



Estimating numerical errors due to operator splitting in global atmospheric chemistry models: Transport and chemistry



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ABSTRACT

We present upper bounds for the numerical errors introduced when using operator splitting methods to integrate transport and non-linear chemistry processes in global chemical transport models (CTM). We show that (a) operator splitting strategies that evaluate the stiff non-linear chemistry operator at the end of the time step are more accurate, and (b) the results of numerical simulations that use different operator splitting strategies differ by at most 10%, in a prototype one-dimensional non-linear chemistry–transport model. We find similar upper bounds in operator splitting numerical errors in global CTM simulations.

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1. Introduction

Global tropospheric chemistry transport models (CTM) are used to address important issues ranging from air quality to climate change. In order to continuously improve their performance, it is of crucial importance to understand and quantify the diverse sources of uncertainties and errors present in them. We group these in three different categories, (i) errors and uncertainties coming from observations and data used in our models (such as emission inventories, wind fields, reaction rates); (ii) errors coming from our choice of governing equations (or mathematical model), parametrizations, and the level of complexity of the physical modules included in our formulation; and (iii) numerical errors coming from the choice of algorithms we use to solve the governing equations using computers [5,30].

In this study, we focus our attention on estimating the magnitude of numerical errors (iii), in particular, those arising from the choice of operator splitting technique utilized to integrate in time the transport and chemistry operators in real-life global CTMs. In order to achieve this, we numerically extend the results introduced for the linear diffusion–reaction case in [26], to a non-linear 1-D chemistry–transport numerical model. The latter numerical results provide us with a framework to estimate upper bounds for operator splitting errors in the fully non-linear 3-D state-of-the-art global CTM: GEOS-Chem [2]. To the best of our knowledge, our contribution is the first in estimating operator splitting errors in the context of real-life global atmospheric chemistry simulations.

CTMs simulate the dynamics of chemical species in the atmosphere by numerically integrating a set of coupled nonlinear partial differential equations of the type:

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$$\frac{\partial C_i}{\partial t} + \nabla \cdot (\mathbf{u} C_i) = \nabla \cdot \left(\rho K \nabla \frac{C_i}{\rho} \right) + P_i(C_j) - C_i L_i(C_j) + Q_i - S_i \quad (1)$$

for $i = 1, \dots, N$; where $C_i(\mathbf{x}, t)$ represents the spatio-temporal evolution of the concentration of species i (typically over a hundred species are considered), $\mathbf{u}(\mathbf{x}, t)$ is the wind velocity, ρ is the air density, K the eddy diffusivity matrix, P_i are the nonlinear production terms, L_i are the destruction terms, Q_i are the volume emission sources, and S_i are the sinks (ex. precipitation or in-cloud removal). See [27] for a detailed description of these equations.

Due to the dimensions of grid boxes in global CTMs, like GEOS-Chem (with hundreds of kilometers in the horizontal versus tens to hundreds of meters in the vertical), inertial vertical transport processes in this global models are simulated (a) using vertical mass fluxes schemes that ensure that the horizontal air flow is divergent-free ($\nabla_{hor} \cdot \mathbf{u} = 0$), (b) using convection parametrizations, and (c) using a boundary layer mixing algorithm [14,1,29,20]. In addition, horizontal diffusion due to numerical errors in transport schemes are typically higher than their Eddy diffusivity counterpart, as measured by aircraft missions [19,29,23,25]. As a consequence, the first term of the right-hand side of equation (1), which models the dynamics of inertial vertical transport as an eddy diffusion process, is not explicitly integrated in global CTMs; and the governing equations (1) are sometimes written [23–25] in a simplified way as

$$\frac{\partial C_i}{\partial t} + \mathbf{u} \cdot \nabla C_i = P_i(C_j) - C_i L_i(C_j) + Q_i - S_i. \quad (2)$$

The chemistry operator on the right-hand-side of equations (2) models the chemical interaction of atmospheric species whose lifetimes range from milliseconds to many years. The chemistry operator is very stiff as a consequence of this large range of time-scales and thus, implicit-in-time methods are an appropriate choice to integrate equations (1). Traditional methods, such as the method of lines, aimed at achieving this task in realistic 3D simulations, involve solving for an enormous number of degrees of freedom at each time step in a coupled fashion ($10^8 \approx 100$ chemical species in $\sim 10^6$ grid cells, for a $1^\circ \times 1^\circ$ spatial resolution). This is due to the inter-species coupling in the chemistry operator and the spatial coupling in the transport operator. In practical situations, however, efficient computational algorithms to integrate equations (1) use operator splitting strategies that allow the explicit time-integration of the transport and implicit time-integration of the chemistry operators separately and sequentially, thus, reducing significantly the degrees of freedom solved in a coupled fashion at a given time step. This is done at the expense of a loss of accuracy in the approximate solution [8].

Estimating the magnitude of the numerical errors introduced by the time-integration of equations (1) in realistic 3-D computer simulations is a hard task since no relevant analytic solution can be used as a reference to estimate them. In theory, estimates of these errors depend directly on the regularity properties of the analytic solution of equations (1), the set of initial and boundary conditions, and the chosen numerical scheme [7,9,6,3]. In this study, we assume that the analytic solution of equations (1) is unique and regular enough so that numerical error estimates can be expressed as inequalities of the form (3). Operator splitting errors, as well as numerical errors arising from the time-integration of the chemistry operator depend explicitly on the magnitude of the chosen time steps, while numerical errors coming from the time-integration of the transport operator depend both on the time step and on the grid size. This fact, in combination with an expression of the analytic solution of equations (1), is exploited to obtain the exact magnitude of operator splitting errors in our one-dimensional proto-type transport–chemistry numerical model.

Our one-dimensional numerical experiments show three main results: (a) operator splitting sequences where the stiff non-linear chemistry operator is evaluated at the end of the time step are more accurate than those where the transport is evaluated lastly, independently of the operator splitting time-step, as in the linear case introduced in [26]; (b) the results of numerical simulations that use different operator splitting strategies differ by at most 10%; and (c) numerical errors coming from the integration of the transport operator are much bigger than those coming from the operator splitting technique for spatial and temporal scales comparable to those used in global CTM. We use this fact, and evidence from papers such as [29,23,20,25], to suggest that in realistic 3D simulations, errors due to operator splitting are much smaller than those introduced by transport schemes.

2. Numerical error estimation

Upper bounds of the numerical errors introduced by solving partial differential equations with regular boundary and initial conditions, using a given numerical scheme, can be expressed by inequalities represented as

$$\|C(x, t) - C_h(x, t)\|_{V_1} \leq M_1 \Delta t^\alpha + M_2 \Delta x^\beta \quad (3)$$

where $C(x, t)$ is the true solution of the partial differential equation, $C_h(x, t)$ the numerical approximation, Δt and Δx are the time step and grid size respectively, α and β are exponents (typically larger than one) that determine the order of convergence of the method in time and space respectively, M_1 and M_2 are constants that depend on the regularity of the true solution $C(x, t)$ and parameters in the equation, and $\|\cdot\|_{V_1}$ is the norm in the appropriate Banach space V_1 . For a convergent method, as $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, the numerical error vanishes, (i.e. $\|C - C_h\|_{V_1} \rightarrow 0$) and the numerical approximation C_h converges to the true solution C , in the normed space V_1 . More details about the integral representation (equation (3)) of numerical errors due to discretization of partial differential equations can be found in [7,9,6,3].

For the specific set of partial differential equations (1), operator splitting errors and errors coming from the numerical integration of the chemistry operator (where no coupling in space exists) contribute to the first term on the right-hand-side

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