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Positivity Issues in Adaptive Solutions of Detailed Chemical Schemes for Engine Simulations

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Abstract

Reliable and efficient solution of chemical kinetics is one of the main computational kernels in engine simulations. The chemical schemes are characterized by high degrees of stiffness, due to the very different reaction rates, and include intermediate species with low density, whose accurate solution is needed to well understand the combustion process. In this context, the non-negativity property of numerical methods for ordinary differential equations is crucial to avoid spurious numerical instabilities and very high accuracy requests. In this work we discuss results obtained by using a recent version of the VODE package, which allows to impose non-negativity constraints on the solution, in simulations of combustion when a moderate size chemical scheme is used. The impact of positivity requirements on the total mass preservation and the computational cost is analyzed for a classic model problem for which experimental data are available for validation.

Keywords: `detailed reaction schemes, stiff ODE solvers, positivity preservation, combustion modeling.`

1. Introduction

In the last decade, due to the adverse effect of emissions from internal combustion engines on human health and on the environment, the amount of pollution tolerated by Government laws have been strongly reduced. Manufacturers have therefore to adopt proper engine design and technological solutions to keep such emissions within the fixed limits. In this frame-

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work, modeling activities are expected to give reliable details on combustion dynamics and they represent helpful tools for the design of future engines. As a result, the use of detailed kinetics reaction mechanisms in multidimensional diesel engine simulations has become a popular choice, thanks to its potentiality to describe combustion development and incorporate models for pollutants formation. On the other hand, with the adoption of detailed kinetic schemes some computational issues arise, as discussed in the following.

Mathematical models for simulations of modern internal combustion engines involve unsteady Navier-Stokes equations for turbulent multicomponent mixtures of gases, coupled with model for fuel spray and combustion. Operator splitting is usually used for the numerical solution of the overall model, where different physical phenomena are decoupled and different sub-models are solved independently, at each splitting interval, on 3D computational meshes representing the engine cylinder. One of the main computational kernels in this framework is the solution of the combustion sub-model. It describes chemical reactions involving a high number of chemical species, characterized by very different reaction rates. We focus on the positivity and total mass density preservation issues for effective solution of the non-linear systems of ordinary differential equations (ODEs) in combustion simulations for diesel engines. This work takes place in the context of activities devoted to designing and developing efficient and robust algorithms and software for realistic simulations of internal combustion engines [2,4].

2. Numerical Issues of Detailed Chemical Schemes

The non-linear ODE system, describing the rate of change of the chemical species concentration due to reactions, has the following form:

$$(1) \qquad \dot{\rho}_m = W_m \sum_{r=1}^{R} (b_{mr} - a_{mr})\, \dot{\omega}_r\, (\rho_1, \ldots, \rho_M, T)\,, \quad m = 1, \ldots, M$$

where M is the number of chemical species, R is the number of chemical reactions, $\dot{\rho}_m$ is the production rate of species m, W_m is its molecular weight, a_{mr} and b_{mr} are integral stoichiometric coefficients for reaction r, $\dot{\omega}_r$ is the kinetic reaction rate and T is the temperature. This system, coming from the mass balance equations for the different species (molecules and radicals) involved in the combustion process, is characterized by a high degree of stiffness due to the strongly different reaction rates of the species, and its solution is required for each grid cell of the overall discretization grid. During a diesel combustion process, the mathematical features of system (1) change, since two main combustion phases can be identified:

1. a *low temperature phase* or *autoignition*, the period from the start of fuel injection to ignition. In this phase, system (1) is characterized by a high degree of stiffness, due to chemical reactions involving some intermediate species with very low density and very short destruction time. Some of these intermediate species are responsible for ignition starting, then their accurate solution is needed to well understand the combustion process and the formation of pollutants.
2. a *high temperature phase* or *combustion* from ignition onwards. This phase is characterized by a smoother kinetic dynamics, and a lot of intermediate species are rapidly damped.

