Operator splitting and commutativity analysis in the Danish Eulerian Model

I. Dimov
Bulgarian Academy of Science, Sofia

I. Faragó and Á. Havasi
Eötvös Loránd University, Budapest

Z. Zlatev
National Environmental Research Institute, Roskilde, Denmark

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Abstract

In this paper the splitting error arising in the Danish Eulerian Model is investigated. Sufficient conditions under which the local splitting error vanishes are formulated for the continuous case. The numerical solution of the model problem introduces several other error sources, which makes the task of determining the effect of the splitting error more complicated. Therefore, we need numerical examples which will allow us to separate the splitting errors from the other errors in order to evaluate both the magnitude of these errors and the relationships between splitting errors and other errors for different values of the discretization parameters. Several such examples have been constructed and analysed. The appropriate conclusions were drawned. The experiences obtained from these experiments can be a starting step towards a total error analysis of the numerical solution of split systems of partial differential equations.

1 Introduction

Large air pollution models are based on the numerical solution of the transport-chemistry equations [2], describing all important physical and chemical processes that can cause changes in the concentrations of the different air pollutants. The Danish Eulerian Model (DEM) is a representative of such a kind of models. The reliable forecast of the pollutant concentrations in time and space requires efficient solution techniques for the transport-chemistry equations. This system contains several terms having completely different mathematical properties, which necessitates the application of operator splitting [7]. This procedure allows us to solve a few simpler systems instead of the original, complicated one.

Several splitting methods are used in large air pollution models. The procedure called physical splitting [1, 3] is based on a separation of the different "physical" sub-processes of pollution transport, namely, advection, turbulent diffusion, emission, deposition and chemical reactions. In each time-step of the numerical integration the systems describing these sub-processes are solved successively while they are coupled to each other through the initial conditions.

An alternative method is the one which has been implemented among others in the DEM and therefore will be called DEM splitting. This procedure differs from the physical splitting only in the fact that the sub-models are chosen not only on the base of the physical processes, but also on the spatial (vertical and horizontal) directions (see Section 2).

Obviously, the application of operator splitting will in general introduce error in the solution even if the sub-problems are solved exactly. Therefore, it is desirable that this error is zero or at least small in some sense. The splitting error that arises in one time-step, by the assumption that the exact solution is known at the beginning of the time-step, is called local splitting error. The order in which the local splitting error tends to zero as the splitting timestep-size tends to zero for a chosen splitting method is called the order of the applied splitting method [1, 3]. In order to evaluate both the magnitude of the splitting errors and the relationship between splitting errors and other errors for different values of the discretization parameters it is important to separate the splitting errors from other error sources.

In Section 2 we present the splitting procedure applied in the Danish Eulerian Model. In Section 3 we give sufficient conditions under which the splitting error vanishes in the DEM for all initial concentrations (L-commutativity analysis). Since in practice the transport-chemistry system can only be solved numerically, the direct applicability of the L-commutativity analysis is rather limited. The question of how the application of operator splitting influences the numerical results is therefore of great importance from a practical point of view. In Section 4 numerical results of solving simple test problems by using the DEM are introduced and the effect of operator splitting on the numerical solution is investigated. It is important to emphasize that by using these examples we have performed only the first steps in the attempts to evaluate the impact of the splitting errors on the results in comparison with the impact of other discretization errors.

2 Operator splitting in the Danish Eulerian Model

The Danish Eulerian Model (DEM) has been developed for studying the long-range transport of air pollutants over the European region [7, 8]. The model is based on the system of partial differential equations

$$\partial_t c_l + \sum_{i=1}^{3} \partial_i (u_i c_l) = \sum_{i=1}^{3} \partial_i (k_i \partial_i c_l) + E_l + R_l(\mathbf{x}, \mathbf{c}) + \sigma_l c_l, \tag{1}$$

$l = 1, \ldots, m$, with the corresponding initial and boundary conditions. The meanings of the different symbols and terms in (1) can be explained as follows. The symbols ∂_t and ∂_i denote differentiation with respect to the time t and the space variable x_i, respectively.

- The symbol $\mathbf{c} = (c_1, c_2, \ldots, c_m)^T$ denotes the unknown function $\mathbb{R}^4 \to \mathbb{R}^m$ if c_l is the concentration of the lth species and m is the number of species taken into account in the model; u_j, $j = 1, 2, 3$, denotes the jth component of the velocity vector $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$, and $k_j = k_j(\mathbf{x}, t)$, $j = 1, 2, 3$, the diffusion coefficient in the direction x_j.

- The second term on the left-hand side describes transportation due to the velocity field and is called advection term.

- The first term on the right-hand side expresses turbulent diffusion.
- The symbol E_l denotes the emission for the lth pollutant.
- Term $R_l(\mathbf{x}, \mathbf{c})$ represents chemical reactions w.r.t. the lth species which take place during the atmospheric transport of the pollutants. We remark that this term differs from the others in two important properties: 1. as opposed to the others, it is a usually non-linear (often quadratic) operator, and 2. it is the only term in (1) that depends not only on the concentration of the given species, but also that of the others, so the functions R_l map from $\mathbb{R}^{m+3}$ to $\mathbb{R}^m$. Without chemistry, the m equations in (1) would be independent of each other, i.e., instead of a system, we would have m scalar equations.
- The residual term $\sigma_l c_l$ describes the process of deposition, where σ_l is the deposition coefficient belonging to the lth species.

Let us denote with $\mathbf{E}$ and $\mathbf{R}$ the $\mathbb{R}^m$-valued functions with coordinate functions $E_1, E_2 \ldots, E_m$ and $R_1, R_2 \ldots, R_m$, respectively, and with σ the diagonal matrix $diag[\sigma_1, \ldots, \sigma_m]$. We will sometimes also use the notation $\mathbf{x}_h$ and $\mathbf{u}_h$ for the the horizontal space vector component (x_1, x_2) and the horizontal velocity vector component (u_1, u_2), respectively. Furthermore, if a differential operator D is applied to $\mathbf{c} : \mathbb{R}^4 \to \mathbb{R}^m$, this should be understood as the vector function $D\mathbf{c} := (Dc_1, Dc_2, \ldots, Dc_m)$, where the components $Dc_l, l = 1, \ldots, m$ are either scalar or $\mathbb{R}^3$-valued vector functions, e.g., $D\mathbf{c} := \sum_{i=1}^2 \partial_i(u_i\mathbf{c})$ means $(\sum_{i=1}^2 \partial_i(u_i c_1), \ldots, \sum_{i=1}^2 \partial_i(u_i c_m))$.

