possible to test such complex interactions in a model without a mathematical framework and the mathematical tools to achieve that are commonly called sensitivity analysis techniques.

2. Conventional Techniques

The conventional sensitivity analysis techniques are reviewed for example in [1] and have been used in the field of plasma simulation e.g. [2]. This method is essentially a finite difference method as it relies on calculation of partial derivatives of each model output with regard to each model input. For a better example, let us try to consider the sensitivity of number density of species n_i to reaction rates in a kinetic model (reaction rates considered inputs with given uncertainties). This number density is a complicated function of the values of all the rate coefficients

$$n_i = n_i(k_1, \dots, k_N) \tag{1}$$

The sensitivity of the density n_i to a rate coefficient of reaction *r* would be calculated as

$$S_i(k_r) = \frac{k_r}{n_i}\frac{\partial n_i}{\partial k_r} \tag{2}$$

The advantage of the method is its robustness and the fact that it is relatively easy to assess its convergence (the step in the input coefficient k_r is being decreased until the change in the sensitivity coefficient S_{ir} is small). The disadvantage is the incapability to predict second-order coupling between the model inputs. For example, the output n_i may seem non-sensitive to input k_{30} but becomes sensitive to it if the magnitude of input k_{45} is decreased). This is because the derivatives in equation (1) are calculated at constant values of the other input parameters.

As an alternative to the conventional methods described above, the so-called **elementary effects (EE) method** was developed [3] which is discussed in the following paragraphs. It should be pointed out that the EE method is not a replacement of the conventional sensitivity analysis method but rather an alternative.

3. Elementary Effects Method

The method of elementary-effects was introduced by Morris et al. [3]. Unlike the conventional method described above, it does not attempt to calculate the exact values of the derivative in equation (1). Instead, it relies on sampling of the *k*-dimensional space of the *k* model, thereby also reducing the number of model runs necessary (in the EE method, it is approximately proportional to *k*

while in the conventional methods, it is proportional to k^2).

Instead of the finite partial differences, the EE methods operates with so-called *elementary effects*. Firstly, we introduce weight coefficients w_r, by which corresponding model inputs k_r are multiplied. The algorithm then begins at a random position in the k-dimensional space of the weight coefficients, changes one of them coefficient by a value Δ and calculates the elementary effect of r-th input on an i-th output as

$$d_i(w_r) = \frac{f(w_1,\dots,w_r+\Delta,\dots w_k) - f(w_1,\dots,w_r,\dots w_k)}{\Delta} \quad (3)$$

The algorithm then proceeds onto another input (one that has not yet been modified in the current trajectory). In this manner, m trajectories in the k-dim space of the input parameters are generated, which should cover as much of it as possible. The expression for the elementary effect is not equivalent to expression (2) as each elementary effect with regard to input r is calculated at different values of other inputs.

In the EE method, it is necessary to uniformly populate the phase space of the input coefficients, as thoroughly discussed in [4]. Once it is done and several elementary effects have been obtained for each input (several trajectories were generated), the mean value μ_i and their standard deviation σ_i are calculated and then act as a measure of sensitivity.

$$\mu_i = \frac{1}{m}\sum_{r=1}^{m} d_i(w_r) \quad (4)$$

$$\sigma_i = \sqrt{\frac{1}{r-1}\sum_{r=1}^{m}(d_i(w_r) - \mu_i)^2} \quad (5)$$

Simply speaking, the value of μ_i is high when the input influences the model linearly and σ_i is high if the input influences the result depending on another input.

Figure 1 provides an illustration how the population of the phase space with trajectories could look like in a simple case of a few input parameters. An elementary effect is calculated in each point of the trajectory which is not its starting point.

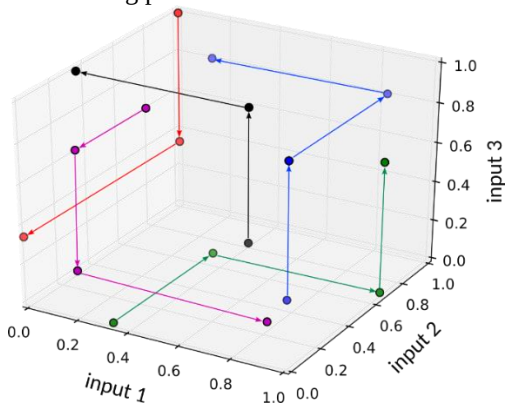

Fig. 1: Population of 3-dim phase space of the model inputs by trajectories.