A general-purpose ODE stiff solver for system (1) is likely to introduce negative species densities values at some point, because of rounding and truncation errors, particularly when densities are very small. Therefore, the positivity preserving property is crucial for avoiding spurious numerical instabilities, especially in the low temperature combustion phase. Positivity is often obtained by applying the so-called clipping approach, where negative values are projected to zero, but this approach can seriously affect mass density preservation. Another approach to get positivity as side effect is to use very low absolute tolerances in the stopping criterion of the numerical procedure. In this case, computational work can dramatically increase and the solution is strongly dependent on user's choices.

In this work we analyze the performance of the VODE_F90 package [12] in the solution of system (1), when a moderate size chemical reaction model for combustion simulations is considered. Let $\mathbf{y}(t) = (\rho_1(t), \ldots, \rho_M(t))$ be the vector of unknowns and $\mathbf{f}(\mathbf{y}(t))$ the right hand side of (1), our problem assumes the general form of an autonomous system of ODEs:

$$\frac{d}{dt}\mathbf{y}(t) = \mathbf{f}(\mathbf{y}(t)), \quad t > 0.$$

VODE_F90 is a Fortran 90 extension of the well-known VODE package [5] for the solution of stiff and non-stiff, autonomous and non-autonomous systems of ODEs. In the stiff case, it uses variable coefficient stiffly stable Backward Differentiation Formulas (BDF) [8]:

$$\sum_{i=0}^{q} \alpha_{n,i}\mathbf{y}^{n-i} + h_n\beta_n\mathbf{f}^n = 0,$$

of order q ranging from 1 to 5, with an automatic, adaptive technique for the selection of step sizes. In the above formulas, $\mathbf{y}^{n-i} \simeq \mathbf{y}(t_{n-i})$, $\mathbf{f}^n = \mathbf{f}(\mathbf{y}^n)$ and $h_n = t_n - t_{n-1}$. The stopping criterion of both solvers is based on a componentwise error control of the following type:

$$e_m \leq |y_m| Rtol_m + Atol_m, \quad m = 1, \dots, M, \tag{2}$$

where $\mathbf{Rtol} = (Rtol_1, \dots, Rtol_M)$ and $\mathbf{Atol} = (Atol_1, \dots, Atol_M)$ are two vectors representing relative and absolute error control tolerances, respectively. VODE_F90 allows the users to impose constraints on the solution, such as the non-negativity ones. The approach to impose constraints on the solution was to modify the original VODE predictor-corrector scheme in the following way:

i the predicted solution $\tilde{\mathbf{y}}^n$ is obtained by an explicit method as in VODE, but within an iterative procedure, where the step size is halved until the imposed solution constraints are verified;

ii the corrected solution $\mathbf{y}^n$ is found by solving the non linear system of equations $\mathbf{G}(\mathbf{x}) = 0$, where:

$$\mathbf{G}(\mathbf{x}) = \mathbf{x} - \tilde{\mathbf{y}}^n - h_n \beta_n / \alpha_{n,o} (\mathbf{f}(\mathbf{x}) - \mathbf{f}(\tilde{\mathbf{y}}^n)),$$

applying modified Newton iterations which are stopped when both the VODE componentwise error control in (2) and the imposed solution constraints are verified.

In our experiments, we set both the original VODE and VODE_F90 with $maxstep = 2500$ the maximum number of internal iterations, whereas a suitable order choice is demanded to the solver. Experimental results show that two different failure cases occur during our simulations, where both the solvers stop and make available a diagnostic of the failure as well as relevant information related to the state of the integration. In these cases, the last value of the solution is used as starting point for a new call to the solver on the rest of the current interval, using one of the two following restarting strategies:

Increasing iterations If $maxstep$ has been reached before completing the integration task on the current interval, the integration is attempted, maintaining the last order and step size used by the solver before the failure, within other 2500 internal iterations. This choice is related to the need of high accuracy in the solution of the intermediate species responsible of the ignition. In case of failure after the second solver call, the integration task on the rest of the current interval is attempted, within no more than 2500 internal iterations, by using the one-order formula (Backward Euler method), as also suggested by the solver in the diagnostic of the failure.

Changing formula If repeated error test failures occur on one attempted time step, we immediately consider the problem due to highly oscillating components, therefore the integration task is restarted by using the one-order formula. Also in this case $maxstep = 2500$.

