Sensetivity Analysis

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Abstract

Adjoint sensitivity analysis of ignition delay time for a zero-dimension reactor is presented in this work. A developed work package based on the algorithmic differentiation technique is used to provide accurate jacobins. The numerical jacobians provided by algorithmic differentiation are similarly accurate as analytical ones encounter the approximated derivatives using finite difference schemes. The framework is extendable for different configurations without extra effort. The proposed approach provides a superior accurate and robust computational method for the sensitivity of any parameter contribute to the governing equations (Arrhenius, thermodynamic, etc.).

Keywords:
Sensitivity analysis, Uncertainty quantification, Enthalpy of formation, Standard entropy, Heat capacity

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1. Introduction

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2. Primal problem

The governing equations that describe an ideal homogeneous zero-dimensional isochoric reactor are as follows,

$$\frac{\partial Y_i}{\partial t} = \frac{1}{\rho}\dot{\omega}_i \tag{1}$$

$$\frac{\partial T}{\partial t} = \frac{1}{\rho C_v}\dot{\omega}''_T \tag{2}$$

where Y_i, is the species mass fraction vector $i = [1, ..., N]$, C_v, ρ are the heat capacity at constant volume, the density respectively, $\dot{\omega}_i$ is the rate of consumption or production for the different species and $\dot{\omega}''_T$ is the heat released rate which is defined by,

$$\dot{\omega}''_T = -\sum_{i=1}^{N}\dot{\omega}_i u_i, \tag{3}$$

knowing that u_i is the total internal and chemical energy and driven from the enthalpy,

$$u_i = h_i - RT. \tag{4}$$

The reaction rate of different species i due to the set of reactions N_r is expressed as,

$$\dot{\omega}_i = \sum_{j=1}^{N_r}\dot{\omega}_{ij}. \tag{5}$$

The consumption/production rate of species based on each reaction is $\dot{\omega}_{ij} = q_j M_i \nu_{ij}$ where M_i is the molecular weight of species i, ν_{ij} is the stoichiometric molar balance between reactants and products of species i involves in reaction j, $\nu_{ij} = \nu''_{ij} - \nu'_{ij}$. The reaction rates q_j are modelled as follow,

$$q_j = k_{f_j}\prod_{i=1}^{N}[X_i]^{\nu'_{ij}} - k_{r_j}\prod_{i=1}^{N}[X_i]^{\nu''_{ij}}, \tag{6}$$

where the forward and reverse reaction rate constants of reaction j are k_{f_j} and k_{r_j} respectively, and the molar concentration of species i is $[X_i]$. The thermodynamic quantities are computed based on NASA polynomial empirical model add ref. The ideal gas equation $p = \frac{\rho RT}{\bar{M}}$ is used to close the system, as $\bar{M}$ is the average molecular weight and R is the universal gas constant.

2.1. reaction rates models

The forward rate coefficients are generally computed using Arrhenius parameters. Depending on how the forward rate constants change with the pressure, additional reaction types, such as three-body and uni-molecular/recombination fall-off reactions, are also considered. Lindemann and Troe forms are used to express the rate constants of pressure-dependent fall-off reactions.The reverse rate constants are related to the forward rate constants through the equilibrium constants or through own Arrhenius parameter in case explicitly mentioned in the mechanism data.

2.2. Mechanisms

2.2.1. H2/O2
The first scheme under consideration is the hydrogen oxidation mechanism described by Ó Conaire et al. [29]. It includes 40 reactions among 10 species consisting of 5 elements, i.e. O, H, C, N, and Ar.

2.2.2. GRI 3.0
The second examined scheme is the well-known gri3.0 [30] reaction scheme. The model includes 325 reactions and 53 species.

3. Methodology

The most common method in sensitivity analysis is based on the gradient descendant technique for continuous, differentiable, and convex functions add ref, and this is also the case for our model. As there are several approaches to compute the gradients (brute force, Forward sensitivity, and Adjoint, etc.), and each one has its advantages and disadvantages, a detailed comparison is provided in add ref. The adjoint approach scales with the number of the objective functions/quantity of interests(QOI) independent of the system parameters number based on that the adjoint approach was chosenadd ref.

