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An approach to chemical reactions in the atmosphere

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1. Introduction

We discuss an approximate approach to simulate time series reactions in the atmosphere. At first, we write a reaction at definition time-t, as A+B=C. Next, we suppose that densities of the compounds are written by Gaussians. The Gaussian is a solution for general small particles diffusion processes. The time-t is discrete about the interval is dt. If 2 particles of compound A and B are interacted within the interval, the reaction reaches equilibrium, and a compound C is generated.

2. Descriptions

Considering properties of the atmosphere, we adopt Gaussian having different parameters for the horizontal and vertical directions.

$GA\{A\}(r,z)=QA\{A\}\exp\{-\alpha A\ (r-rA)^2-\beta A(z-zA)^2\}$, (1)

The suffix A corresponds to compound A. The Q is density and the unit is [M/volume] of compounds. In case of uncertain compounds chemically, it is replaced by [kg/volume]. A vector r is for x- and y-coordinates, and z is for z-coordinate. The function exp(whose arguments is 3-dimensional distance) is a kind of the volume. Eq. (1) is a relation of [M]; that is, a reaction equation, which is defined at any time.

The α and β (which are positive) are diffusion parameters and they depend with elapsed time from the generation. The dependency is very complex and the evaluation is difficult. In the puff-model approach, it is calculated by many turbulence parameters. However; we wonder that model is significant in case of very diffused case. We wish to adopt Lagrangian particles (L-particles), where alpha-beta-parameters are not, and effects of the turbulence are expressed by random numbers.

L-particles are a finite volume of the air, and have no shape. Therefore; we redefine it to be Gaussian. The multiply of Gaussians is a Gaussian; it is an appropriate function to express reactions.

Under the representation, alpha-beta-parameters are fixed coefficients to define a unit volume. They are a kind of mesh intervals. The re-defined Gaussians are moved by meteorological fields, as if they were L-particles. The Gaussian is like as a mesh-unit in Euler approach, which has a finite volume. They are in a space, and are moved by wind fields; however, they are not arranged orderly in Euler approach. Here, if the arrangement is introduced as following;

A transformation between L-particle and Euler-mesh:

Q(mesh coordinates)=Integral{GA(r,z)G(on mesh)dv},

{GA(r,z)}–>{Q(on mesh)}.

The transformation seems to be usable to evaluate diffused mist.

3. Reactions

In an interval time, chemical equilibrium is,

Keq=[C]/([A][B]). (2)

For every times,

QA(t+dt)=QA(t)-QC(t), QB(t+dt)=QB(t)-QC(t), (3)

rA (t+dt)=rA (t)+{u,v}Adt+Rand(), (4)

ZA (t+dt)=ZA (t)+{w}Adt+Rand(), (5)

Where, a vector {u,v,w} is wind speeds. Rand() is normal distributed random numbers.

In another reaction, A+B=C+D, we get,

Keq=([C][D])/([A][B]), (6)

Since the distributions of C and D are same at the first step,

$GC=GD=(KeqGAGB)^{0.5}$. (7)

4. Progress of the research

We try to simulate some reactions in the atmosphere now.

Keywords: atmospheric reaction, SPM, L-particle