3. Test Case

When a complete diesel engine simulation is performed, the effective ignition delay - defined as the time from the start of fuel injection to the time of pressure rise (when the absolute maximum value for temperature derivative is reached) - results not only from the gas phase kinetics evolution, but also from the spray break up and evaporation dynamics. Moreover, the phenomenon is highly non-homogeneous, thereby also the spatial distribution of chemical species, depending on the flow turbulence, affects the full simulation results. In order to isolate the effect of reaction kinetics, neglecting additional phenomena also relevant for engine simulations, a simplified environment has been chosen as preliminary test bench. In this way a preliminary validation of the combustion model can be performed and it is possible to focus on main numerical issues in very short computing times. The physical domain is an adiabatic constant volume vessel. Homogeneous initial conditions are applied, with an equivalence ratio (i.e. the ratio of the fuel-to-oxidizer ratio to the stoichiometric fuel-to-oxidizer ratio) equal to 0.5. Initial temperature and pressure have been chosen to resemble conditions relevant to diesel autoignition: initial temperature is fixed at $714K$ and initial pressure is equal to 42 bar. The adopted reaction scheme is a skeletal mechanism developed in [11] and involving $M = 44$ species and $R = 185$ reactions. It was reduced from a more detailed mechanism involving 168 species and 1008 elementary steps for the ignition and combustion of n-heptane [3]. Experimental data of the heptane ignition delay time at the mentioned initial conditions are available from shock tube experiments [6].

Numerical experiments have been carried out by interfacing both VODE and VODE_F90 with the KIVA3V-II code [1], in order to restart the solver at each splitting interval of the operator splitting procedure, applied for the solution of the Navier-Stokes equations modeling internal combustion engines. The CHEMKIN package [10] is used for setting the ODE systems describing the chemical scheme. The experiments have been carried out on an Intel Itanium 2 (Madison - 1.4 Ghz) processor, running Linux Red Hat Enterprise Rel. 3 and GNU 2.3.2 suite of compilers.

VODE with clipping strategy and VODE_F90, where positivity constraints were imposed, are compared in terms of:

- *accuracy* by means of temperature profile and OH mass fraction evolution. Observe that the OH radical can be considered as a combustion marker, indeed the OH mass fraction reaches its absolute maximum value when the high temperature phase starts;

- *computational efficiency* by means of the following counters: the number of integration step (NSTEP), the number of function evaluations (NFE), the number of Jacobian evaluations (NJE) and the number of LU factorizations (NLU) performed by the solvers during the simulation;
- *mass densities preservation* by means of the frequency distribution of the relative error values on the total mass density computed at the end of each time splitting interval.

In the first set of experiments, we compared the two solvers with different accuracy requests. While the values of the **Atol** components were set to 10^{-12} for the intermediate species and to 10^{-6} for the initial species and the main combustion products, all the components of **Rtol** were set to 10^{-2} in Fig. 1.(a),(c) and to 10^{-3} in Fig. 1.(b),(d). The global temperature profile produced by both the solvers is acceptable, the absolute maximum value of the temperature is reached at the times reported in Table 1 corresponding to the times where OH mass fraction reaches its absolute maximum values (see Fig. 1.(c) and 1.(d)). We observe that for each solver, when **Rtol** components decrease, the ignition point is advanced. However, in the VODE case, decreasing accuracy requests produces a greater loss of total mass density than VODE_F90, as we can see by Fig. 2, where the frequency distribution of the relative error on the total mass density is shown, and by Table 2, where the means E and the standard deviation σ of these distributions are reported. Therefore, as expected, total mass density preservation is a key issue in capturing ignition starting.

