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DEC 78 Z HULEWICZ, Z JACHLEWSKI, K EKSANOW  
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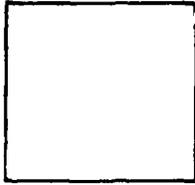


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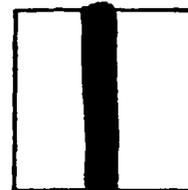
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# THE ATMOSPHERE POLLUTION CAUSED BY THE TECHNOLOGICAL LIQUID GASES EVAPORATION

Zbigniew Hulewicz, Zygmunt Jacklewski and Kamil Eksanow

The calculation method of the atmospheric dispersion of the pollution, caused by the liquid gas evaporation, when this process takes place in the open space, has been discussed and illustrated.

## 1. INTRODUCTION

The problem of the gas dispersion in the atmosphere during the present intensive development of the world economy becomes a very important problem involving consideration of numerous specialists from different branches of sciences and life. This problem comprises also systematical and willful gas ejection into the atmosphere as well as unpredictable gas penetration into the atmosphere as the result of reservoir damages, industrial installations, etc.

The problem of systematical and controlled gas exhaust into the atmosphere, mostly from industrial chimneys, is theoretically pretty well worked out giving details connected with this problem. The computational methods of this type of the pollution spread is known. However, the scientists are short on the descriptions concerning the cases of emergency, when the liquid gases, especially the toxic ones, which dispersing in the atmosphere, can cause the life threat even in the places located far away from the source of dispersion.

The present study gives the sketch describing the method of the computation of the gaseous cloud dimensions as well as the area, where the life threat can exist. This method can be useful for drafting the threat maps in the area of the existing installations or the installations under construction or in the area with the liquid gas reservoirs depending on the meteorological, and regional conditions and on the sort of gas. This method can serve for the evaluation of the precise location of new constructions.

## 2. FUNDAMENTAL PRINCIPLES

The case of the reservoir damage with the liquid gas is being considered.

This damage caused the whole amount of the liquid gas being ejected outside. However, the ejection time was so short that it can be neglected. It is presumed that the liquid gas, thrown out of the reservoir, makes "a blot" having round shape and coating uniform thickness all over the surface and the surface coated with the liquid gas is horizontal and non-absorbable. The liquid gas blot which was formed in this way can be considered as an intermittently continuous pointed source of emission. The source output depends on the evaporation speed of the liquid gas which is presumed to be constant.

The gaseous pollution cloud, resulting from the liquid gas evaporation, undergoes diffusion in the atmosphere according to the vorticity diffusion laws. After the liquid gas is evaporated completely, the gaseous cloud keeps moving in the direction of the wind and with a wind speed until its complete diffusion. Of the main interest is the area where the gaseous concentrations exceeding the permissible ones are being observed.

The problem of the vorticity diffusion in the atmosphere ground layer is a complex problem, comprising not only meteorological factors but also topographical. In order to simplify the calculations it is presumed that during the process of the liquid gas evaporation and spreading the gaseous cloud, the meteorological conditions remain unchanged and the process is taking place in the plane area which is partially covered with trees and partially constructed.

The solution of the problem requires considering three separate processes, namely - the liquid gas evaporation, the evaporated gas spread at the moment of evaporation, that is from the emission continuous source and the gas spread when the evaporation is over.

### 3. THE SPEED OF THE LIQUID GAS EVAPORATION

On the basis of the boundary layer theory Leibenson /1/ has introduced the empirical equation for the liquid evaporation speed from the free surface in the open space which has the following form:

$$q = 0,265 D \frac{MP_s}{RT_s} b R_s^{0.5} P_s^{0.3}, \quad (1)$$

where  $q$  - liquid evaporation speed /g/s/;  
 $D$  - diffusion coefficient of the liquid steam in the air /cm<sup>3</sup>/s/;  
 $M$  - molecular mass of the liquid / g/mol /;  
 $P_n$  - pressure of the liquid saturated steam under the  $T_0$  temperature /mm/Hg /;  
 $T_0$  - surrounding temperature /K/;  
 $R$  - ga. constant which is equal to  $6.237 \cdot 10^4$  cm<sup>3</sup>. mmHg/K.mol;  
 $b$  - width of the surface of the evaporating liquid / cm /;  
 $Re$  - Reynolds number ( $Re = ul_p/\nu$ );  
 $u$  - wind speed / cm/s /;  
 $l_p$  - length of the surface of the evaporating liquid / cm /;  
 $\nu$  - kinematic viscosity of the liquid steam / cm<sup>2</sup>/s /;  
 $Pr$  - Prandtl number ( $Pr = \nu/D$ ); 0.265 - experimental coefficient.