In the paragraphs below, we give specific examples, how the Elementary Effects method can be used to understand and optimize a specific numerical model of processes in an atmospheric pressure plasma jet, which has been developed earlier.

4. Use case: Sensitivity of a Gas Dynamics Model to Experimental Inputs

We have previously developed a model of gas dynamics applicable to atmospheric-pressure plasma jets. This model solves the Navier-Stokes equations coupled to a diffusion equation describing the mixing of the gaseous components (usually a rare gas and air), heat equation and, optionally advection-diffusion-reaction equations for active species in the afterglow. This model has previously been employed to explain certain experimental observations related to the gas flow in the APPJ [5–7]. Figure 2 shows an example output from the model

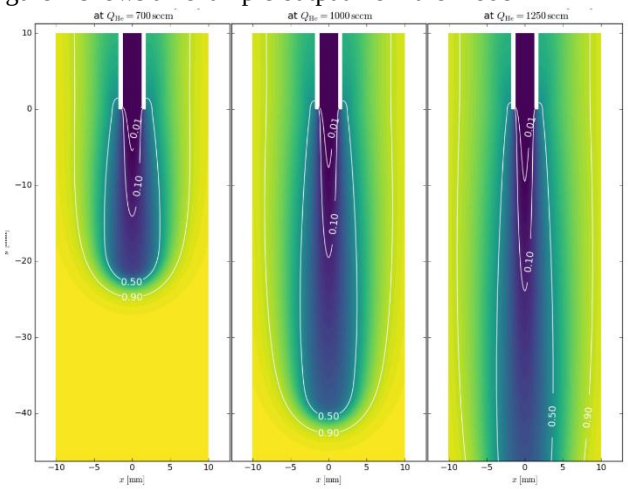

Fig. 2: Example output from the gas flow model – gas composition outside the APPJ, adapted from [6].

The model has several inputs, which are either estimated or provided from experiment but in any case, can potentially impact the result because their uncertainty is quite high. In this section, we chose to study only the sensitivity with regard to 4 input parameters, to make the procedure more transparent and possible to correlate with a physicist's intuition. The four parameters and their uncertainties are the following:

- Gas temperature at APPJ orifice T_g,can range from 20 to 70°C in a typical APPJ
- Ambient temperature T_a,can range from 18 to 28°C
- Inner diameter of the jet r_{jet}, manufacture tolerances introduce uncertainty of +/- 0.1 mm.
- Air impurity in the rare gas x_{air}, from 0 to 1%, depending on the tubing

As the output parameter, we chose the axial distance z_0, which is the distance where the air molar fraction reaches 10%. The elementary effects algorithm was run for 5 trajectories with 5 steps each, meaning that it required 25

model runs. Figure 3 then shows the output of the algorithm, which is a 2D scatter plot of μ_i and σ_i.

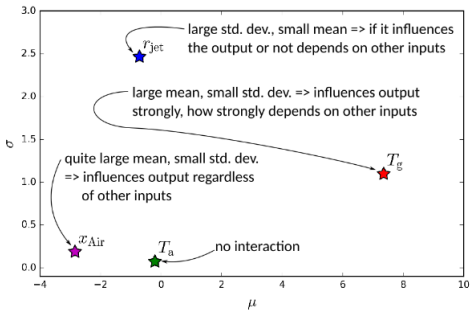

Fig. 3: 2D scatter plot of elementary effects mean and standard deviation for the 4 model inputs considered.

By looking at the plot, we can make the following conclusions:

1. The ambient temperature has negligible effect on the mixing outside the APPJ
2. Air impurity shows mostly linear interaction – it influences the output regardless of the values of other inputs
3. r_{jet} and T_g show non-linear interaction – they influence the solution depending on the value of the other parameter. Their effects can cancel out (increasing both r_{jet} and T_g appropriately leads to the same gas velocity) but generally do not cancel out.

These conclusions are clearly consistent with one's intuition which suggests that the elementary effects method provides reliable results when performing the sensitivity analysis. In the following section, we apply the method to a model with a notably higher number of input parameters.

