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ECOLOGICAL SAFETY PREDICTIVE MODELING CONCERNING FINE COCOA DUST DISPERSION, RELEASED BY CONFECTIONERY MANUFACTURE

[1]Valentina Iurchenko, [1]Elena Lebedeva, [2]Svitlana Ponomaryova

[1]Kharkov National University of Civil Engineering and Architecture
40, Sumskaya Str., Kharkiv, 61002, Ukraine
[2]Ukrainian Research Institute of Environmental Problems
6, Bakulyna Str., Kharkiv, 61002, Ukraine
yurchenko.valentina@gmail.com

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Abstract. In order to predict ecological safety conserning cocoa dust emission ($PM_{2,5}$ and PM_{10}), the mathematical modeling of its dispersion was performed considering the atmosphere turbulent diffusion. Necessary gravity sedimentation rate of cocoa dust for modeling was identified during the experimental researches. Obtained results indicate the necessity of intensification of fine particles emission clean-up in the observed confectionery factory.

Key words: cocoa fine dust, dispersion, ecological safety, mathematic modeling, atmosphere turbulent diffusion.

1. Introduction

Confectionery enterprises area significant emission source of suspended particulate organic substances (organic dust). Free-running organic substances (flour, starch, sugar, cocoa) are used in most technological processes. During confectionary products production emissions with sugar, flour, cocoa, starch dust invade in the open air. Forthe confectionary factories carbon intensities of organic dust, that is undeferential in composition for each kind of manufacture, are set (Table 1) [1].

The suspended particulate matters with the sizeto 10 um (PM_{10} according to [2]) and to 2.5 um ($PM_{2,5}$ according to [2], that prevail in the emissions of confectionary [3]), are specifically environmentally hostile.

Atmospheric air pollution with $PM_{2,5}$, PM_{10} influences over health even in very low concentration. Practically there is no lowest observed effect level whereby any health effects are not occurred. [4]. Due to the small size, such matters are able to get in not only upper respiratory airway, but in lungs, that causes effects such as: depression of pneumonic function, sensation of upper respiratory airway, cough, difficulty in breathing, asthma exacerbation, arrhythmia, nonfatal infarction, untimely death of people with cardiopulmonary diseases.

Table 1

Carbon intensities of suspended particulate organic matters, that are undeferential in composition in production of confectionary products per ton of end products [1]

No.	Confectionary production type	Carbon intensity, gr/t	
		min	max
1	Cocoa powder	2674	4081
2	Panned sweets	941	1050
3	Chocolate	834	1050
4	Candies	510	1169
5	Chocolate bar	245	412
6	Oriental sweets	242	297
7	Caramel	236	292
8	Marshmallow	136	261
9	Biscuits	124	136
10	Butter scotch	45	48
11	Halva	15	35
12	Waffles	13	29
13	Candied fruit jelly	7	7
14	Pastries (cakes, muffins), kg/year	6	23

Performed analysis of scientific and technical literature revealed that suspended particulate organic substances (organic dust) have certain special features. They are able to cause allergies due to the presence of protein and vegetal, microbiotic matters, fragments of insects, mineral fertilizer etc. [5]. According to WHO, every fifth resident of the earth suffers from allergy, in big cities – up to 60 % of population. In Ukraine, unfortunately, such statistics is not carried out. The suspended particulate organic substances are by nature indirect emission source of CO_2, in which all organic matters acetify, and consequently, they are potential greenhouse gases. Particles PM_{10} and $PM_{2,5}$ are able to be taken to extra-long distances, to deteriorate visibility, damage plants, get directly into impoundments or ground, and then to be washed off into water bodies by overland runoff and to change pH [6]. Getting to the water body such particles influence its ecosystem. The authors [7, 8] undertook the study and confirmed, that the water ecosystem can be greatly defenseless, if the particles $PM_{2,5}$ get into it, as such particles generally accumulate in the impoundments due to setting out and washing off with rainfalls, upon that increasing concentration and treatment impact.

Based on the above, the regulatory actions, emissions monitoring of $PM_{2,5}$, PM_{10}, including of organic origin, and also forecasting of negative impact of these emissions are key factors of monitoring and control of such emissions regarding ecological safety of equipment sites for environment as a whole and a human being in particular. Moreover, it is impossible to evaluate correctly impact consequences of the particular type $PM_{2,5}$, PM_{10} on a man and environment without data on content of $PM_{2,5}$, PM_{10} in gas emissions of certain types of factories.