If the evaporating liquid surface has round shape with the  $d$  diameter, then the following dependence is compulsory:

$$b = l_p = \sqrt{\frac{\pi d^2}{4}} = 0,885d.$$

Equation /1/ is not being solved in the Reynolds number optional scope. However, it is possible to arrive at a certain generalization of equation /1/, introducing the variable quantities of the  $k$  experimental coefficient as well as these of the  $n$  power factor under the Reynolds number. At that time this equation becomes:

$$q = kD \frac{MP_n}{RT_0} b Re^n \sqrt{Pr}. \quad (2)$$

Equation /2/ can be transformed to:

$$\frac{qRT_0}{DMP_n b \sqrt{Pr}} = k Re^n. \quad (3)$$

The left side of this equation is a certain dimensionless quantity designated as  $A$  and in this case one obtains:

$$A = k Re^n. \quad (4)$$

On the basis of equations /3/ and /4/ it becomes possible to calculate, using the experimental data, the values of the A dimensionless number for different values of the Reynolds number. The  $A = f(Re)$  (tab. 1) empirical dependence, obtained in the above-mentioned way, is being used for the calculation of the liquid evaporation speed:

$$q = AD \frac{MP^*}{RT_s} \sqrt[3]{\nu Pr}. \quad (5)$$

Table 1. Dependence of dimensionless number A on the Re

Re	A	Re	A	Re	A
6·10 <sup>2</sup>	21,6	3·10 <sup>3</sup>	218	5·10 <sup>6</sup>	16500
8·10 <sup>2</sup>	25,1	5·10 <sup>3</sup>	315	1·10 <sup>7</sup>	30000
1·10 <sup>3</sup>	28,5	1·10 <sup>4</sup>	525	2·10 <sup>7</sup>	61000
1,5·10 <sup>3</sup>	35,5	2·10 <sup>4</sup>	900	3·10 <sup>7</sup>	93000
2,5·10 <sup>3</sup>	48,3	3·10 <sup>4</sup>	1275	5·10 <sup>7</sup>	165000
3,5·10 <sup>3</sup>	57,5	5·10 <sup>4</sup>	1975	1·10 <sup>8</sup>	355000
5·10 <sup>3</sup>	70,1	1·10 <sup>5</sup>	3600	2·10 <sup>8</sup>	810000
1·10 <sup>4</sup>	107	2·10 <sup>5</sup>	6650	3·10 <sup>8</sup>	1050000
2·10 <sup>4</sup>	175	3·10 <sup>5</sup>	9700		

#### 4. GASEOUS CLOUD SPREAD DURING THE EVAPORATION OF THE LIQUID GAS BLOT

On the analogy of the 2nd law of the Fick diffusion, the changes of the gaseous pollution concentration in the atmosphere can be represented by the following equation:

$$\frac{de}{dt} + u \frac{de}{dx} + v \frac{de}{dy} + w \frac{de}{dz} = \frac{d}{dx} k_x \frac{de}{dx} + \frac{d}{dy} k_y \frac{de}{dy} + \frac{d}{dz} k_z \frac{de}{dz}, \quad (6)$$

where:

e- gas concentration;

u, v, w - components of the wind speed in the direction of the X, Y, Z axis of the co-ordinate rectangular system;

$k_x, k_y, k_z$  - component of the coefficient of the vorticity diffusion in the direction of the X, Y, Z axis.