In the Danish Eulerian Model the system (1) is split into five simpler systems with the following sub-operators:

1. the operator of horizontal advection $A_1(\mathbf{c}) = -\sum_{i=1}^2 \partial_i(u_i\mathbf{c})$;
2. the operator of horizontal diffusion $A_2(\mathbf{c}) = \sum_{i=1}^2 \partial_i(k_i\partial_i\mathbf{c})$;
3. the deposition operator $A_3(\mathbf{c}) = \sigma\mathbf{c}$;
4. the operator of emission and chemistry $A_4(\mathbf{c}) = \mathbf{E} + \mathbf{R}(\mathbf{x}, \mathbf{c})$
5. and the operator of vertical transport $A_5(\mathbf{c}) = -\partial_3(u_3\mathbf{c}) + \partial_3(k_3\partial_3\mathbf{c})$.

This splitting procedure will be simply referred to as DEM splitting in the sequel.

3 L-commutativity of the operators in the DEM splitting

3.1 Splitting error and the notion of L-commutativity

The main aim of the first part of this paper is to formulate conditions under which the splitting error in the DEM vanishes for all initial concentrations. In this section we introduce some basic notions that will be frequently used in the sequel.

Let $\mathbf{S}$ be some normed space of mappings $\mathbb{R}^4 \to \mathbb{R}^m$ and A and B differentiable operators of type $\mathbf{S} \to \mathbf{S}$. The operator

$$E_{A,B}(\mathbf{s}) := (B'(\mathbf{s}) \circ A)(\mathbf{s}) - (A'(\mathbf{s}) \circ B)(\mathbf{s}) \tag{2}$$

is called *commutator* of the operators A and B. (Here $'$ refers to the derivative, so $A'(\mathbf{s})$ and $B'(\mathbf{s})$ are continuous linear operators of type $\mathbf{S} \to \mathbf{S}$.) We say that the operators A and B L-commute on the element $\mathbf{s} \in \mathbf{S}$, if $E_{A,B}(\mathbf{s}) = 0$. If $E_{A,B}(\mathbf{s}) = 0 \ \ \forall \mathbf{s} \in \mathbf{S}$, then we say that the operators A and B *L-commute*. We remark that if A and B are linear operators, then $A'(\mathbf{s}) = A$ and $B'(\mathbf{s}) = B$ for all $\mathbf{s} \in \mathbf{S}$. In this case the commutator of the operators means

$$E_{A,B}(\mathbf{s}) = (B \circ A)(\mathbf{s}) - (A \circ B)(\mathbf{s}), \tag{3}$$

i.e., the L-commutativity is equivalent to the usual commutativity.

The splitting error is strongly related to the above commutativity notion: the complicated error analysis (by use of the Baker–Campbell–Hausdorff formula [5]) shows (see for example [2]) that the splitting error vanishes *for all* initial functions if and only if all pairs of the sub-operators L-commute. In the next section we shall analyse the conditions of L-commutativity for all pairs of the sub-operators in the DEM splitting.

In order to analyse the conditions under which the sub-operators $A_i : \mathbf{S} \to \mathbf{S}, i = 1, \ldots, 5$, introduced in Section 2 for the DEM splitting, L-commute, we compute the derivatives of these operators.

All split operators, with the exception of A_4, are linear, therefore the relation $A_i'(\mathbf{c}) = A_i \quad \forall \mathbf{c} \in \mathbf{S}$ holds for $i = 1, 2, 3$ and 5. The emission term

in the operator A_4 is independent of the concentration vector, and so has a zero derivative. Consequently, the derivative of A_4 is equal to the derivative of the chemistry term.
Let $R_c(\mathbf{x}, \mathbf{c})$ denote the Jacobi matrix of the chemistry function $\mathbf{R}(\mathbf{x}, \mathbf{c}) = (R_1(\mathbf{x}, \mathbf{c}), R_2(\mathbf{x}, \mathbf{c}), \ldots, R_m(\mathbf{x}, \mathbf{c}))$ w.r.t. the variables $c_1, c_2, \ldots, c_m$, i.e.

$$(R_c(\mathbf{x}, \mathbf{c}))_{i,j} := \partial_j^c R_i(\mathbf{x}, \mathbf{c}), \quad i, j = 1, \ldots, m,$$

where the symbol ∂_j^c refers to differentiation w.r.t. the variable c_j. By using this notation, clearly we have

$$A_4'(\mathbf{c}) = R_c(\mathbf{x}, \mathbf{c}) \ \ \forall \mathbf{c} \in \mathbf{S}.$$

Here we need some further remarks concerning notation. Since the chemical function $\mathbf{R}(\mathbf{x}, \mathbf{c})$ depends on $\mathbf{c}$, and $\mathbf{c}$ depends on $\mathbf{x}$, $\mathbf{R}$ generally depends both explicitly and implicitly on $\mathbf{x}$. This may lead to some misunderstanding when using the symbol ∂_i. To avoid this, we introduce the symbol ∂_i^x to refer to differentiation w.r.t. the variable x_i, while ∂_i will denote differentiation w.r.t. the ith variable. For $i \in \{1, 2, 3\}$, the relation

$$\partial_i^x R_l(\mathbf{x}, \mathbf{c}) = \partial_i R_l(\mathbf{x}, \mathbf{c}) + \sum_{j=1}^{m} \partial_j^c R_l(\mathbf{x}, \mathbf{c}) \partial_i c_j \tag{4}$$

holds. This relation will be often used in the following. (Obviously, if $f = f(\mathbf{x})$, then $\partial_i f = \partial_i^x f$.) Moreover, for the sake of brevity, we will use the notation $E_{i,j} := E_{A_i, A_j}$ in the sequel.