In Ukraine the regulatory actions for $PM_{2,5}$, PM_{10} are only in the development stage, although control of these values has been carried out by State Statistics Committee of Ukraine since 2004. Due to implementation of EU Directive 2008/50 / European Parliament and Council of air quality and clean air for Europe the regulatory legal acts regarding setting of the standards of suspended materials concentration ($PM_{2,5}$, PM_{10}) in the open air and provision of their monitoring in the open air will be worked out.

For the present, according to [9] in Ukraine the standards of safe reference level of impact (SRLI) for flour, sugar, starch and cocoa dust are valid, which are shown in Table 2.

Table 2

SRLI of pollutants into the atmosphere of aggregations

Ser. No.	Matter	SRLI	
		mg/m³	mkg/m³
859	Flour dust	0.06	60
939	Sugar dust (sucrose)	0.1	100
878	Cocoa dust	0.06	60
890	Starch dust	0.1	100

Recommendations and standards of different countries of the world for $PM_{2,5}$ and PM_{10}, are shown in Table 3.

Table 3

Critical concentration of $PM_{2,5}$ and PM_{10} in the atmosphere according to recommendations [4, 10–13]

Name of the country or organization	Concentration, mkg/m³			
	PM_{10}		$PM_{2,5}$	
	$C_{d.c.}$	$C_{a.c.}$	$C_{d.c.}$	$C_{a.c.}$
European Union [4]	35–25	28–20	–	17–12
WHO [10]	50	20	25	10
USA [11]	150	–	35	12
Canada [16]	–	–	28	10
Australia [12]	50	–	25	8
Japan[13]	100	–	35	15

Note. $C_{d.c.}$ – daily average concentration, $C_{a.c.}$ – annual average concentration.

As seen, SRLI values for the cocoa dust are 60 mkg/ m³. Considering that the cocoa dust mostly consists of the particles $PM_{2,5}$, critical concentration should comply with values of daily average concentration$C_{d.c.}$ for $PM_{2,5}$ according to the Table 3. Consequently, it should not exceed value 35 mkg/m³.

For forecasting of harm impact of $PM_{2,5}$, PM_{10} emission on the environment and the human, it is necessary to choose evaluation method of the given emissions distribution in the atmosphere, that will take into consideration in maximum special features of pollutants and physical factors, that influence the transport process of the given pollutant in the atmosphere.

The research object is mathematic modelling of cocoa dust dispersion by the confectionary factory, considering the atmospheric turbulent diffusion.

2. Objects and research methods

The research object is a real confectionary factory, that is situated in the urban area and produces cocoa dust emission 3.918 g/s. Calculation of this dust dispersion and mapping of dispersion were conducted on a Fortran software package based on a numerical model that takes into account wind-induced transport, atmospheric turbulent diffusion, and gravity (gravitational dust settling).

3. Results and discussion

The characteristics of environmental pollution with the fine dust, released by the confectionary factories, can be determined by means of mathematical model formulation of dust transport in the atmosphere.

Initial equation

Transport process of the dust in the atmosphere occurs under the effect of the following physical factors:

1. Transportation under the effect of wind;

2. Transportation under the effect of atmospheric turbulent diffusion;
3. Gravity transportation(dust gravity sedimentation)

For mathematical modeling of the dust dispersion process in the atmosphere, considering indicated factors, equation of Marchuk G. I. [14, 15] was applied:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial nC}{\partial y}+\frac{\partial (w-w_S)C}{\partial z}+kC=$$
$$=\frac{\partial}{\partial x}\left(m_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(m_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(m_z\frac{\partial C}{\partial z}\right)+\sum q_i d(x-x_i)d(y-y_i)d(z-z_i), \quad (1)$$

where C – dust concentration; u, v, w – vector components of air environment motion speed; w_s – speed of pollutant gravity sedimentation(dust); m_x, m_y, m_z – coefficients of atmospheric turbulent diffusion; k – coefficient, considering dust washing off with rainfalls [14]; x_i, y_i, z_i – Cartesian coordinates of position of dust emission source; q_i –rate of pollutant emission, depending on the time; $d(x-x_i)d(y-y_i)d(z-z_i)$ – identification of delta function of Dirac.

For modeling of pollutant washing off process from the atmosphere with rainfalls the following empirical equation can be applied [14]:

$$k = k_r \cdot k_0 \cdot I,$$

where s – parameter of pollutant washout with rainfalls, that depends on rainfall type; k_r – standard value of total wash off capability of rain ($k_r = 10^{-5}\, h/(mm\cdot s)$); k_0 – nominal wash off capability of rainfalls of other types, is presented in Table 4; I – rainfall intensity, $I = 1\, mm/h$.