The principal element of the theory of the gaseous pollution dispersion in the atmosphere is a proper interpretation of the diffusion coefficient in the

direction of the Z axis, since the kind of surface, where the vorticity diffusion takes place, influences significantly this diffusion. From the Lajchtman<sup>[2]</sup> studies, it turns out that the kind of the basis influences first of all the air vertical currents. According to the halfempirical theory of vorticity, the  $k_z$  diffusion coefficient is expressed by the following equation:

$$k_z = l^2 \frac{u^2}{dz}, \quad (7)$$

where  $l$  is the length of the agitation way.

The dependence of the agitation way on the height is expressed in /3/

$$l = \gamma \left( \frac{z}{z_0} \right)^{1-\epsilon} z_0, \quad (8)$$

where:  $\gamma$  - constant empirical coefficient (0,40);

$z_0$  - parameter characterizing the basis roughness, which represents the height over the Earth surface where the wind speed is equal to 0 /m/;

$z$  - height over the Earth surface /m/;

$\epsilon$  - parameter characterizing the degree of the atmosphere vertical stability represented by the following function:

$$\epsilon = f \left( \frac{\Delta t}{u^2} \right). \quad (9)$$

In our geographical latitude the  $\epsilon$  values fluctuate from -0.3 up to +0.3, then:

$$\epsilon = - \frac{\Delta t}{u^2}, \quad (10)$$

where:

$\Delta t$  - temperature difference at the 50 and 200 cm height /°C/;

$u$  - wind speed at the  $z$  height / m/s /.

Dependence of the wind speed on the height /3,4/ is represented by the following equation:

$$\frac{u}{u_1} = \frac{\ln z/z_0}{\ln z_1/z_0}, \quad (11)$$

where  $u_1$  wind speed at the  $z_1$  height /m/;

After the transformation one can obtain from equations /7/,/8/,/11/ the following:

$$k_z = \left( \frac{\varepsilon u_1 z_0^2 z_1^{1-\varepsilon}}{z_1^2 - z_0^2} \right) \left( \frac{z}{z_1} \right)^{1-\varepsilon}. \quad (12)$$

The expression in the first brackets represents the  $k_1$  diffusion coefficient in the vertical direction at the  $z_1$  height and in this case one can write

$$k_z = k_1 \left( \frac{z}{z_1} \right)^{1-\varepsilon}. \quad (13)$$

For  $z_1=1$  one obtains:

$$k_z = k_1 z^{1-\varepsilon}. \quad (14)$$

It appears from this that in order to calculate the  $k_z$  coefficient, it is necessary to know the  $k_1$  coefficient. If in the equation determining the  $k_1$  coefficient, the product of all quantities except  $u_1$  is designated as  $p$ , then one obtain

$$k_1 = pu_1. \quad (15)$$

For different values of the  $\varepsilon$  and  $z_0$  parameters one can calculate the  $p$  values and from them it is possible to calculate values of the  $k_1$  coefficient. The  $z_0$  parameter usage is complicated because it changes depending on  $\varepsilon$ , that is on the atmosphere condition. Lajchman /4/ has introduced the roughness parameter designated as  $z_{00}$  which depends completely on the basis condition he also calculated the values of the  $k_1/u_1$  quotient for different values of  $\varepsilon$  and  $z_{00}$ . The  $z_0$  and  $z_{00}$  parameters are connected between each other with the following dependences:

$z_0 = z_{00}$  in the case of isothermality;

$z_0 = 2z_{00}$  in the case of convection;

$z_0 = \sqrt[3]{2} z_{00}$  in the case of inversion

Table 2 presents different values of the  $z_{00}$  parameter for different kinds of the basis. Fig. 1 presents the nomogram of the  $p = k_1/u_1 = f(\varepsilon, z_{00})$  function.