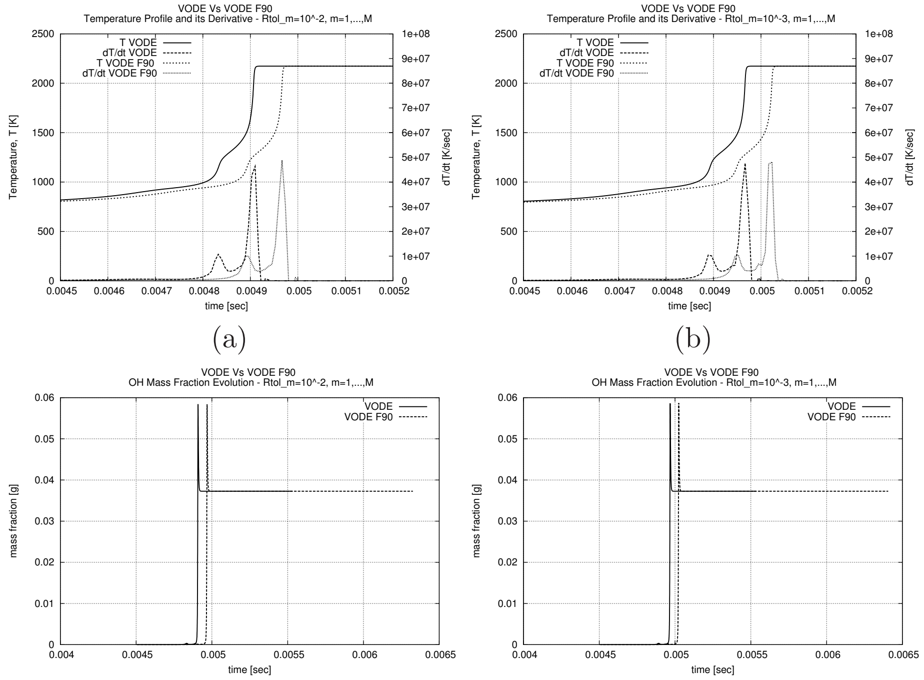
Table 1. Absolute maximum points for temperature

	$Rtol_m = 10^{-2}, \quad m = 1, \ldots, M$	$Rtol_m = 10^{-3}, \quad m = 1, \ldots, M$
VODE	4.91 ms	4.97 ms
VODE_F90	4.97 ms	5.02 ms

Table 2. Expectation and standard deviation of the relative error on the total mass density

	$Rtol_m = 10^{-2}, \quad m = 1, \ldots, M$		$Rtol_m = 10^{-3}, \quad m = 1, \ldots, M$	
	E	σ	E	σ
VODE	$0.79 \cdot 10^{-09}$	$0.18 \cdot 10^{-08}$	$0.14 \cdot 10^{-09}$	$0.15 \cdot 10^{-09}$
VODE_F90	$0.28 \cdot 10^{-13}$	$0.42 \cdot 10^{-13}$	$0.466 \cdot 10^{-14}$	$0.99 \cdot 10^{-14}$

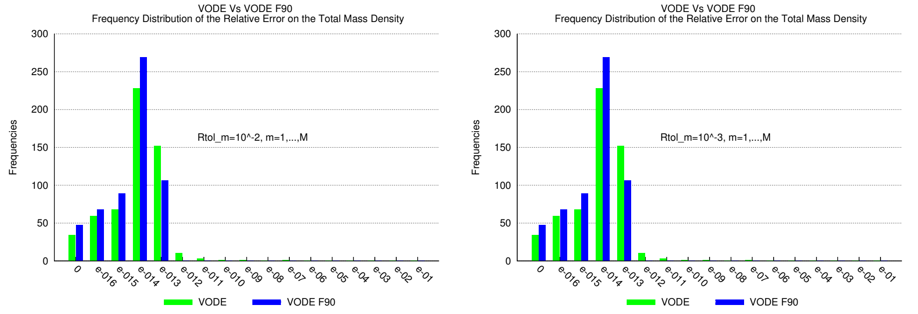
In Tab. 3, we show results related to computational efficiency. We note that



(a) (b)

(c) (d)

Fig. 1. *Temperature (and its derivative) values and OH mass fraction evolution when* $Rtol_m = 10^{-2}, \quad m = 1, \ldots, M$ *(a),(c) and* $Rtol_m = 10^{-3}, \quad m = 1, \ldots, M$ *(b),(d) are used for the solvers*



(a) (b)