3.2 Analysis of the commutators in the DEM splitting

In the sequel we move on to the investigation of the commutators of all pairs of sub-operators in the DEM splitting and formulating conditions under which these commutators vanish.

Clearly, for the first two operators we have

$$(E_{1,2}(\mathbf{c}))_l = \sum_{i,j=1}^{2} \partial_i(k_i \partial_i[-\partial_j(u_j c_l)]) + \sum_{i,j=1}^{2} \partial_i(u_i[\partial_j(k_j \partial_j c_l)]),$$

$l = 1, \ldots, m$. Aiming at getting a sufficient condition of commutativity, we impose the condition

$$\partial_i k_j = 0, \ i, j = 1, 2 \ \text{ and } \ \sum_{i=1}^{2} \partial_i u_i = 0. \tag{5}$$

(The latter condition expresses that the horizontal velocity field is divergence-free.) Then we are led to the result

$$(E_{1,2}(\mathbf{c}))_l = -\sum_{i,j=1}^{2} 2k_i(\partial_i u_j)\partial_i\partial_j c_l - \sum_{i,j=1}^{2} k_i(\partial_i^2 u_j)\partial_j c_l.$$

Consequently, when

$$\partial_j u_i = 0, \quad i,j = 1,2 \tag{6}$$

(i.e.,the horizontal velocity field is independent of the horizontal space coordinates), the operators A_1 and A_2 commute.

The commutator of the horizontal advection and deposition operators reads

$$(E_{1,3}(\mathbf{c}))_l = \sum_{i=1}^{2} \sigma_l(-\partial_i(u_i c_l)) + \sum_{i=1}^{2} \partial_i[u_i(\sigma_l c_l)] = \sum_{i=1}^{2} u_i c_l \partial_i \sigma_l.$$

Therefore, they commute if and only if the horizontal gradients of each deposition coefficients are orthogonal to the horizontal velocity field, i.e. the condition

$$\sum_{i=1}^{2} u_i \partial_i \sigma_l = 0 \tag{7}$$

holds for $l = 1, \ldots, m$.

For the commutator of the operators A_1 and A_4 we have

$$(E_{1,4}(\mathbf{c}))_l = [\sum_{i=1}^{2} R_c(\mathbf{x},\mathbf{c})(-\partial_i(u_i\mathbf{c}))]_l + \sum_{i=1}^{2} \partial_i^x[u_i R_l(\mathbf{x},\mathbf{c})] + \sum_{i=1}^{2} \partial_i(u_i E_l). \tag{8}$$

By a simple transformation, we get

$$[\sum_{i=1}^{2} R_c(\mathbf{x},\mathbf{c})(-\partial_i(u_i\mathbf{c}))]_l = \sum_{j=1}^{m}\sum_{i=1}^{2} (R_c(\mathbf{x},\mathbf{c}))_{l,j}(-\partial_i(u_i c_j)) =$$

$$-\sum_{j=1}^{m}\sum_{i=1}^{2} \partial_j^c R_l(\mathbf{x},\mathbf{c})((\partial_i c_j)u_i + c_j\partial_i u_i). \tag{9}$$

Then, by use of (4), the second term of (8) can be written as

$$\sum_{i=1}^{2} \partial_i^x[u_i R_l(\mathbf{x},\mathbf{c})] = \sum_{i=1}^{2} R_l(\mathbf{x},\mathbf{c})\partial_i u_i + \sum_{i=1}^{2} u_i \partial_i R_l(\mathbf{x},\mathbf{c}) + \sum_{i=1}^{2} u_i \sum_{j=1}^{m} \partial_j^c R_l(\mathbf{x},\mathbf{c})\partial_i c_j. \tag{10}$$

For the last term of (8) we have

$$\sum_{i=1}^{2} \partial_i(u_i E_l) = \sum_{i=1}^{2}(\partial_i u_i)E_l + \sum_{i=1}^{2} u_i\partial_i E_l. \tag{11}$$

Combining (9), (10) and (11) we obtain that

$$(E_{1,4}(\mathbf{c}))_l = -\sum_{j=1}^{m}\sum_{i=1}^{2} \partial_j^c R_l(\mathbf{x},\mathbf{c})c_j\partial_i u_i + \sum_{i=1}^{2} R_l(\mathbf{x},\mathbf{c})\partial_i u_i +$$

$$\sum_{i=1}^{2} u_i\partial_i R_l(\mathbf{x},\mathbf{c}) + \sum_{i=1}^{2}(\partial_i u_i)E_l + \sum_{i=1}^{2} u_i\partial_i E_l.$$

Suppose that the horizontal velocity field is divergence-free. Then $(E_{1,4}(\mathbf{c}))_l$ turns into zero if and only if

$$\sum_{i=1}^{2} u_i\partial_i R_l(\mathbf{x},\mathbf{c}) + \sum_{i=1}^{2} u_i\partial_i E_l = 0$$

for all $l = 1,\dots,m$. Therefore, if

$$\sum_{i=1}^{2} \partial_i u_i = 0, \quad R_l = R_l(\mathbf{c}) \;\text{ and } \partial_i E_l = 0, i = 1,2, \tag{12}$$

i.e., the velocity field is divergence-free, the functions R_l are explicitly independent of the horizontal space coordinates, and the horizontal gradients of each emission functions are orthogonal to the horizontal velocity field, then the operators A_1 and A_4 L-commute.

The commutator of the operators A_1 and A_5 has the form

$$(E_{1,5}(\mathbf{c}))_l = -\partial_3(u_3[-\sum_{i=1}^{2}\partial_i(u_i c_l)]) + \partial_3(k_3\partial_3[-\sum_{i=1}^{2}\partial_i(u_i c_l)]) +$$

$$\sum_{i=1}^{2}\partial_i(u_i[-\partial_3(u_3 c_l + \partial_3(k_3\partial_3 c_l))]).$$

Assume that the horizontal velocity is independent of height. Then we get

$$(E_{1,5}(\mathbf{c}))_l = -\sum_{i=1}^{2}\partial_3[(u_i c_l)\partial_i u_3] + \sum_{i=1}^{2} u_i(\partial_i\partial_3 k_3)\partial_3 c_l + \sum_{i=1}^{2} u_i(\partial_i k_3)\partial_3^2 c_l. \tag{13}$$

Then under the conditions

$$\partial_i u_3 = 0,\ \ i = 1,2 \ \text{ and } \partial_i k_3 = 0,\ \ i = 1,2, \tag{14}$$

i.e., the vertical velocity is independent of the horizontal space coordinates and the vertical diffusion coefficients are independent of the horizontal space coordinates, the operators A_1 and A_5 commute.