**Table 2. Dependence of roughness parameter  $\epsilon_{00}$  vs. the kind of covering of the terrain**

Kind of covering of the terrain	Height (thickness) of covering	Roughness parameter
	[m]	[m]
Close-land-surface with no plants	---	0,010
Idle land	0,05-0,1	0,022
Grass	0,3	0,039
	0,2	0,032
	0,1	0,025
	0,05	0,015
Ripe corn	1,2-1,3	0,045
Equal snow-covering of considerable thickness	—	0,050
Unequal snow-covering of average thickness	---	0,010
Single buildings, clumps of bushes and trees, small woods	do 10	0,100

The vorticity diffusion coefficients in the  $k_x$  and  $k_y$  horizontal surface have the same value and are independent from the height. They are designated by the  $k_0$  joint symbol. As opposed to the vertical direction, the diffusion in the horizontal direction is not a subject to the basis hampering influence. Therefore, at small heights the  $k_z$  coefficient has to be smaller than the  $k_0$  coefficient. The  $k_z$  coefficient is increasing along with the height increase, whereas the  $k_0$  coefficient remains constant. At a certain height in the layer which is called the isotropic vorticity layer one can see the  $k_z$  and  $k_0$  coefficient equalization. It is assumed that the isotropic vorticity appears at the height where the relation of the squares of the horizontal component of the wind speed to the squares of the vertical one reaches the minimum /5/. The experience indicated that for the isotherm, the isotropic vorticity takes place at the 12-14 m height /6/. Generally, it is assumed that the isotropic vorticity height is equal to 13m. Using this assumption one can calculate the  $k_0$  diffusion coefficient, which is:

$$k_0 = k_z = k_1 \cdot 13^{1-\epsilon}. \quad (16)$$

This relation can be used in the inversion condition for a small wind speed.

Knowing  $k_z$  and  $k_0$  one can solve the differential equation /6/ which for this purpose is better to transform introducing  $k_z$  according to formula /13/ as well as from  $k_x = k_y = k_0$  one obtains:

$$\frac{\partial c}{\partial \tau} + u \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} \left[ k_1 \left( \frac{z}{z_1} \right)^{1-\epsilon} \frac{\partial c}{\partial z} \right] + k_0 \left[ \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right]. \quad (17)$$

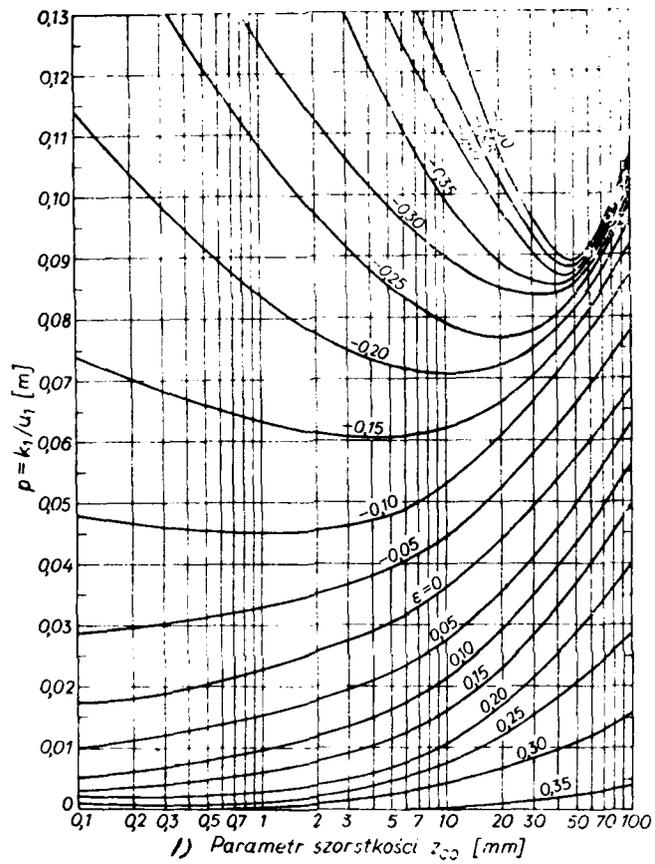


Fig. 1. Nomogram of the function of  $p = k_1/u_1 = f(\epsilon, z_{00})$

Key: 1) Roughness Parameter

Equation /7/ is being solved while maintaining the following boundary conditions:

a) it is assumed that there is no gas absorption through the basis, that is

$$\lim_{z \rightarrow 0} \frac{\partial \sigma}{\partial z} = 0;$$

b) at the  $\tau = 0$  time the gas concentration in all points of the space is equal to zero, except for the initial point of the co-ordinate system where there is the source:

$$\lim_{\tau \rightarrow 0} \sigma(\tau, x, y, z) = 0 \quad \text{for} \quad \tau = 0, \quad x = 0, \quad y = 0, \quad z = 0;$$

c) at the distance infinitely remote from the source, the gas concentration is always equal to zero:

$$\lim_{r \rightarrow \infty} \sigma(\tau, x, y, z) = 0, \quad r = \sqrt{x^2 + y^2 + z^2};$$