Table 4

Nominal wash off capability of rainfalls of other types

Type of rainfalls	k_0
rain	1
storm rain	1.1
rain shower	2.6
snow	3.0

In the developed computational model the following dependencies for assignment of the wind profile and vertical atmospheric diffusion coefficient are applied [14]:

$$u = u_1\left(\frac{z}{z_1}\right)^p,\ m_z = k_1\left(\frac{z}{z_1}\right)^m,$$

here u_1 – wind speed at height z_1 (set z_1=10m); k_1=0.2; p=0.4 (for the urban area [15]); m≈1.

For calculation of other atmospheric diffusion coefficients the following empirical dependencies were applied [14, 15]:

$$\mu_y = \mu_x,$$
$$\mu_y = \kappa_0 u.$$

Solution of the equation (1) will be defined numerically.

Boundary conditions

For obtaining single valued solution of the current task it is necessary to formulate the particular boundary conditions for the equation, indicated above. The conditions are the following[15]:

On the border of air flow in put the condition is set in the calculation area:

$$C\big|_{boundary} = C_в,$$

where $C_в$ – known value of dust concentration in the atmosphere (in the calculations $C_в$ = 0 is set).

On the output bound the “mild” boundary condition is set in the computational model. For example, in the different format the given condition for x = L_x, (L_x – the distance where output boundary is located) is written that way

$$C(i+1,j,k) = C(i,j,k),$$

where(*i+1,j,k*) – final (boundary) different zone, (*i,j,k*) – foregoing different one.

On the upper boundary H = const, the boundary condition has format C = 0 [15].

On the bottom surface/boundary – ground surface the boundary condition is set in formula

$$\frac{\partial C}{\partial n} = 0,$$

where *n* – outward normal to a surface.

Initial condition

As the equation (1) is unstable, that for its solution it is necessary to set the initial condition. This condition is taken up in the following formula: dust load in the whole calculation area $C = 0$ at t = 0. Physically it defines zero pollution in the initial time in the calculation area.

Method of solution

For numerical integration of the equation (1) the cryptic difference scheme of breakage will be applied. Do consider the principle of its structure [16].

The convective derivatives are presented in the formula:

$$\frac{\partial uC}{\partial x}=\frac{\partial u^+C}{\partial x}+\frac{\partial u^-C}{\partial x},$$

$$\frac{\partial vC}{\partial y}=\frac{\partial v^+C}{\partial y}+\frac{\partial v^-C}{\partial y},$$

$$\frac{\partial wC}{\partial z}=\frac{\partial w^+C}{\partial z}+\frac{\partial w^-C}{\partial z},$$

where $u^+ = \frac{u+|u|}{2}$; $u^- = \frac{u-|u|}{2}$; $v^+ = \frac{v+|v|}{2}$; $v^- = \frac{v-|v|}{2}$; $w^+ = \frac{w+|w|}{2}$; $w^- = \frac{w-|w|}{2}$.

For approximation of the convective derivatives the formula is applied [16]:

$$\frac{\partial u^+ C}{\partial x} \approx \frac{u^+_{i+1,j,k} C^{n+1}_{i,j,k} - u^+_{i,j,k} C^{n+1}_{i-1,j,k}}{\Delta x} = L_x^+ C^{n+1},$$

$$\frac{\partial u^- C}{\partial x} \approx \frac{u^-_{i+1,j,k} C^{n+1}_{i+1,j,k} - u^-_{i,j,k} C^{n+1}_{i,j,k}}{\Delta x} = L_x^- C^{n+1},$$

$$\frac{\partial n^+ C}{\partial y} \approx \frac{n^+_{i,j+1,k} C_{i,j,k} - n^+_{i,j,k} C_{i,j-1,k}}{\Delta y} = L_y^+ C^{n+1},$$

$$\frac{\partial n^- C}{\partial y} \approx \frac{n^-_{i,j+1,k} C_{i,j+1,k} - n^-_{i,j,k} C_{i,j,k}}{\Delta y} = L_y^- C^{n+1},$$

$$\frac{\partial w^+ C}{\partial z} \approx \frac{w^+_{i,j,k+1} C_{i,j,k} - w^+_{i,j,k} C_{i,j,k-1}}{\Delta z} = L_z^+ C^{n+1},$$

$$\frac{\partial w^- C}{\partial z} \approx \frac{w^-_{i,j,k+1} C_{i,j,k+1} - w^-_{i,j,k} C_{i,j,k}}{\Delta z} = L_z^- C^{n+1},$$

where $L_x^+ = \frac{u^+_{i+1,j,k} C^{n+1}_{ijk} - u^+_{ijk} C_{i-1,j,k}}{\Delta x}$,

$$L_x^- = \frac{u^-_{i+1,j,k} C^{n+1}_{i+1jk} - u^-_{ijk} C^{n+1}_{ijk}}{\Delta x},$$

$L_y^+, L_y^-, L_z^+, L_z^-$ – designation of difference operators under approximation of the convective derivatives.