3.1. Forward solution

The forward solution of the primal problem are split into two main steps reading the chemical mechanism files including thermodynamic properties and set up the numerical framework

3.2. Adjoint approach

There are several adjoint approaches as fully continuous, fully discrete, and semi discrete add ref. The studied system is zero-dimensional so only fully continuous/discrete techniques are applicable. for this study, the fully continuous method is considered. The general derivation of adjoint equations for system of non linear coupled ordinary differential equations(ODE) as follow, consider an objective function of multiple imputes and single outputs, $y = J(q_i, g_j)$, where $y \rightarrow R$ as $q_i \rightarrow R^n$, $g_j \rightarrow R^m$ are the state vector and system parameters(thermodynamic, Arrhenius ,etc.) respectively. The objective function could represent any quantity of interest (QoI) produced by the system like ignition delay time or average temperature etc. The Lagrangian function is used to remove the dependencies between the state variables and system parameters,

$$\mathcal{L}(q_i, \mathbf{g}) = J - \lambda \cdot \int_0^{t_f} (\frac{\partial q_i}{\partial t} - F(q_i \mathbf{g}))dt - a_i \cdot (q_i - q_0)\big|_{t=0}, \tag{7}$$

where λ and a are the lagrangian variables vectors , $F(q_i, \mathbf{g})$ are the governing equations right hand side and $(q_i - q_0)\big|_{t=0}$ are the initial conditions, taking the derivative of $\mathcal{L}(q_i, \mathbf{g})$ with respect to q_i leads to the following adjoint equations.

$$\frac{\partial \mathcal{L}(q_i, \mathbf{g})}{\partial q_i}\delta q_i = \frac{\partial J}{\partial q_i}\delta q_i - \lambda_i \int \frac{\partial \delta q_i}{\partial t} - \frac{\partial F(q_i, \mathbf{g})}{\partial q_i}\delta q_i dt - a_i \delta q_i\big|_{t=0}, \tag{8}$$

applying integration by parts to the above equation,

$$\frac{\partial \mathcal{L}(q_i, \mathbf{g})}{\partial q_i}\delta q_i = \frac{\partial J}{\partial q_i}\delta q_i + \delta q_i \int \frac{\partial \lambda_i}{\partial t} + \lambda_j \frac{\partial F_j}{\partial q_i}dt - a_i \delta q_i\big|_{t=0} - \lambda_i \delta q_i\big|_{t=0}^{t_f} \tag{9}$$

in case J is an integral QoI then it can be expressed as $J = \int h dt$ and by substituting in the above equation

$$\frac{\partial \mathcal{L}(q_i, \mathbf{g})}{\partial q_i}\delta q_i = \delta q_i \int \frac{\partial h}{\partial q_i} + \frac{\partial \lambda_i}{\partial t} + \lambda_j \frac{\partial F_j}{\partial q_i}dt - a_i \delta q_i\big|_{t=0} - \lambda_i \delta q_i\big|_{t=0}^{t_f} \tag{10}$$

then by cancelling the perturbation δq_i the adjoint equation is as follow,

$$0 = \frac{\partial h}{\partial q_i} + \frac{\partial \lambda_i}{\partial t} + \lambda_j \frac{\partial F_j}{\partial q_i}. \tag{11}$$

Eliminating the perturbation δq_i at $t = 0$ and $t = t_f$, as the values of λ_i are known at $t = t_f$, this imposes an initial conditions for the above equations $\lambda_i = 0\big|_{t=t_f}$, due to these initial conditions the adjoint equations are integrated backward in time, which requires a very dense mesh to achieve high accuracy add ref.

Computing the jacobians for highly non-linear systems requires checking pointing that is stored during the forward solution of the primal problem, because of the asynchronous between the forward and the backward time integration. A high-order interpolation function is used to overcome the fidelity difference.