Applying again the definition of the commutator, we have

$$(E_{2,3}(\mathbf{c}))_l = \sum_{i=1}^{2} \sigma_l(\partial_i[k_i(\partial_i c_l)]) - \sum_{i=1}^{2} \partial_i(k_i[\partial_i(\sigma_l c_l)]) =$$

$$-\sum_{i=1}^{2} k_i(\partial_i c_l)\partial_i \sigma_l - \sum_{i=1}^{2} \partial_i(k_i c_l \partial_i \sigma_l).$$

This yields that the operators A_2 and A_3 commute if and only if

$$\partial_i \sigma_l = 0, \quad i = 1,2 \tag{15}$$

is satisfied for all $l = 1, \ldots, m$, i.e. $\sigma_l = const$ along horizontal planes.

The lth component of the commutator of the operators A_2 and A_4 has the form

$$(E_{2,4}(\mathbf{c}))_l = [R_c(\mathbf{x},\mathbf{c})\sum_{i=1}^{2}(\partial_i[k_i\partial_i\mathbf{c}])]_l - \sum_{i=1}^{2}\partial_i^x[k_i\partial_i^x R_l(\mathbf{x},\mathbf{c})] - \sum_{i=1}^{2}\partial_i(k_i\partial_i E_l) =$$

$$\sum_{j=1}^{m}\sum_{i=1}^{2}\partial_j^c R_l(\mathbf{x},\mathbf{c})(\partial_i[k_i\partial_i c_j]) - \sum_{i=1}^{2}\partial_i^x[k_i\partial_i^x R_l(\mathbf{x},\mathbf{c})] - \sum_{i=1}^{2}\partial_i(k_i\partial_i E_l). \tag{16}$$

Using the relation $\partial_i^x R_l(\mathbf{x},\mathbf{c}) = \partial_i R_l(\mathbf{x},\mathbf{c}) + \sum_{j=1}^{m}\partial_j^c R_l(\mathbf{x},\mathbf{c})\partial_i c_j$, the expression (16) can be written as

$$(E_{2,4}(\mathbf{c}))_l = -\sum_{i=1}^{2}\partial_i^x(k_i\partial_i R_l(\mathbf{x},\mathbf{c})) - \sum_{j=1}^{m}\sum_{i=1}^{2}[\partial_i[\partial_j^c R_l(\mathbf{x},\mathbf{c})]k_i\partial_i c_j]$$

$$-\sum_{j=1}^{m}\sum_{r=1}^{m}\sum_{i=1}^{2}\partial_r^c\partial_j^c R_l(\mathbf{x},\mathbf{c})(\partial_i c_r)k_i\partial_i c_j - \sum_{i=1}^{2}\partial_i(k_i\partial_i E_l). \tag{17}$$

By use of (17) one can see that if the conditions

$$\partial_1 R_l(\mathbf{x},\mathbf{c}) = \partial_2 R_l(\mathbf{x},\mathbf{c}) = 0 \text{ and } \partial_r^c \partial_j^c R_l(\mathbf{x},\mathbf{c}) = 0 \text{ for all } r,j = 1,\dots,m \tag{18}$$

are simultaneously satisfied and

$$\partial_i E_l = 0, i = 1,2 \tag{19}$$

then the operators L-commute. The equation (19) can be replaced by the two conditions

$$k_1(\mathbf{x},t) = k_2(\mathbf{x},t) = const \text{ and } \sum_{i=1}^{2} \partial_i^2 E_l = 0. \tag{20}$$

In turn, we have

$$(E_{2,5}(\mathbf{c}))_l = -\partial_3(u_3 \sum_{i=1}^{2}[\partial_i(k_i\partial_i c_l)]) + \partial_3(k_3\partial_3 \sum_{i=1}^{2}[\partial_i(k_i\partial_i c_l)]) +$$
$$\sum_{i=1}^{2} \partial_i(k_i\partial_i[\partial_3(u_3 c_l) - \partial_3(k_3\partial_3 c_l)]).$$

In order to simplify our task, we impose the conditions

$$\partial_j u_3 = 0,\ j = 1,2,3 \text{ and } \partial_3 k_i = 0,\ i = 1,2, \tag{21}$$

i.e., the vertical velocity is independent of space and the horizontal diffusion coefficients are independent of height. Then for the commutator we get

$$(E_{2,5}(\mathbf{c}))_l = -\sum_{i=1}^{2}(\partial_i k_i)(\partial_i\partial_3 k_3)\partial_i c_l - \sum_{i=1}^{2} k_i(\partial_i^2\partial_3 k_3)\partial_3 c_l - \sum_{i=1}^{2} 2k_i(\partial_i\partial_3 k_3)\partial_i\partial_3 c_l -$$
$$\sum_{i=1}^{2}(\partial_i k_i)(\partial_i k_3)\partial_3^2 c_l - \sum_{i=1}^{2} k_i(\partial_i^2 k_3)\partial_3^2 c_l - \sum_{i=1}^{2} 2k_i(\partial_i k_3)\partial_i\partial_3^2 c_l, \quad (i = 1,2).$$

Therefore, if in addition we assume that

$$\partial_j k_3 = 0,\ j = 1,2, \tag{22}$$

i.e., the vertical diffusion coefficient is independent of the horizontal space coordinates, then the operators A_2 and A_5 commute.