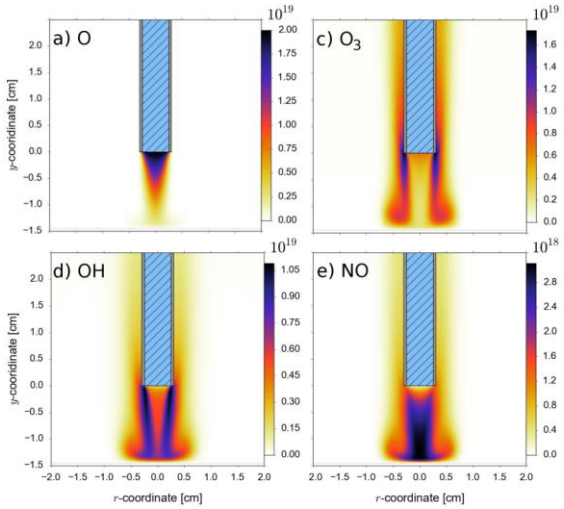

Fig. 4: Outputs from 2D afterglow chemistry model, adapted from [7]

5. Use case: Reduction of an Afterglow Reaction Scheme

The gas flow numerical model which has been discussed above can also be complemented with a model of 2D afterglow chemistry, as illustrated in figure 4 and reference [7].

The reaction scheme which was used for the calculation contains 125 reactions which could be important in the afterglow and which have already been manually pre-selected based on the works by Murakami *et al.* [8]. The question, however, remains if this reaction scheme can be further reduced and optimized. The motivation in this case is only partially reduction of the computation costs. More importantly, many of the reaction rates are have a large error or are only estimated based on an analogy. If we eliminate the reactions which are of little importance at relevant conditions, we can focus on refining the important reaction rates, thereby making the model more accurate.

For the purpose of sensitivity analysis and optimization, we did not solve the model in the 2D geometry but simplified it to 0D time-dependent. Compared to the previous case, we still have many more model outputs – the densities of all the species that the model solves for as a function of time – and many more model inputs – rate coefficients – so the sensitivity plots look much more chaotic, see figure 5.

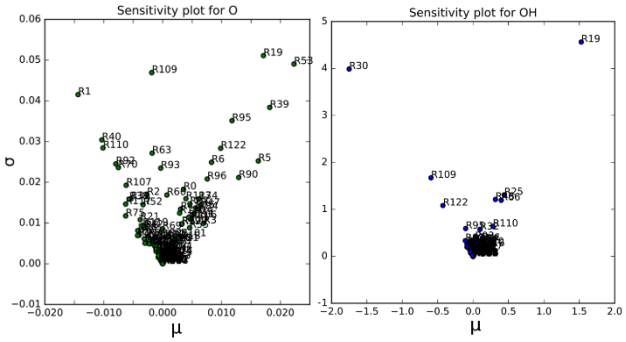

Fig 5: Sensitivity plots for oxygen radical and OH radical densities.

In figure 5 above, each labelled point corresponds to a specific reaction. Those reactions, which are close to point (0,0) do not influence the concentration of the corresponding species but may still influence the concentration of other species.

We further analysed the sensitivity coefficients for all the species and eventually removed 62 reactions which had close to zero interaction for all of the species, thereby reducing the already optimized reaction scheme almost by a half. As figure 6 illustrates, the time-dependent concentrations of the species were nearly unaffected by this, meaning that the elementary effects method correctly identified the reactions, to which the model is not sensitive.

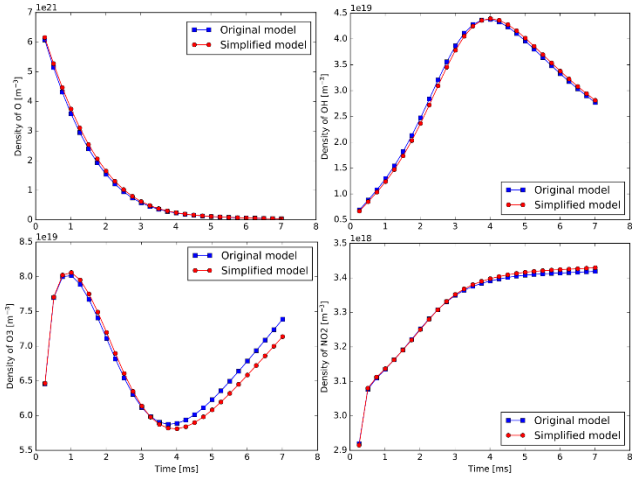

Fig. 6: Verification that the reduction of the reaction scheme from 125 to 62 reactions did not change the results.

6. Conclusion

On two examples, we have illustrated that the elementary effects method can be used for sensitivity analysis and sensitivity analysis-based optimization of numerical models in plasma physics. In subsequent work, we will focus on applying this method to even much larger reaction schemes with the aim to optimize them, eventually making the numerical models more transparent.

7. References

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Acknowledgement

AO is a Brno PhD Talent – funded by Brno municipality. ZB acknowledges the support of the Czech Science Foundation (GACR contract no. 15-04023S).