3.3. Computing derivatives

There are several methods to compute the derivatives that construct the jacobians, one of the most common techniques is the Fréchet derivative add ref. Although it is easy to implement, this method is error-prone which is accurate depending on the proposed perturbation value similar to the FD method. Complex step differentiation (CSD) prevents the loss of precision inherited in the traditional finite difference, however, still not so accurate and on top of that, the main disadvantage is the high computational time consumption for both of the methods. These disadvantages make FD and CSD are out of scope, especially for large systems. To achieve high accuracy affordably a working package based on algorithmic differentiation (AD) method is coded up from scratch in Julia Language likewise the governing equations ??. The new AD tool provides the values of reaction rates and the thermodynamic quantities, and their gradients with respect to all system variables and parametersfast and as accurate as analytical derivatives. It is important to note that, Julia is a new programming language made for facilitating the computation of scientific applications. Julia combines execution speed on a par with statistically-typed languages with the active performance provided by dynamic languages add ref.

3.4. Sensitivity analysis of ignition delay time

The ignition process involves a sudden increase in the temperature accompanies by changes in the species profiles. The variation in the behaviour of the species profile changes according to the mechanism used in the modelled reactor, so it is hard to put a general and identical description to ignition based on the specific field. But globally the rapid increase in the temperature distinguishes the ignition phenomenon independent of the applied mechanism so that the phase shift in the temperature profile could mimic the ignition delay time add ref and the QOI is written as follow

$$J = \frac{1}{\tau} \int (T - T^{shift})^2 dt. \tag{12}$$

The transitioned profile T^{shift} is determined from the relation $T^{shift}(t) = T(t - 10^{-2} \cdot t_r)$, where t_r is the characteristic time of ignition and computed based on the
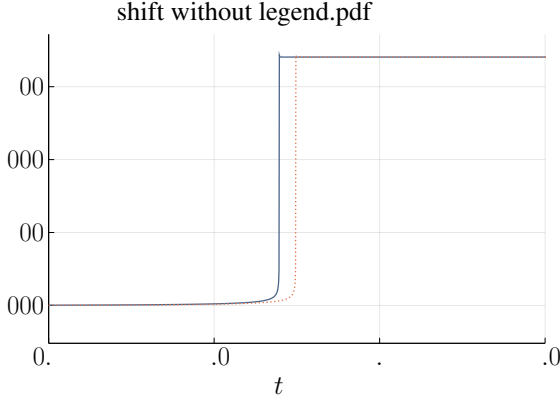
Figure 1: comparison between the reference temperature profile.——, shifted profile; .....

maximum time gradient for temperature $\frac{dT}{dt}\big|_{max}$ leading to the equation

$$tr = \frac{T_{max} - T_0}{\frac{dT}{dt}\big|_{max}}.$$ (13)

Figure 1 visualizes the difference between the original and the delayed profile, showing a schematic vision to the value of t_r.

The gradients of the QOI with respect to system parameter $\frac{dJ}{dg_i}$ is derived from the Lagrangian function add ref as follow

$$\frac{dJ}{dg_i} = \int \frac{\partial h}{\partial g_i} + \lambda_j \frac{\partial F_j}{\partial g_i} dt.$$ (14)

Finally, the sensitivity is normalized and related to $\frac{dJ}{dg_i}$ as follow add ref,

$$S_i = \frac{g_i}{J} \cdot \frac{dJ}{dg_i}$$ (15)

4. Results and Validation

The first step is validating the primal problem **??** implementation in the newly developed AD tool name of the tool. For the sake of validation the *gri*3.0 mechanism is simulated by Cantera and Flame Master add ref with initial mass fractions of $Y_{CH_4} = 0.05$ and $Y_{O_2} = 0.2$ in N_2, as initial temperature $T = 1000K$ at atmospheric pressure condition is used and compared to the results of name of the tool. The perfect matching between temperature and species profiles obtained by different software as shown in figure 2 and figure 3 insures the veracity of the simulation of the governing equations by name of the tool.
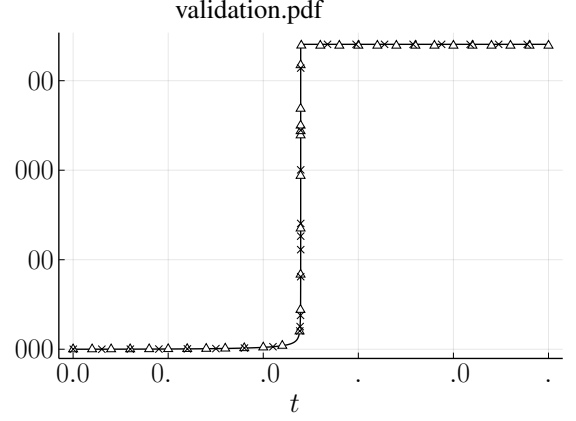