Fig. 2. *Frequency distribution of the relative error on the total mass density with* $Rtol_m = 10^{-2}, \quad m = 1, \ldots, M$ *(a) and* $Rtol_m = 10^{-3}, \quad m = 1, \ldots, M$ *(b)*

counters increase in both solvers, in order to satisfy accuracy requests. In all the tests, when the same accuracy requests are imposed, VODE seems to be more efficient than VODE_F90, because VODE_F90 spends more in terms of NSTEP and NLU during the predictor-corrector procedure described in Section 2, in order to ensure the non-negativity condition. However, we observe that for $Rtol_m = 10^{-2}$, $m = 1, \dots, M$, VODE_F90 requires less values of NFE and NJE than VODE, while VODE for $Rtol_m = 10^{-3}$, $m = 1, \dots, M$, shows NFE, NJE and NLU counters less than that required for $Rtol_m = 10^{-2}, \quad m = 1, \dots, M$. Therefore, a more deep analysis is needed on this point, taking also into account previous considerations on the strong relation between total mass density preservation and accuracy in ignition prediction.

Table 3. Performance of the VODE solver versus VODE_F90 with different values of **Rtol** components

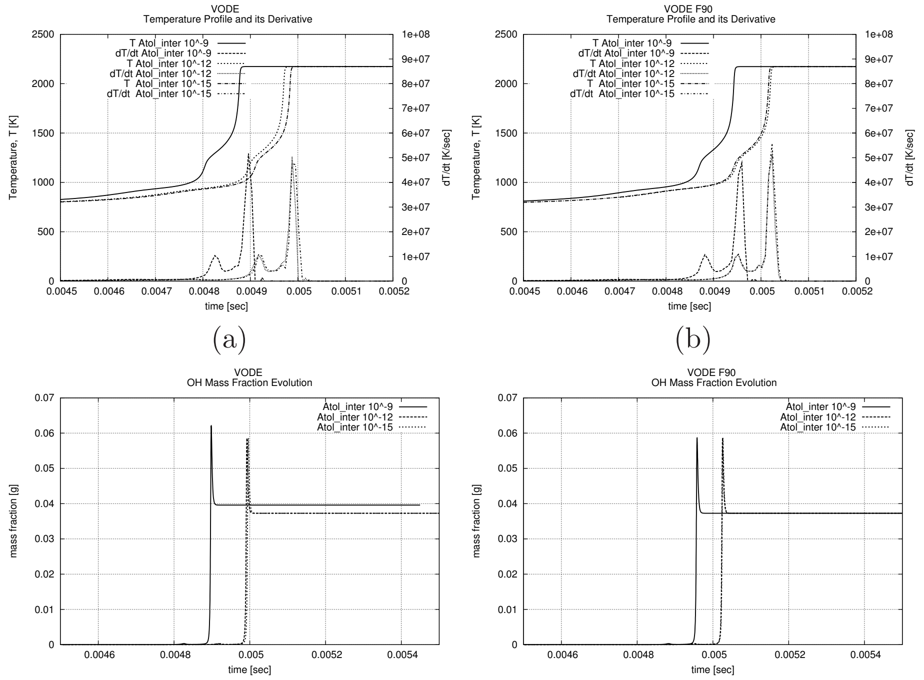
	$Rtol_m = 10^{-2}, \quad m = 1, \dots, M$			
	NSTEP	NFE	NJE	NLU
VODE	8006	44960	765	5819
VODE_F90	9016	38558	589	6804
	$Rtol_m = 10^{-3}, \quad m = 1, \dots, M$			
	NSTEP	NFE	NJE	NLU
VODE	12749	43242	605	5576
VODE_F90	14774	48035	623	6961

In the second set of experiments, we have considered different values of **Atol** components related to intermediates species, in order to enhance total mass density preservation property of the VODE solver. In the following we show results about three tests, in which we set all the vector components of **Rtol** to 10^{-3}, whereas the vector components of **Atol** (say $Atol_{inter}$), corresponding to intermediate chemical species, were set to 10^{-9}, 10^{-12} and 10^{-15}, respectively.

We observe in Fig. 3.(a),(b) that also in this case, increasing absolute tolerance leads to an earlier ignition point, as we can observe also from the times of maximum values for OH mass fraction (see Fig. 3.(c),(d)). The global temperature profile produced by both the solvers is compatible with the typical temperature behaviour for this test case, but decreasing absolute tolerances delays ignition time with respect to experimental measure, as we can see also from Table 4.