The lth component of the commutator of the operators A_3 and A_4 reads

$$(E_{3,4}(\mathbf{c}))_l = [R_c(\mathbf{x},\mathbf{c})(\sigma\mathbf{c})]_l - \sigma_l R_l(\mathbf{x},\mathbf{c}) - \sigma_l E_l =$$

$$\sum_{j=1}^{m}[\partial_j^c R_l(\mathbf{x},\mathbf{c})]\sigma_j c_j - \sigma_l R_l(\mathbf{x},\mathbf{c}) - \sigma_l E_l.$$

Consequently, the operators A_3 and A_4 do not L-commute in any realistic case.

The lth component of the commutator for the operators A_3 and A_5 has the form

$$(E_{3,5}(\mathbf{c}))_l = -\partial_3(u_3\sigma_l c_l) + \partial_3[k_3\partial_3(\sigma_l c_l)] - \sigma_l[-\partial_3(u_3 c_l) - \partial_3(k_3\partial_3 c_l)] =$$

$$-u_3 c_l\partial_3\sigma_l + k_3(\partial_3 c_l)\partial_3\sigma_l + \partial_3(k_3 c_l\partial_3\sigma_l).$$

Therefore, if

$$\partial_3\sigma_l = 0 \tag{23}$$

i.e., the deposition coefficients are independent of height, then the operators A_3 and A_5 commute.

The lth component of the operators A_4 and A_5 can be written as

$$(E_{4,5}(\mathbf{c}))_l = -\partial_3^x[u_3 R_l(\mathbf{x},\mathbf{c})] + \partial_3^x[k_3\partial_3^x R_l(\mathbf{x},\mathbf{c})]$$

$$-[R_c(\mathbf{x},\mathbf{c})(-\partial_3[u_3\mathbf{c}] + \partial_3[k_3\partial_3\mathbf{c}])]_l - \partial_3(u_3 E_l) + \partial_3(k_3\partial_3 E_l) =$$

$$-u_3\partial_3 R_l(\mathbf{x},\mathbf{c}) - R_l(\mathbf{x},\mathbf{c})\partial_3 u_3 + k_3\partial_3^x(\partial_3 R_l(\mathbf{x},\mathbf{c})) + (\partial_3 k_3)\partial_3 R_l(\mathbf{x},\mathbf{c}) +$$

$$k_3\sum_{j=1}^{m}\partial_3[\partial_j^c R_l(\mathbf{x},\mathbf{c})]\partial_3 c_j + k_3\sum_{r=1}^{m}\sum_{j=1}^{m}\partial_r^c\partial_j^c R_l(\mathbf{x},\mathbf{c})\partial_3 c_r\partial_3 c_j$$

$$+\sum_{j=1}^{m}\partial_j^c R_l(\mathbf{x},\mathbf{c})c_j\partial_3 u_3 - E_l\partial_3 u_3 - u_3\partial_3 E_l + k_3\partial_3^2 E_l + (\partial_3 k_3)\partial_3 E_l. \tag{24}$$

So, under the assumptions

$$\partial_3 u_3 = 0, \quad \mathbf{R} = \mathbf{R}(x,y,\mathbf{c}), \quad \partial_l^c\partial_j^c R_l(\mathbf{x},\mathbf{c}) = 0 \ \text{ and } \partial_3\mathbf{E} = 0, \tag{25}$$

i.e., the vertical velocity, $\mathbf{R}$ (explicitly) and the emission are independent of height, and for $\mathbf{R}$ also the third condition is satisfied, then the operators A_4

and A_5 L-commute.

In Table 1 we summarize the conditions of the L-commutativity of each pair of operators in the DEM splitting.

Table 1. Conditions of L-commutativity in the DEM.

Pair of operators	Condition
A_1, A_2	(5), (6)
A_1, A_3	(7)
A_1, A_4	(12)
A_1, A_5	(14)
A_2, A_3	(15)
A_2, A_4	(18), (20)
A_2, A_5	(21), (22)
A_3, A_4	do not L-commute
A_3, A_5	(23)
A_4, A_5	(25)

4 Test problems for investigating the effect of the splitting error

As it was mentioned in the previous section, if the sub-operators L-commute in a splitting procedure, then the local splitting error is zero, so the exact solution of the sequence of problems obtained by splitting gives the exact solution of the original problem. However, if the operators do not L-commute, then usually some error arises from the application of splitting. The situation is more complicated when the sub-problems are solved numerically, which is usually the case in practice. Then generally five error sources may influence the results: 1. the error of the spatial discretization method, 2. the error of the time integration method, 3. the rounding errors, 4. the splitting error and 5. inconsistencies arising when boundary conditions are imposed to the sub-problems. (It is shown in ([3]) that defining boundary conditions for the sub-problems is not a trivial task and usually causes error in the solution.) In general, the effects of these error sources cannot be separated from each other. In practice, when the exact solution is unknown, even the total error is very difficult to quantify.

In this section we construct such test problems of partial differential equations for the DEM, which will allow us to draw general conclusions about the interaction of the different error sources. Further, it is highly desirable to check by numerical experiments that the theoretically derived results for the continuous sub-problems are not deteriorated when these problems are discretized and handled numerically. However, this is only the beginning procedure and much more efforts are needed for investigating the effect of the splitting error on the numerical results. For simplicity, only advection and emission terms are present. The advection is given by the Molenkampf–Crowley operator defined as

$$A_1(c) = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y}. \tag{26}$$

This describes a circular motion of the pollutant particles with constant angular velocity around the origin. This type of advection has widely been used for testing numerical algorithms developed for solving the advection equation [7].

An important common feature of the chosen test examples was the knowledge of the analytic solutions of a) the original problem, b) the sequence of problems obtained by splitting and c) each of the sub-problems. We defined pure initial value problems, because the introduction of boundary conditions makes the task rather complicated.