Figure 2: comparison between the temperature profile obtained by different software .——, AD tool; x, Cantera; Δ, Flame Master
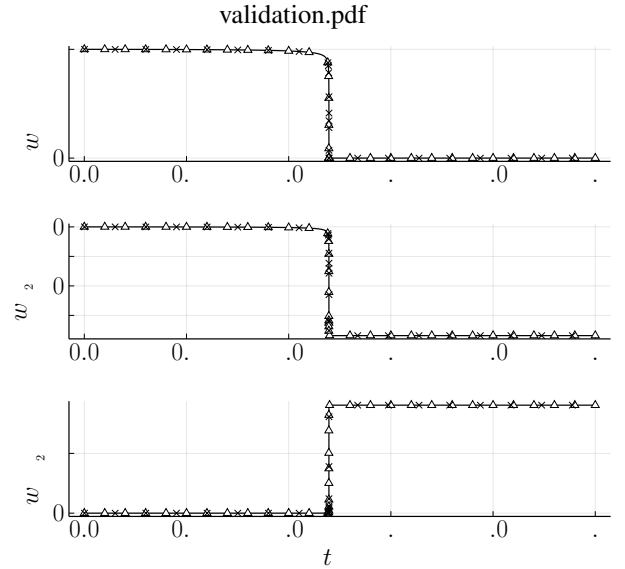

Figure 3: comparison between different species profiles obtained by different software .——, AD tool; x, Cantera; Δ, Flame Master
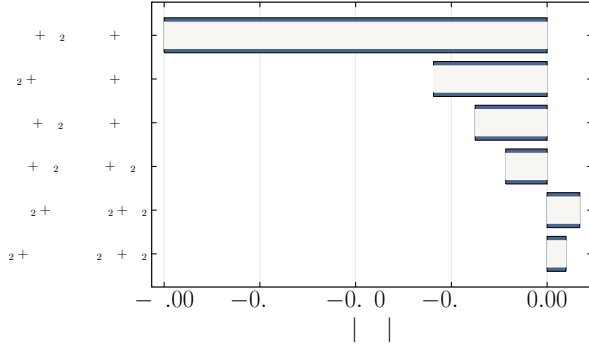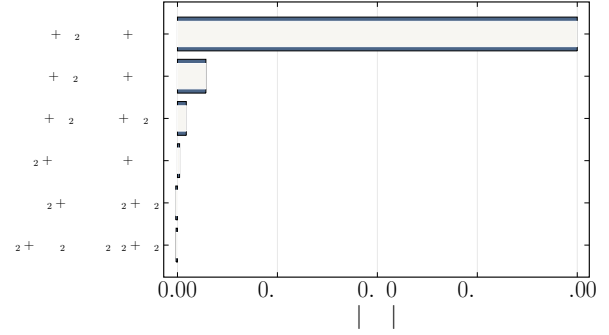
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Figure 4: sensitivity analysis of ignition delay time with respect to A for most dominant ten reactions

Figure 5: sensitivity analysis of ignition delay time with respect to β for most dominant ten reactions
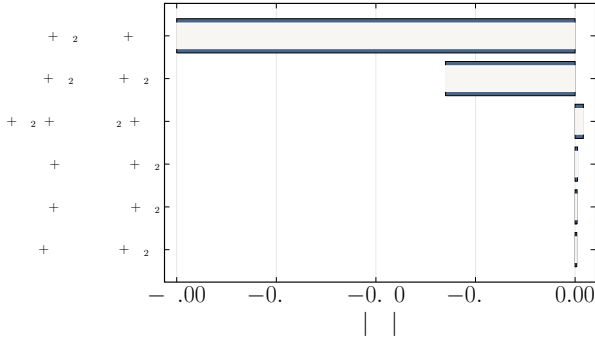