The total amount of the gas released through the source is located in the atmosphere:

$$Q = q\tau_p = \int_0^{\infty} dz \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} \sigma(\tau, x, y, z) dx,$$

where:  $q$  - the emission source output is equal to the evaporation speed of the liquid gas /g/s/;

$\tau_p$  - evaporation time of the liquid gas /s/;

$\sigma(\tau, x, y, z)$  - gas concentration at the point of the  $x, y, z$  co-ordinates after the time  $\tau$  since the moment of evaporation beginning /g/m<sup>3</sup>/.

The solution of equation /17/ after taking into consideration all above-mentioned boundary conditions will look like:

$$\sigma_{(x,y,z)} = \frac{q(u_1 z_1^2 k_1^{-1} m^{-2})^{1/m}}{2 \sqrt{\pi k_0 u z_1} \Gamma\left(1 + \frac{1}{m}\right) x^{1/2 + 1/m}} \exp\left\{-\frac{u}{4x} \left[\frac{y^2}{k_0} + \frac{4(z/z_1)^m z_1^2}{k_1 m^2}\right]\right\}, \quad (18)$$

where:  $m = 1 + \epsilon$  is the index of the atmosphere stability;  $\Gamma(1 + 1/m)$  is gamma function of the  $1 + 1/m$  argument;

Assuming that  $z_1 = 1$ , equation /18/ will be reduced to the following:

$$\sigma_{(x,y,z)} = \frac{q(u_1/k_1 m^2)^{1/m}}{2 \sqrt{\pi k_0 u} \Gamma\left(1 + \frac{1}{m}\right) x^{1/2 + 1/m}} \exp\left[-\frac{u}{4x} \left(\frac{y^2}{k_0} + \frac{4z^m}{k_1 m^2}\right)\right]. \quad (19)$$

Equation /19/ enables to calculate the gas concentration originating from the emission source with the  $q$  constant output. This calculation can be made at any point with the  $x, y, z$  co-ordinates.

#### 4. GAS CLOUD DIFFUSION AFTER EVAPORATION IS OVER.

The gas cloud, created as the result of the liquid gas evaporation after the reservoir or installation was damaged, will detach from the emission source after the  $\tau_p$  time which is equal to the evaporation time. After the emission is over, the gas cloud will keep diffusing as the result of stormy atmospheric diffusion.

The formula for the calculation of the gas in atmosphere at different distances from the emission source after the optional  $\tau$  time expiration, can be introduced by means of the integration of equation /17/ while maintaining the  $a, b, c$  boundary conditions as well as the approximative condition which presumes that the total amount of the liquid gas after evaporation composes the cloud with complete dimensions.

Equation /17/ after being solved (assuming that  $z_1=1$ ) acquires the following form in this case:

$$c_{(x,y,z)} = \frac{Q \exp\left(-\frac{x^2 + y^2}{4k_0\tau_u + r^2} - \frac{z^m}{k_1 m^2 \tau_u + h^m}\right)}{\pi I' \left(1 + \frac{1}{m}\right) (k_1 m^2 \tau_u + h^m)^{1/m} (4k_0\tau_u + r^2)}, \quad (20)$$

where:  $Q$  - amount of gas in the cloud /g/;  $\tau_u$  - time measured since the moment of the evaporation end /s/;  $r, h$  - specific dimensions of the gas cloud ( $r$  - radius of the horizontal profile on the Earth level;  $h$  - height /m/);

The gas cloud moves in the direction of the wind with its speed. In the same way the co-ordinate system where equation /20/ is mandatory, has to move in the same way. It is assumed that the beginning of the co-ordinate system is covered with the gravity center of the gas cloud.