The second derivatives are approximated with the following formulas [16]:

$$\frac{\partial}{\partial x}\left(m_x \frac{\partial C}{\partial x}\right) \approx m_x \frac{C^{n+1}_{i+1,j,k} - C^{n+1}_{ijk}}{\Delta x^2} - m_x \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i-1,j,k}}{\Delta x^2} = M^-_{xx} C^{n+1} + M^+_{xx} C^{n+1},$$

$$\frac{\partial}{\partial y}\left(m_y \frac{\partial C}{\partial y}\right) \approx m_y \frac{C^{n+1}_{i,j+1,k} - C^{n+1}_{ijk}}{\Delta y^2} - m_y \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i,j-1,k}}{\Delta y^2} = M^-_{yy} C^{n+1} + M^+_{yy} C^{n+1},$$

$$\frac{\partial}{\partial z}\left(m_z \frac{\partial C}{\partial z}\right) \approx m_z \frac{C^{n+1}_{i,j,k+1} - C^{n+1}_{ijk}}{\Delta z^2} - m_z \frac{C^{n+1}_{i,j,k} - C^{n+1}_{ij,k-1}}{\Delta z^2} = M^-_{zz} C^{n+1} + M^+_{zz} C^{n+1}.$$

In the given formulas

$M^+_{xx} = -m_x \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i-1,j,k}}{\Delta x^2}$, $M^-_{xx} = m_x \frac{C^{n+1}_{i+1,j,k} - C^{n+1}_{i,j,k}}{\Delta x^2}$,

M^+_{yy}, M^-_{yy}, M^+_{zz}, M^-_{zz} – designations of difference operators under approximation of the second derivatives. With consideration of the designations, the difference analogue of the three-dimensional equation of impurities transportation will have the formula:

$$\frac{C^{n+1}_{i\,jk} - C^{n}_{i\,jk}}{\Delta t} + L_x^+ C^{n+1} + L_x^- C^{n+1} + L_y^+ C^{n+1} + L_y^- C^{n+1} + L_z^+ C^{n+1} + L_z^- C^{n+1} + s\ C^{n+1}_{i\,jk} =$$
$$= \left(M^+_{xx} C^{n+1} + M^-_{xx} C^{n+1} + +M^+_{yy} C^{n+1} + M^-_{yy} C^{n+1} + M^+_{zz} C^{n+1} + M^-_{zz} C^{n+1}\right).$$

Time derivative is presented at this rate:

$$\frac{\partial C}{\partial t} \approx \frac{C^{n+1}_{i\,j} - C^{n}_{i\,j}}{\Delta t}.$$

Upon integrating on the time slot *dt* splittance of the given equation will be performed in the following way [16]:

in the first step $k = n + \frac{1}{4}$:

$$\frac{C^{k}_{i,j,k} - C^{n}_{i,j,k}}{\Delta t} + \frac{1}{2}\left(L_x^+ C^k + L_y^+ C^k + L_z^+ C^k\right) + \frac{s}{4} C^k_{i,j,k} =$$
$$= \frac{1}{4}\left(M^+_{xx} C^k + M^-_{xx} C^n + M^+_{yy} C^k + M^-_{yy} C^n + M^+_{zz} C^k + M^-_{zz} C^n\right), \qquad (3.1)$$

in the second step $k = n + \frac{1}{2}$; $c = n + \frac{1}{4}$:

$$\frac{C^{k}_{i,j,k} - C^{c}_{i,j,k}}{\Delta t} + \frac{1}{2}\left(L_x^- C^k + L_y^- C^k + L_z^- C^k\right) + \frac{s}{4} C^k_{i,j,k} =$$
$$= \frac{1}{4}\left(M^-_{xx} C^k + M^+_{xx} C^c + M^-_{yy} C^k + M^+_{yy} C^c + M^-_{zz} C^k + M^+_{zz} C^c\right), \qquad (3.2)$$

in the third step $k = n + \frac{3}{4}$; $c = n + \frac{1}{2}$ formula is applied (3.2);

in the fourth step $k = n + 1$; $c = n + \frac{3}{4}$ formula is applied (3.1).