4.1 The numerical discretization of the test problems

The examples were treated both directly and by using splitting. The same numerical method was applied to the solution of the problems in all cases: we used linear finite elements for the space discretization and a fourth-order predictor-corrector scheme for the time integration. It was necessary to define a limited spatial domain and boundary conditions for the numerical disretization of the test problems. The spatial domain was chosen to be the unit square in the 2-D case and the unit cube in the 3-D case. If we want to reveal the relationship between the errors caused by the discretization parameters and the splitting errors, then we must try to eliminate the effect due to the need of boundary conditions in the numerical procedures. An attempt to eliminate the effect of errors caused by imposing boundary conditions during the numerical treatment of the discretized problems (or sub-problems) has been made by using Dirichlet boundary conditions (both for the original problem and the sub-problems, when appropriate), which are equivalent to the values of the exact solutions of the treated problems (sub-problems) on the boundary. In this way the numerical solution of the problem (sub-problem) will always be sufficiently accurate when the discretization parameters are sufficiently small. when comparing the numerical and the theoretical results.

Different equidistant grids were used during the numerical solutions. Assume that N_x and N_y are the numbers of grid-points in the Ox and Oy axes, respectively. Then at every time-step n, $n = 1, 2, \ldots, N_t$, approximations of the solution at the $N_x \times N_y$ grid-points are to be calculated. We shall denote these approximations

$$c_{i,j,n} \approx c(x_i, y_j, t_n), \quad i \in 1, 2, \ldots, N_x, \ \ j \in 1, 2, \ldots, N_y, \ \ n \in 1, 2, \ldots, N_t. \tag{27}$$

and the error ERR_n at time-step n is evaluated by

$$ERR_n = \frac{DIFFERENCE_n}{MAXVALUE_n} \tag{28}$$

where

$$DIFFERENCE_n = \max_{i=1,2,\ldots,N_x,\ j=1,2,\ldots,N_y} (\mid c_{i,j,n} - c(x_i, y_j, t_n) \mid) \tag{29}$$

and

$$MAXVALUE_n = \max_{i=1,2,\ldots,N_x,\ j=1,2,\ldots,N_y} (\mid c(x_i, y_j, t_n) \mid). \tag{30}$$

The global error ERRMAX (which is the error over the whole time-integration interval) is evaluated by

$$ERRMAX = \max_{n=1,2,\ldots,N_t} (ERR_n). \tag{31}$$

The values of $ERRMAX$, rounded to the third digit, will be considered in the following part.

4.2 Test problems with two-dimensional advection

In this section we consider two problems of the form

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + E(x, y, t). \tag{32}$$

We split the right-hand side into the sum of the Molenkampf–Crowley advection term $A_1(c) = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y}$ and the emission term $A_4(c) = E$.

4.2.1 Problem 1

First we set $E = 1$ and consider the initial value problem
Problem 1

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + 1, \quad t \in (0, 1] \qquad c(x, y, 0) = x^2 + y^2. \tag{33}$$

Clearly, in this case, due to (12) the commutator turns into zero, so no splitting error arises in the continuous case. This problem has the exact solution

$$c(x, y, t) = x^2 + y^2 + t. \tag{34}$$

Assume that the calculations have been performed up to some time level t_{n-1} and the solution at time t_n has to be found.

When Problem 1 is solved without splitting, in the nth time-step we use the boundary condition, corresponding to the exact solution (34).

Due to the linearity in time, the time integration scheme does not cause any error in this case, but the space discretization with linear finite elements may cause errors. Thus, it is expected that refining the spatial grid leads to a reduction of the error, while reducing the time-step has no effect on the error.

When Problem 1 is solved by using splitting, the calculations in each time-step are carried out in two parts. (The splitting time-step equals the time-step of the time integration.) First the advection part is handled, which means that the problem

$$\frac{\partial c_n^{(1)}}{\partial t} = y\frac{\partial c_n^{(1)}}{\partial x} - x\frac{\partial c_n^{(1)}}{\partial y}, \qquad c_n^{(1)}(x, y, t_{n-1}) = c_{n-1}^{(2)}(x, y, t_{n-1}) \tag{35}$$

is solved, where the lower index n denotes that the function should be considered on the time interval $[t_{n-1}, t_n]$. The second part of the work consists of the solution of

$$\frac{\partial c_n^{(2)}}{\partial t} = 1, \quad c_n^{(2)}(x, y, t_{n-1}) = c_n^{(1)}(x, y, t_n), \tag{36}$$

which is trivial.

There should be no errors due to the application of this splitting procedure and no errors due to the time integration method. The errors are caused by a.) the use of linear finite elements in the advection parts and b.) the rounding errors. Some results which were obtained in the treatment of Problem 1, are given in Table 2 and 3.

The results that are given in Table 2 show that the rounded to the third digit values of $ERRMAX$ are the same for the two cases. Moreover, it is seen that the errors are decreasing as the grid is refined.

The results given in Table 3 show that the errors do not depend on the lenght of the time-steps.

Table 2. The values of $ERRMAX$ obtained when Problem 1 is solved without splitting and with splitting (the values for the same grid are equal when rounded to three digits because all computations are carried out in double precision). The factors by which the errors are reduced when the grids are refined are given in the fourth column. The discrepancies, $100(Expected\ factor - Computed\ factor)/(Expected\ factor)$, are given in brackets (all discrepancies are less than 16%). The expected reduction factors are given in last column.

Grid	Without splitting	With splitting	Computed factor	Expected factor
16×16	1.47E-3	1.47E-3	-	-
32×32	3.97E-4	3.97E-4	3.70 (7.5%)	4
96×96	4.67E-5	4.67E-5	31.48 (13.9%)	36
288×288	5.35E-6	5.35E-6	274.77 (15.2%)	324
480×480	1.94E-6	1.94E-6	757.73 (15.8%)	900

Table 3. The values of $ERRMAX$ obtained when Problem 1 is solved by using different time-steps Δt without splitting and with splitting. The 16×16 grid is used in the discretization of the spatial derivatives. The experiment shows that the values of $ERRMAX$ does not depend on the lenght of time-steps. As in the previous table, these values remain the same both when no splitting is used and when splitting is applied.