The  $r$  and  $h$  parameters introduced in equation /20/ are not absolute dimensions of the gas cloud. In order to determine the values of these parameters, equation /20/ can be logarithmated which gives the following result:

$$\ln c = \ln A - \frac{x^2 + y^2}{4k_0 \tau_u + r^2} - \frac{z^m}{k_1 m^2 \tau_u + h^m}, \quad (21)$$

where

$$A = \frac{Q}{\pi \Gamma\left(1 + \frac{1}{m}\right) (k_1 m^2 \tau_u + h^m)^{1/m} (4k_0 \tau_u + r^2)}$$

If the cloud section is being regarded in the  $z = \text{const.}$  plane, then

$$\ln c = \ln AB - \frac{x^2 + y^2}{4k_0 \tau_u + r^2}, \quad (22)$$

where

$$B = \exp\left(-\frac{z^m}{k_1 m^2 \tau_u + h^m}\right).$$

Equation /22/ can be written in the form:

$$x^2 + y^2 = (4k_0 \tau_u + r^2) \ln \frac{AB}{c}. \quad (23)$$

This is the circle equation with the radius:

$$R^2 = (4k_0 \tau_u + r^2) \ln \frac{AB}{c}. \quad (24)$$

From equation /24/ it appears that if  $\tilde{u}=0$  and  $ABc^{-1}=e$ , then  $r^2=R^2$ .

If in this case  $z=h$ , then  $B=e^{-1}$  and in the result  $e=Ae^{-2}$ . Therefore,  $r$  and  $h$  are such specific cloud dimensions for which the gas concentration in the atmosphere at the  $\tilde{u}=0$  moment amounts to:

$$c = \frac{Q}{\pi \Gamma\left(1 + \frac{1}{m}\right) h r^2} e^{-2}. \quad (25)$$

## 5. GENERAL METHOD OF CALCULATIONS

The basic data for calculations to be determined are the parameters

characterizing the liquid gas, such as: the gas sort and amount, molecular mass, pressure of the gas saturated under the temperature for which calculations will be done, density, kinematic viscosity, the diffusion coefficient under the same temperature, permissible gas concentration in the air; the parameters characterizing the atmosphere condition: the wind speed and direction, the air temperature at the 50 and 200 cm height; and finally the parameter of the basis roughness designated as  $z_{00}$ . It is necessary to evaluate the size of the liquid gas blot.

The gas physical and chemical parameters are stabilized and given for the standard temperatures. Values of these parameters for other temperatures can be calculated from the formulas given in the literature.

After the determination of the basic data, it becomes possible to calculate the Reynolds number, as well as the Prandtl number and A number from formula/5 / which is a formula of the evaporation speed of the liquid gas which determines at the same time the output of the emission source.

The calculation of the size of the area where the gas concentration in the air exceeds the permissible concentration lies in the determination from equation /19/ the x,y,z coefficients of the space points where  $c(x,y,z) = c_d$  ( $c_d$  - permissible concentration). The y co-ordinates are being calculated for the following x co-ordinates (e.g. the pitch is every 10 m) within the scale from  $x=0$  up to  $x = \bar{t}_p u$  ( $\bar{t}_p$  - evaporation time; u - wind speed at a given height). The calculations are being conducted for different z heights or for the chosen height. However, the most frequently chosen height is 2 meters, since in this atmospheric layer the human being is threatened mostly.

The coordinates of the points where  $c=c_d$ , calculated in this way, denote the cloud dimensions at the moment when the evaporation is over. After the evaporation is over, the cloud is moving in the direction of the wind. The cloud location and dimensions after the  $\bar{t}_u$  optional time, calculated from the moment of the evaporation termination, are being calculated from formula /20/. However, there are two problems, whose solution, is conditioned by a correct interpretation of the calculation results. The first problem is the determination of the r and h specific dimensions of the gaseous cloud, that is the parameters which are necessary when equation /20/ is being used.

