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METHODS OF THE WET DEPOSITION DESCRIPTION IN AIR POLLUTION DISPERSION MODELS

In this article, two methods of the parameterisation of wet deposition are described. The simple method can be used for each type of air pollution dispersion model. A more advanced method is based on an independent cloud module and built into numerical pollution dispersion models.

1. INTRODUCTION

A wet deposition is the process during which pollutants are captured by hydrometeors and brought to the earth surface. Hydrometeors are the sets of water deoplets or ice crystals suspended in the atmospheric air or falling to the earth such as clouds, fog, rain or snow.

The absorption of pollutants taking place in clouds is called *the in-cloud scavenging*. The absorption of pollutants by precipitation taking place below the cloud base is called *the below-cloud scavenging*. Sometimes a third type of the wet deposition called *the cloud/fog interception* is distinguished. It takes place in the upper parts of mountains when air masses move up the hills and pollutants are captured directly by the earth surface and plants.

In this article, the methods of a wet deposition parameterisation in air pollution dispersion models are described. There are two methods: a simple one, which can be used in any type of model, and a more advanced one, which is used in more complex numerical models.

2. SIMPLE METHOD

A simple method is the oldest one. It is used to describe the wet deposition of aerosol particles and soluble gases. In this method, the a change in the pollutant concentra-

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tion with time due to wet deposition is approximated by an ordinary differential equation of the first order:

$$\left(\frac{dC}{dt}\right)_w = -\lambda C, \tag{1}$$

where:

C – the air pollutant concentration,

t – the time,

λ – the scavenging parameter.

In this approach, the wet deposition rate depends linearly on the pollutant concentration in the atmosphere. This simple method can be applied in any type of air pollution dispersion model. However, it is employed in different ways, depending on a model structure. Some examples of air pollution models of different types in which the simple method is used are given in the table.

Table

The examples of air pollution dispersion models in which a simple method of wet deposition parameterisation is used

Model type	Model subtypes	Model examples
Eulerian models	Box model	Model of MCMAHON et al. [3], model of SCRIVEN and FISHER [4]
	Analytical model	Model of FAY and ROZENZWEIG [5]
	Numerical model	LOTOS [6], RTM-III model (*Regional Transport Model*) [7]
Lagrangian models	Box model	EMEP-ozone model (*European Monitoring and Evaluation Programme Model*) [8]
	Particle model	ARCO (*Atmospheric Release in Complex Terrain Model*) [9] and LPD (*Lagrangian Particle Dispersion Model*) [10]
Gaussian models	Traditional plume model	URFOR (Urban Air Quality Forecasting Model) [11], REGSIM (*REGional SIMulation Model*) [12]
	New-generation model	ADMS (*Atmospheric Dispersion Modelling Systems*) [13]
	Segmented plume or puff model	SPM (*Segmented Plume Model*) [14] AVACTA [15]

The models are grouped into classed based on mathematical criteria such as: the co-ordinate system and model assumptions. In general, two classes of models are distinguished based on the first criterion: Eulerian models in which a co-ordinate system is fixed to the ground and Lagrangian models in which a co-ordinate system is moving with the air masses. The third class of models, called the Gaussian-type models, is separated from Lagrangian type models because of practical reasons. A further division of models based on the second criterion is listed in the table. A detailed description of the models is given by MARKIEWICZ [1], [2].

Typical values of the parameter λ for gaseous pollutants and aerosol particles cover the range from 10^{-3} to 10^{-5} 1/s [16] and depend on a type and characteristics of pollutant and precipitation. They are determined based on the results of field experiments or theoretical analysis [17]. For example, for SO_2 BEILKE [18] suggest the following relationships: $\lambda = 17 \cdot 10^{-5} J^{0.6}$ [1/s], where J [mm/h] is the precipitation intensity. For atmospheric aerosol ENGELMANN [19] suggests the following relationship: $\lambda = 16 \cdot 10^{-5} J^{0.8}$ [1/s].

3. MODELLING OF THE WET DEPOSITION OF ATMOSPHERIC POLLUTANTS

Advanced methods of the wet deposition parameterisation were applied to numerical air pollution dispersion models in the late eighties. In this approach, the following processes are described: the formation of clouds and other hydrometeors, chemical processes in water phases and participation of clouds and other hydrometeors in the removal of pollutants from the atmosphere. Each of these processes is usually simulated by a specific module. The description of these processes is relatively detailed.

Cloud modules are developed to describe the formation of clouds and precipitation. Although the cloud modules differ in some details, their structure and general rules of their performance are similar. Usually the processes taking place in clouds are simulated using one-dimensional model, which is activated when clouds in a vertical column of the atmospheric air are encountered. The modules of this type are incorporated into the STEM II model (*Sulphur Transport and Emission Model*) [20], RADM model (*Regional Atmospheric Deposition Model*) [21] and ADOM model (*Atmospheric Deposition Oxidant Model*) [22].