Table 4. Absolute maximum points for temperature

	$Atol_{inter} = 10^{-9}$	$Atol_{inter} = 10^{-12}$	$Atol_{inter} = 10^{-15}$
VODE	4.88 ms	4.97 ms	4.99 ms
VODE_F90	4.95 ms	5.02 ms	5.03 ms



(a) (b)

(c) (d)

Fig. 3. *Temperature (and its derivative) values and OH mass fraction evolution with different values of* $Atol_{inter}$*, carried out by VODE (a-c) and VODE_F90 (b-d)*

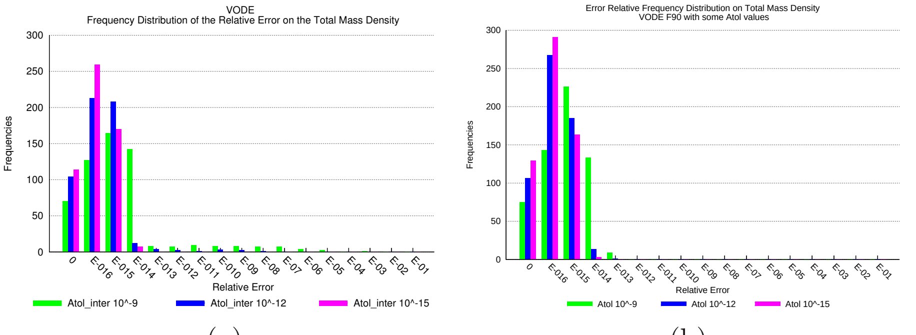
In Fig. 4.(a), 4.(b) and in Table 5, as expected, a sensible reduction of the total mass density loss can be observed for VODE, when $Atol_{inter}$ values are reduced. On the other hand, decreasing $Atol_{inter}$ values produce an increase of the computational cost of both solvers (see Table 6).

Table 5. Expectation and standard deviation of the relative error on the total mass density

	$Atol_{inter} = 10^{-9}$		$Atol_{inter} = 10^{-12}$		$Atol_{inter} = 10^{-15}$	
	E	σ	E	σ	E	σ
VODE	$0.93 \cdot 10^{-06}$	$0.21 \cdot 10^{-04}$	$0.22 \cdot 10^{-10}$	$0.35 \cdot 10^{-09}$	$0.69 \cdot 10^{-15}$	$0.10 \cdot 10^{-14}$
VODE_F90	$0.55 \cdot 10^{-14}$	$0.22 \cdot 10^{-13}$	$0.11 \cdot 10^{-14}$	$0.76 \cdot 10^{-14}$	$0.61 \cdot 10^{-15}$	$0.10 \cdot 10^{-14}$

4. Some conclusions and future work

In this work we carried out a preliminary analysis on the impact of positivity and total mass density preservation properties of some stiff ODE solvers on the prediction of ignition in numerical simulation of combustion.



(a) (b)

Fig. 4. *Frequency distribution of the relative error on the total mass density with different values of* $Atol_{inter}$ *produced by VODE (a) and VODE_F90 (b)*

Table 6. Performance of the VODE solver versus VODE_F90 with different values of $Atol_{inter}$ and $Rtol_m = 10^{-3}, \quad m = 1, \ldots, M$

	VODE			
$Atol_{inter}$	NSTEP	NFE	NJE	NLU
10^{-9}	10876	48210	755	5014
10^{-12}	18331	52757	676	6431
10^{-15}	21648	60800	773	7445
	VODE_F90			
$Atol_{inter}$	NSTEP	NFE	NJE	NLU
10^{-9}	12371	45618	616	6083
10^{-12}	22538	64918	756	9021
10^{-15}	29232	82081	930	12006

We have seen that ignition prediction is strongly related to total mass density preservation of the numerical method. On the other hand, positivity requirements imposed in the solution process, as in the VODE_F90 solver, guarantee better mass density preservation without recurring to very stringent absolute and relative error control tolerances. This can have a relevant impact on the computational cost of the simulations, since although positivity constraints in the ODE solution process introduce additional computational efforts than the usual clipping strategy, it reduces the needs of stringent accuracy requests leading to reduced overall computational costs. Future works will be devoted to carry on the above analysis for numerical simulation of combustion, when more detailed reaction schemes are involved.

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