Time-step Δt	Without splitting	With splitting
$3.33E-3$	1.47E-3	1.47E-3
$6.67E-3$	1.47E-3	1.47E-3
$6.67E-4$	1.47E-3	1.47E-3

4.2.2 Problem 2

In the second example we choose the emission operator as

$$E(x, y, t) = 1 + x - y, \tag{37}$$

and consider the problem

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + 1 + x - y, \quad t \in (0, 1], \qquad c(x, y, 0) = x + y. \tag{38}$$

In this case the advection and the emission operator do not L-commute, and the local splitting error is $\mathcal{O}(\tau^2)$. The exact solution of this problem is given by

$$c(x, y, t) = x + y + t. \tag{39}$$

Neither the time integration scheme causes error in this case, nor the linear finite elements. Thus, the solution obtained when no splitting is applied is the exact one (apart from the rounding errors) for all grids and for any number of time-steps which ensures stable computations. This fact is illustrated by the second coloumn of Table 4.

In the case when splitting is used, first the following sub-problem is solved on the interval $[t_{n-1}, t_n]$:

$$\frac{\partial c_n^{(1)}}{\partial t} = y\frac{\partial c_n^{(1)}}{\partial x} - x\frac{\partial c_n^{(1)}}{\partial y}, \tag{40}$$

$$c_n^{(1)}(x, y, t_{n-1}) = c_{n-1}^{(2)}(x, y, t_{n-1}). \tag{41}$$

Note that the exact solution of (40) (by assuming calculations without rounding errors during the whole splitting procedure, starting from the initial value $c(x, y, 0) = x + y$ is

$$c_n^{(1)}(x, y, t) = x[\cos(t-t_{n-1}) - \sin(t-t_{n-1})] + y[\cos(t-t_{n-1}) + \sin(t-t_{n-1})] + t_{n-1}. \tag{42}$$

The values of this exact solution at the boundaries of the space domain are used to determine the boundary conditions during the advection part.

The second part of the work in the nth time-step consists of the solution of the problem

$$\frac{\partial c_n^{(2)}}{\partial t} = 1 + x - y, \quad c_n^{(2)}(x, y, t_{n-1}) = c_n^{(1)}(x, y, t_n), \tag{43}$$

which is trivial.

The two sub-problems obtained when the above splitting procedure is applied are treated without any errors (apart from the rounding errors) for any spatial grid and for any number of time-steps (providing that the number is sufficiently large, so that the stability of the computations is ensured). However, the splitting procedure may produce errors, because the advection and the emission operator do not L-commute in this case.

Some results, which have been obtained in the treatment of Example 2, are given in Table 4 and Table 5.

The results that are given in Table 4 show that the values of $ERRMAX$ are about 10 order bigger when splitting is applied, however they are practically the same for the different grids both when splitting is used and when no splitting is applied.

The results that are given in Table 5 show that the errors depend on the number of time-steps when splitting is used, while these remain practically the same when no splitting is used. As we mentioned before, the local splitting error is first order. It is seen from Table 5 that the value of $ERRMAX$ is inversely proportional to the number of time-steps (proportional to the length of the splitting time-step), so the global error seems to be only $\mathcal{O}(\tau)$.

Table 4. The values of $ERRMAX$ obtained when Example 2 is solved without splitting and with splitting (the number of time-steps is 1500 for all grids, but the values of $ERRMAX$ are rather insensitive to variations of the number of the time-steps when no splitting is used). The values of $ERRMAX$ are close to the machine precision when no splitting is used. The values of $ERRMAX$ are of order $O(10^{-4})$ for all grids when the splitting procedure is applied.

Grid	Without splitting	With splitting
8×8	3.34E-14	1.70E-4
16×16	3.79E-14	1.80E-4
32×32	3.99E-14	1.80E-4
96×96	7.21E-14	1.97E-4
288×288	4.57E-14	1.99E-4
480×480	4.28E-14	1.99E-4

Table 5. The values of $ERRMAX$ obtained when Example 2 is solved by using different numbers of time-steps without splitting and with splitting. The 16×16 grid is used in the discretization of the spatial derivatives. The experiment shows that the values of $ERRMAX$ does not depend on the number of time-steps when no splitting is used, while in the case where splitting is applied, the values of $ERRMAX$ are reduced when the number of steps is increased.

Steps	Stepsize	Without splitting	With splitting
10	0.1	4.35E-14	2.42E-2
100	0.01	4.36E-15	2.39E-3
1000	0.001	5.76E-14	2.39E-4
10000	0.0001	7.24E-13	2.39E-5

4.3 A test problem with three-dimensional advection

In this sub-section we consider a problem of the form

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + w(x,y,z,t)\frac{\partial c}{\partial z} + E(x,y,z,t), \quad t \in (0,1] \tag{44}$$

$$c(x,y,z,0) = c_0(x,y,z), \tag{45}$$

which describes concentration changes in a velocity field whose horizontal projection is the Molenkampf–Crowley rotation. We remark that in this case the algorithms of the physical splitting and the DEM splitting are different.

By direct substitution into (8), (13) and (24) we obtain that the exact condition of L-commutativity of all three pairs of operators in the above problem with constant vertical velocity ($w = 1$) in the DEM splitting is

$$y\frac{\partial E}{\partial x} - x\frac{\partial E}{\partial y} = 0, \quad \text{and} \quad \frac{\partial E}{\partial z} = 0, \tag{46}$$

while for the physical splitting we obtain the condition

$$y\frac{\partial E}{\partial x} - x\frac{\partial E}{\partial y} + \frac{\partial E}{\partial z} = 0. \tag{47}$$

This condition is satisfied if and only if E has the form

$$E(x, y, z, t) = \phi(y\cos z + x\sin z, -y\sin z + x\cos z, t), \tag{48}$$

where ϕ is any sufficiently smooth function of three variables.

Let us consider an example of the case when the operators L-commute in the physical splitting, but not in the DEM splitting:

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + \frac{\partial c}{\partial z} + y(\cos z - \sin z) + x(\sin z + \cos z) \quad t \in [0, 1] \tag{49}$$

$$c(x, y, z, 0) = e^z(x^2 + y^2) \tag{50}$$

The solution of this problem is

$$c(x, y, z, t) = e^{z+t}(x^2 + y^2) + t[y(\cos z - \sin z) + x(\sin z + \cos z)]. \tag{51}$$

Both the time-integration scheme and the linear finite elements may cause errors in this case. Since the applied time-integration method is of order 4, the errors caused by the spatial discretization are dominant (in fact, if the calculations are stable, then it practically does not matter how large is the timestep-size).