Meteorological data, vertical profiles of the concentrations of gaseous and aerosol pollutants are needed in cloud modules as input data. The concentrations are obtained from the air pollution dispersion model, while meteorological data from observations [22] or from the meteorological model [20], [21]. Meteorological data include:

- the precipitation rates at the earth surface,
- the vertical profile of temperature or the temperature at the earth surface,
- the vertical profile of moisture or the height of the cloud base, or the height of the lifting condensation level (LCL), or the height of the cloud top.

In cloud modules, water occurs in two or three phases. In simpler modules, water is usually grouped into three classes such as: the water vapour, cloud droplets and rain droplets. In more complex modules, water is grouped into five or more classes as, in addition, ice crystals in clouds, snow and graupel are taken into account. The most detailed representation of water, in which its droplets and crystals are grouped additionally into classes of different sizes, is not applied in air pollution models because of computer limitations. However, such complex cloud modules were developed and applied as separate models. They are described by FLOSSMANN et al. [23], RUTLEDGE et al. [24], CHAUMERLIAC [25], FLOSSMANN [26] and GEREMY et al. [27].

The output data from the cloud module include:

- vertical profiles of water content in each of the phases considered,
- the distributions of clouds and precipitation,
- the velocity of vertical movements in clouds,

and in the case of more complex modules, the following parameters are additionally calculated:

- hydrometeor gravitational falling velocities,
- the rates of the hydrometeor interconversion.

The processes connected with the changes of water phases and the transformations taking place in a specific phase are considered in the calculation of hydrometeor interconversion rates. In the case of grouping the water into four classes (the water vapour, cloud droplets, rain droplets, snow), the following conversion mechanisms are considered: condensation, evaporation, absorption, desorption, autoconversion, accretion, freezing, melting and riming. It has to be noticed that a number of conversion mechanisms, which need to be taken into account, grows with a number of the water classes under consideration. The processes taking place in convective and stratiform clouds are modelled separately because of the differences in their parameterisation. These methods are described in detail by PIELKE [28] and ORVILLE [29] and in the papers presenting specific models [30], [31].

The methods of the description of wet removal of atmospheric pollutants from the atmosphere and the chemical processes taking place in the hydrometeors depend on the structure and performance of the cloud module. In the case of simpler cloud modules, the changes of concentrations due to wet deposition and chemical processes in the liquid phase are calculated by the box type model [20], [32].

In the case of more complex cloud modules [21], [33], the influence of wet deposition and chemical processes taking place in the liquid phase are described as follows. The terms describing an exchange of the *i*-th pollutant mass between the gaseous phase and hydrometeors, chemical processes in a geseous phase and emission of the *i*-th gaseous pollutant into the atmosphere are introduced to a gaseous phase pollution transport equation (partial differential equation of the second order). As a result the set of equations of the form given by equation (2) is obtained. The circulation of pollutants in water phases is described by the set of analogous equations. In each of these equations, the terms representing a wet deposition process are introduced. They describe the exchange of mass of the *i*-th substance between hydrometeors, the exchange of mass of the *i*-th substance between hydrometeors and a gaseous phase as well as chemical processes in water phases. A whole set of equations has the following form:

$$\frac{\partial C_i}{\partial t}+\frac{\partial}{\partial x}(uC_i)+\frac{\partial}{\partial y}(vC_i)+\frac{\partial}{\partial z}(wC)_i$$
$$=\frac{\partial}{\partial x}\left(K_x\frac{\partial C_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C_i}{\partial z}\right)+R_i+\sum_p G_{i,p}+Q\,, \qquad (2)$$

$$\frac{\partial(L_{w,p}C_{i,p})}{\partial t}+\frac{\partial(uL_{w,p}C_{i,p})}{\partial x}+\frac{\partial(vL_{w,p}C_{i,p})}{\partial y}+\frac{\partial[(w-v_{f,p})uL_{w,p}C_{i,p}]}{\partial z}$$
$$=\frac{\partial}{\partial x}\left(K_{x,p}C_{i,p}\frac{\partial L_{w,p}}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{y,p}C_{i,p}\frac{\partial L_{w,p}}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{z,p}C_{i,p}\frac{\partial L_{w,p}}{\partial z}\right)$$
$$+R_{i,p}-G_{i,p}+Q_{i,p},\quad i=1,\dots,N_i,\quad p=1,\dots,N_h, \qquad (3)$$

where:

C_i – the concentration of the *i*-th substance in the atmospheric air in mass units of pollutant per volume units of air,

$L_{w,p}$ – the constant of water in the hydrometeor *p* in mass units per volume units of air,

$C_{i,p}$ – the nondimensional concentration of the *i*-th substance in the hydrometeor *p* in mass unit of pollutant per mass units of water,

u, *v*, *w* – the components of the wind vector in a co-ordinate system fixed to the ground (*x*, *y*, *z*),

$v_{f,p}$ – the average gravitational velocity of the hydrometeor *p* (for clouds $v_{f,p} = 0$),

K_x, K_y, K_z – the components of the turbulent diffusion coefficient,

$K_{x,p}$, $K_{y,p}$, $K_{z,p}$ – the components of the turbulent diffusion coefficient for the hydrometeor *p*,

R_i, $R_{i,p}$ – the change of the concentration of the *i*-th substance in a gaseous phase and in the hydrometeor *p* connected with chemical processes,

$G_{i,p}$ – the change of the concentration of the *i*-th substance in the hydrometeor *p* connected with an exchange of mass between the hydrometeor and a gaseous phase,

Q_i – the emission of the *i*-th substance into the atmosphere,

$Q_{i,p}$ – the change of the concentration of the *i*-th substance in the hydrometeor *p* connected with an exchange of mass between the hydrometeor *p* and other hydrometeors,

N_i – the number of the substances considered,

N_h – the number of hydrometeors considered (usually $N_h = 3$, $p = 1$ for cloud droplets, $p = 2$ for rain droplets, $p = 3$ for snow).

The exchange of the mass of the substance *i*-th between hydrometeors ($Q_{i,p}$) is calculated using the parameters describing the rates of conversion of hydrometeors, which are calculated in the cloud module. In the exchange of the mass of the *i*-th gaseous substance between a gaseous phase and hydrometeors containing water in a liquid phase ($G_{i,p}$) (cloud droplets and rain droplets), the limitations in the transport of a gaseous substance between phases can be included [34].

Chemical processes taking place in cloud and rain droplets usually lead to the formation of sulphate(VI) and nitrate(V). A number of the reactions considered depends on a chemical mechanism used and varies from 30 to 60 [21], [35], but it can be smaller [33].

4. SUMMARY

Many difference factors influence the wet deposition of pollutants from the atmosphere. The most important factors are the type and characteristics of pollutant and hydrometeors. Three types of wet deposition are distinguished, i.e., the in-cloud scavenging, below-cloud scavenging and cloud/fog interception.

The description of a wet deposition by air pollution dispersion models is simplified. Two methods are distinguished: the simple one and the more advanced one. In the simple method, which can be applied to any type of the air pollution dispersion model, one parameter is used. In the second method, independent modules describing the formation of clouds and other hydrometeors, chemical processes of pollutants in water phases and participation of hydrometeors in the removal of pollutants from the atmosphere are introduced to an air pollution modelling system. This method is used in numerical models developed after the mid eighties.

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METODY OPISU WYMYWANIA ZANIECZYSZCZEŃ Z ATMOSFERY ZA POMOCĄ MODELI ICH ROZPRZESTRZENIANIA SIĘ

Na przebieg procesu wymywania zanieczyszczeń z atmosfery ma wpływ wiele czynników. Ważny jest zarówno rodzaj substancji usuwanej i jej chemiczne właściwości, jak i rodzaj i charakterystyka hydrometrów, za pośrednictwem których ten proces zachodzi. Zazwyczaj wyróżnia się wymywanie zanieczyszczeń w chmurach, ich wymywanie przez opady atmosferyczne oraz ich przechwytywanie przez podłoże podczas wślizgiwania się mas powietrza po zboczach.

Opis zjawiska wymywania zanieczyszczeń z atmosfery w modelach rozprzestrzeniania się tych zanieczyszczeń jest z konieczności upraszczany. W modelach atmosferycznych rozróżnia się dwie podstawowe metody parametryzacji wymywania zanieczyszczeń. W metodzie pierwszej zjawisko to opisuje się, korzystając z pojedynczego parametru, którym jest współczynnik wymywania zanieczyszczenia z atmosfery (λ). Metoda druga jest znacznie bardziej rozbudowana. Polega na wprowadzeniu do systemu modelowania procesów atmosferycznych współpracujących ze sobą modułów, które opisują powstawanie chmur i opadów, przemiany chemiczne zanieczyszczeń z atmosfery. Moduły te umożliwiają względnie szczegółowy opis procesów zachodzących w chmurach i tych towarzyszących opadom i są realizowane w modelach numerycznych opracowanych pod koniec lat osiemdziesiątych.