In the fifth step of splittance in the discrete model influence of sources on impurity concentration change is considered and calculation dependence in this step has the following form:

$$\frac{\overset{5}{C}{}^{n+1}_{i,j,k}-\overset{5}{C}{}^{n}_{i,j,k}}{\Delta t}=\sum_{l=1}^{N}\frac{Q_l(t^{n+1/2})}{\Delta x\Delta y\Delta z}d_l \ .$$

The function d_l identically becomes zero, except zones, where the 1[st] pollution source is located.

Theinitialconditionforeachequationineachsplittances tepiswrittenintheform [14]:

$$\overset{1}{C}\Big|_{t=t^n}=C\left(x,y,z,t^n\right),$$

$$\overset{k}{C}\Big|_{t=t^n}=\overset{k-1}{C}\Big|_{t=t^{n+1}}, \quad k=2,3,4\ ,$$

$$C\left(x,y,z,t^{n+1}\right)=\overset{5}{C}\Big|_{t=t^{n+1}}\ ,$$

where $\overset{1}{C}, \overset{k}{C}, \overset{5}{C}$ – impurity concentration values in any given calculation step.

Calculation of unknown concentration value C in each fractional step of the examined difference scheme is performed by means of the explicit formula of point-to-point computation.

Modeling of cocoa dust dispersion,
released by the confectionary factory

Cocoa dust emission is examined in the specific confectionary factory. Emission rate of the cocoa dust is 3.918 gr/s, release height is 6 m, wind speed is 5 m/s, atmospheric diffusion coefficient is 3 m^2/s. Speed of cocoa dust gravity sedimentation is set during the special experimental researches [3], it is 0.06 cm/s. The pollution zone of the atmosphere at a height of 1.5 m below the surface is presented in pic. 1, and cocoa dust concentration at a height of 1.5 m from the surface is presented in Table 5.

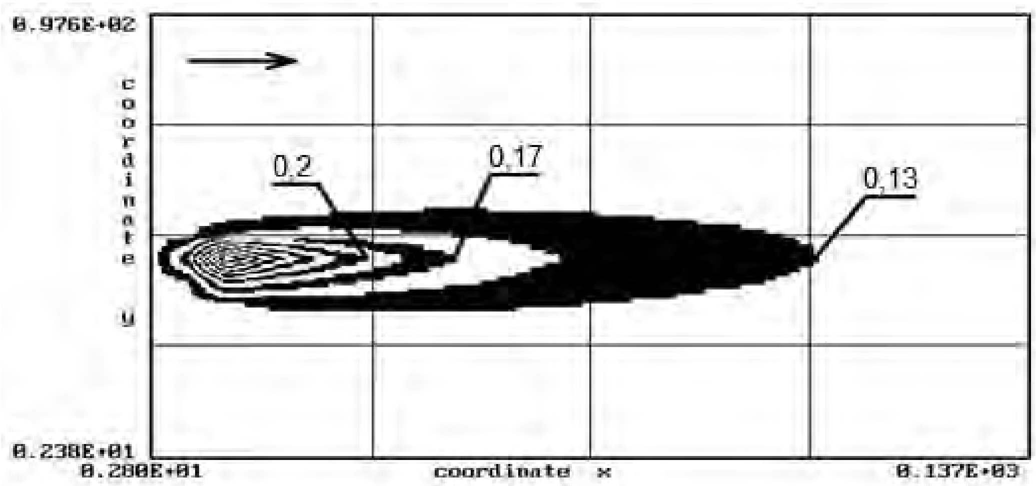

Fig. 1. Pollution of the atmosphere at a level of 1.,5 m

Table 5

Calculated cocoa dust concentration at different distances from emission sources at the confectionary factory

Distance from emission source, m	Concentration, mcg/m^3
40	177
60	167
80	150
100	134
120	120

As it is seen from the represented data, coca dust concentration on the border of the sanitary protection zone of the factory (100 m) exceeds the national standard – suggested no-adverse-response level (60 mcg/ m^3) of the critical concentration $PM_{2,5}$, applied in European Union (35 mcg/m^3).

Conclusions

1. The cocoa dust released by the confectionary factories consists, mainly, of the particles $PM_{2,5}$, critical concentration of which must be no greater that 60 mcg/m^3, according to the national standards (the standards of European Union 35 mcg/m^3).

2. For the first time, applying the equation of Marchuk G. I., and also by means of rate of cocoa dust gravity sedimentation set in the results of the authors' researches the mathematical modeling of cocoa dust dispersion released by the confectionary factory was performed.

3. It was found that under the current emission rate the cocoa dust concentration on the border of the sanitary protection zone of the factory exceeds not only the European standard, but also the national one.

4. Obtained results indicate the necessity of intensification of fine particles emission clean-up in the observed confectionery factory.

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