When physical splitting is applied to Problem 3, then first the advection equation

$$\frac{\partial c_n^{(1)}}{\partial t} = y\frac{\partial c_n^{(1)}}{\partial x} - x\frac{\partial c_n^{(1)}}{\partial y} + \frac{\partial c_n^{(1)}}{\partial z} \tag{52}$$

is solved with the initial condition

$$c_n^{(1)}(x, y, z, t_{n-1}) = e^{z+t_{n-1}}(x^2 + y^2) + t_{n-1}[y(\cos z - \sin z) + x(\sin z + \cos z)]. \tag{53}$$

The second step is the solution of the emission sub-problem

$$\frac{\partial c_n^{(2)}}{\partial t} = y(\cos z - \sin z) + x(\sin z + \cos z) \tag{54}$$

by using the initial condition

$$c_n^{(2)}(x,y,z,t_{n-1}) = c_n^{(1)}(x,y,z,t_n), \tag{55}$$

which is trivial. The calculations at any time-step n are now carried out in three parts. Assume again that the calculations have been completed up to some time-step t_{n-1}.
First the horizontal advection is handled, which means that the following problem is to be solved:

$$\frac{\partial c_n^{(1)}}{\partial t} = y\frac{\partial c_n^{(1)}}{\partial x} - x\frac{\partial c_n^{(1)}}{\partial y} \tag{56}$$

with the initial condition

$$c_n^{(1)}(x,y,z,t_{n-1}) = e^{z+t_{n-1}}(x^2+y^2) + t_{n-1}[y(\cos z - \sin z) + x(\sin z + \cos z)]. \tag{57}$$

The treatment of the emission sub-model is the second action at the nth time-level, i.e., the solution of the problem.

$$\frac{\partial c_n^{(2)}}{\partial t} = y(\cos z - \sin z) + x(\sin z + \cos z) \tag{58}$$

$$c_n^{(2)}(x,y,z,t_{n-1}) = c_n^{(1)}(x,y,z,t_n). \tag{59}$$

The third step consists of the treatment of the vertical advection equation

$$\frac{\partial c_n^{(3)}}{\partial t} = \frac{\partial c_n^{(3)}}{\partial z} \tag{60}$$

with the initial condition

$$c_n^{(3)}(x,y,z,t_{n-1}) = c_n^{(2)}(x,y,z,t_n). \tag{61}$$

With a simple, but cumbersome calculation we can determine the exact solution of the problem, so we can compute the exact errors. Some results, which were obtained in the treatment of Problem 3, are given in Table 6.

Table 6. Values of $ERRMAX$ obtained when Problem 3 is solved with the DEM splitting by using different numbers of time-steps and different spatial grids.

Time-step Δt	16x16x16	32x32x32	64x64x64	128x128x128
8.0E-3	1.58E-2	1.92E-2	unstable	unstable
4.0E-3	7.99E-3	9.03E-3	unstable	unstable
2.0E-3	4.03E-3	4.55E-3	5.07E-3	unstable
1.0E-3	2.22E-3	2.33E-3	2.53E-3	unstable
5.0E-4	1.32E-3	1.22E-3	1.28E-3	1.35E-3
2.5E-4	1.00E-3	6.73E-4	6.58E-4	6.74E-4
1.25E-4	1.02E-3	4.02E-4	3.47E-4	3.43E-4
6.25E-5	1.03E-3	2.96E-4	1.91E-4	1.77E-4
3.125E-5	1.03E-3	2.95E-4	1.14E-4	9.32E-5
1.5625E-5	1.03E-3	2.94E-4	8.11E-5	5.15E-5
7.8125E-6	1.03E-3	2.94E-4	8.09E-5	3.07E-5
3.90625E-6	1.03E-3	2.94E-4	8.08E-5	2.15E-5

Our main conclusions are as follows.

- Assume that no splitting is used and the grid is fixed. Then the results are practically independent of the timestep-size (in the sense that if the time-integration is stable, then the errors are practically the same for all time-stepsizes).

- The observed convergence is nearly linear until the error become comparable with the error achieved when no splitting is used. To check this we are keeping the reduction of the time-stepsize (by increasing the number of time-steps) until the errors in two consecutive runs remain the same for the spatial grid under consideration. When this happens (i.e., when the errors in two consecutive runs remain the same for the spatial grid under consideration), the errors are the same as those obtained when no splitting is used.

- The errors obtained with the same timestep-size are nearly the same for all spatial grids when the splitting errors are the dominating errors and when the time-integration method is stable.

- The time-stepsize must be reduced very considerably in order to avoid completely the influence of the splitting procedure on the results. This is especially true for the refined spatial grids.

4.3.1 Keeping the splitting steps constant

Let us assume that the number of splitting steps is kept constant and the number of time-steps per a splitting step is varied. Some results shown in Table 7 indicate that the error does not depend on the number of time-steps that are carried out per a splitting step when the splitting is causing the dominating error.

Table 7. Values of $ERRMAX$ obtained when Problem 3 is solved with the DEM splitting by using a fixed numbers of spltting steps with different numbers of time-steps per a splitting step. (The upper line contains the values of τ corresponding to each column.)

Time-step Δt	$8.0E-3$	$4.0E-3$	$2.0E-3$	$1.0E-3$	$5.0E-4$	$2.5E-4$
$8.0E-3$	1.59E-2	-	-	-	-	-
$4.0E-3$	1.59E-2	7.99E-3	-	-	-	-
$2.0E-3$	1.59E-2	7.99E-3	4.03E-3	-	-	-
$1.0E-3$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	-	-
$5.0E-4$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	-
$2.5E-4$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.33E-3	1.00E-3
$1.25E-4$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.33E-3	1.01E-3
$6.25E-5$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	1.01E-3
$3.125E-5$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	1.00E-3
$1.5625E-5$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	1.01E-3
$7.8125E-6$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	1.01E-3
$3.90625E-6$	1.59E-2	7.99E-3	4.03E-3	2.22E-3	1.32E-3	1.01E-3

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