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.

\[ G_A(r,z) = Q_A e^{-\alpha_A (r-r_A)^2 - \beta_A (z-z_A)^2}, \]

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

The \(\alpha\) and \(\beta\) (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:

\[ Q(\text{mesh coordinates}) = \text{Integral}\{G_A(r,z)G(\text{on mesh})dv\}, \]

\[ G_A(r,z) \rightarrow \{Q(\text{on mesh})\}. \]

The transformation seems to be usable to evaluate diffused mist.

3. Reactions

In an interval time, chemical equilibrium is,

\[ K_{eq} = [C]/([A][B]), \]

For every times,

\[ QA(t+dt) = QA(t) - QC(t), QB(t+dt) = QB(t) - QC(t), \]

\[ r_A(t+dt) = r_A(t) + \{u,v\} Adt + \text{Rand}(), \]

\[ Z_A(t+dt) = Z_A(t) + \{w\} Adt + \text{Rand}(), \]

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

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

\[ K_{eq} = ([C][D])/(([A][B])), \]

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

\[ GC = GD = (K_{eq}G_A G_B)^{1/2}. \]

4. Progress of the research

We try to simulate some reactions in the atmosphere now.

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