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SECOND AND HIGHER ORDER SEMI-IMPLICIT MEfflODS TO STUDY THE EVOLUTION OF AN AEROSOL BY COAGULATION

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INTRODUCTION

Coagulation is one of the main phenomena that modify aerosol particle size distribution (PSD). As for the monocomponent case, if *nv* is the density function, so that *nv dv* is the number of particles with volumes between *v* and $v + dv$ per air volume unit and $qv = V\, nv$ defines the particle overall volume PSD, we shall obtain a time evolution (Jacobson *et al.,* 1994):

aqv - : r - = lov 13v-vvqv-vn–;;dv-qv l0= l3v–;;nj;dv, (1)
ut o ' o '

being the expression corresponding to the internally mixed multicomponent aerosol similar to this one.

For solving this equation in the common cases in the atmosphere requires PSD was discretized. Then we integrate numerically in the time domain the resultant differential equation system. A usual discretization, directly related to the particle diameter logarithm, will verify for the particle volumes of each interval or bin, k:

$$v_k = v_1 R^{k-1}, \qquad k=l,\cdots,NB, \tag{2}$$

where *R* is a constant, and the particle overall volume *Qk* is associated with hin *k,* and a certain number of particles $Nk = Qk/vk$, The equation system for *Qk,* $k = 1, ..\bullet, NB$, is stiff and should be solved by means of stable methods that do not require small integration time steps to keep the error bounded.

Jacobson *et al.* (1994) have developed a semi-implicit method, non-iterative in each step that is stable and of the first order in time. PSD evolves from a stage *n* corresponding to a time *t,* to a stage $n + 1$, corresponding now to a time $t + \&$, by using:

+l - Q'¡ +& L'=I :E ;;;l Í;,j,k l3i,¡Q?+I Nj (3)
k - 1 +&:E]!!,1 (l-Ík,j,k)l3k,jNj '

so that *Íi,j,k* are partition coefficients among the different bins (refer to Jacobson *et al.,* 1994). We have proved (Fernández-Díaz *et al.,* pub. pending) that this method is approximately of second order with respect to the size discretization.

METHOD

It is interesting to find other methods of higher order with respect to the integration time step. One of those ways could be derived combining expression (3) for time step &, that can be labelled as Q'¡+l[&], and for step &/2, labelled as Q,¡+[1][&/2], by means of:

Q'¡+I = 2Q,¡+l[&/2]- +l[&), (4)

which is of second order in time and self-starting, even though it requires applying three times the expression (3) at each time step &.

Other semi-implicit methods of higher order could be derived from the formulas given by Young and Gregory (1988) to determine the derivative of a variable depending on the values given at previous points. In our case it would be:

(nn+I)' ~ _! (J.m Qn+l-i
i¿k ~ Af L, ı k ,
i=O

where a'(' are fixed constants values. The expression correspondíng to the first order $(m = 1)$ is (3). For the second order in time $(m = 2)$ we would get:

(21+! _ 40t- -! +2AfI,'=I I, ,;;} /;,j,k i,jQ'/+1(2NJ-N';-1) (5)
k - 3+2&I,f!1 (l-Ík,j,k) k,j(2Nj-N';-1) '

that requieres the knowledgement of -t and Ot and therefore it needs an expression such as (4) to start (or may be (3 with very small time steps). We have built other expressions of higher order which have not been described here to be brief. Ali of them are multi-step and semi-implicit, non-iterative (at each time step) ones, and they spend nearly the same calculation time than expression (3) with much smaller error (O(Afm)).

We have proved that in the evolution of an exponential PSD with constant coagulation coefficient (a system with known analytic solution), the error given after applying expressions (4) and (5) decreases vs. the time step Af, and according to the theory.

CONCLUSIONS

We have developed severa! integration methods for the coagulation equation that allow reducing the error yielded in comparison to the methods used until now. Ali of them are compatible with the time-splitting technique used when other phenomena such as condensation and deposition are present.

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REFERENCES

Fernández Díaz *et al.* (Pub. pending). A modified semi-implicit method to obtain the evolution of an aerosol by coagulation. *Atmospheric Environment.*

Jacobson, M.Z. *et al.* (1994). Modeling coagulation among particles of different composition and size. *Atmospheric Environment,* **28,** 1327-1338.

Young, D.M. and Gregory, R.T. (1988). *A Survey of Numerical Mathematics.* Dover Publications, Inc., New York, 478-482.