Figure 6: sensitivity analysis of ignition delay time with respect to E for most dominant ten reactions
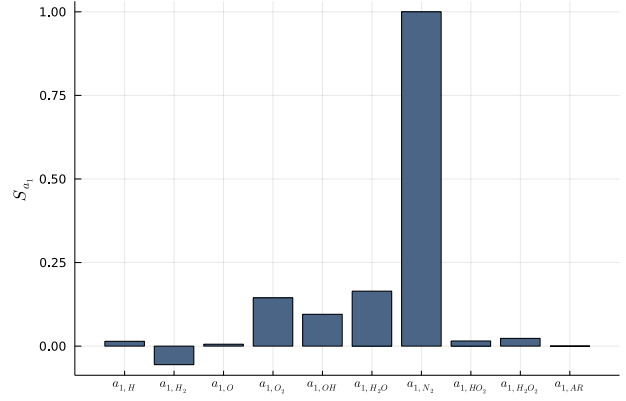

Figure 7: sensitivity with respect to thermodynamic coefficient a_1

The validation of the sensitivity analysis is carried out using CSD, two different mechanisms with various environments are used for this purpose. Starting with the $h2vb$ mechanism as a preliminary step due to the small size of the mechanism and the huge importance of hydrogen fuel. Considering the following initial mass fractions of $X_{H_2} = 0.09$ and $X_{O_2} = 0.18$ in N_2, as initial temperature 1000 K at atmospheric pressure condition is used for all of the $h2vb$ sensitivity results unless different composition is stated. Figure 4 shows a good agreement between the results of name of the tool and CSD. The reaction $H + O_2 => O + OH$ is the dominant reaction in the ignition process in terms of Arrihinieus parameters, showing the importance of the direct oxidation of H_2 on the gradients.

discuss the same results for GRI.

4.1. Fall off and third body reactions parameter

4.2. Thermodynamic parameters

One of the important aspects when analysing the ignition process is not only the reactions behaviour but also,

the effect of the thermodynamic quantities and it's impact on system sensitivities. However, it is not straightforward to extract the derivatives of any QoI with respect to NASA polynomial coefficients, but as AD provides a full accessibility to the gradients with respect to all system parameters, it is possible to provide a full analysis for the sensitivity with respect to Thermodynamic parameters. Figure 7 shows that a_{1N_2} dominating the other species. This can be returned to the large value of Y_{N_2}, which mainly influences the C_v mixture average rather than enthalpy and entropy. As N_2 is an inert species in h_2v scheme. Same results can be found by analysing the other coefficients at low temperature.

Extracting the sensitivities with respect to NASA Polynomial coefficients at high temperature provides a similar behaviour as it is shown in figure 8. On the other hand, a comparison between figure 7 and 8 exhibits an increase in the gradient of Y_{H_2O} which can be related to the increase in the value of Y_{H_2O} due to the combustion process. This demonstrates that thermodynamic properties for diluted mixture is controlled by the
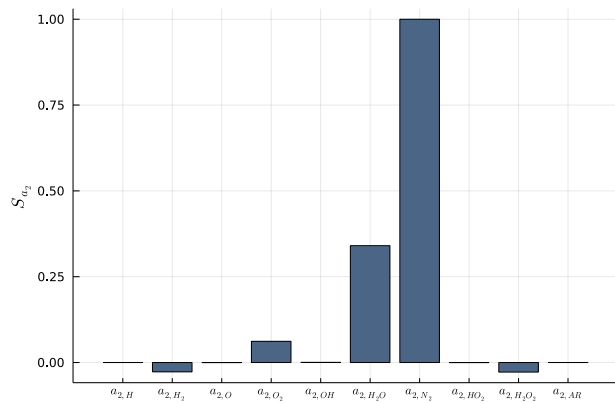
Figure 8: sensitivity with respect to thermodynamic coefficient a_1

diluted species

discuss the same results for GRI.

4.3. Sensitivity evolution in time

5. Conclusions

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Acknowledgments

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