The second problem lies in the non-congruence of the figures obtained as the result of the equation /19/ and /20/ solution.

It is proposed to use the following procedure which represents a conditional, approximative solution of the above-mentioned problems: the figure which is being made by the  $c=\text{const.}$  lines after the  $\tilde{t}_n$  time (solution of equation /19/) should be transferred in proper dimension of the circles. The transposition basis can be maintaining the same area of the surface, circumscribed by the given figure and circle. After obtaining two circles with the  $R_1$  and  $R_2$  radius which correspond to the  $c_1$  and  $c_2$  concentrations, it becomes possible to determine the specific radius of the r-cloud using equation /24/. The specific height  $h$  can be calculated in the same way.

In order to calculate the dimensions of the cloud after <sup>the</sup>  $\tilde{t}_u$  time it is possible to apply equation /24/ or /25/. The circle obtained, as the result of calculations, with the  $R$  radius has to be retransferred (maintaining the same size of the surface area) into the figure similar to the original one.

This procedure enable to determine not only the size of the gaseous cloud but also its shape. However, one must be warned that the assumption of the similarity of the cloud shape at the moment of its diffusion not always can be realized.

## 6. SUMMARY CALCULATIONS

The mentioned method shows the calculations of the results of the damage of the reservoir which contains the liquid chlorine. The calculations were made by means of the Minsk 22 and Odra 1004 digital computers. The basic data are compared in Table 3 and 4.

The  $Re$ ,  $A$  values (Tab.1) and  $q$  values (Formula /5/) calculated on the basis of these data, amount:  $Re = 8.0 \cdot 10^6$ ;  $A = 2.5 \cdot 10^4$ , the evaporation speed  $q = 37.7$  kg/s.

It is assumed that the process of the atmospheric diffusion takes place in the inversion conditions, in the area which is partially covered with forests and partially cultivated. For the inversion the average value of the  $\mathcal{E}$  parameter is .20 ( $m = 1 + \mathcal{E} = 1.2$ ); however, the surface roughness in the

accepted here area amounts <sup>10m</sup>. For these conditions one reads out the value of the  $k_1/u_1$  quotient equal to .04 from <sup>the</sup> monogram (Fig.1). From this value one calculates the value of the  $k_1$  diffusion coefficient when assuming that the wind speed at the 1m height is 1.2 times lower than this one at the 2m height, that is  $u_1 = u_2/1.2$ . These data are compared in Table 5.

Using formula (12) the chlorine diffusion in the atmosphere has been computed. The gaseous cloud dimensions indicate the points where the chlorine concentration reaches the permissible value. It is assumed that the chlorine permissible concentration amounts  $.001\text{mg/dm}^3$ . This value is given by the Polish State Standard PN-56/Z-040030 which identifies the maximum permissible gas concentrations in the air surrounding the working place. The gaseous cloud dimensions after the evaporation was terminated are presented on Fig. 2.

Table 3. Start data for computing

Quantity	Symbol	Numerical value
Amount of chloride	$Q$	1000 kg
Spot diameter	$d$	10 m
Air temperature	$T$	293 K
Wind velocity at a height of 2m	$u_2$	4 m/s
Permissible concentration of $\text{Cl}_2$	$c_d$	0,001 g/m <sup>3</sup>
Toxic concentration of $\text{Cl}_2$	$c_t$	0,012 g/m <sup>3</sup>

Table 4. Physico-chemical properties of chlorine in 20°C

Quantity	Symbol	Numerical value
Molecular mass	$M$	70,91 g/mol
Saturated vapour pressure	$P_n$	4993 mm Hg
Kinetic viscosity	$\nu$	0,0442 cm <sup>2</sup> /s
Diffusion coefficient	$D$	0,124 cm <sup>2</sup> /s

- Table 5

Quantity	Symbol	Numerical value
Roughness parameter	$z_{00}$	0,10 m
Vertical stability parameter of the atmosphere	$\epsilon$	0,20
Index stability of the atmosphere	$m = 1 + \epsilon$	1,20
Diffusion coefficient (eq. (15))	$k_1$	0,133 m <sup>2</sup> /s
Diffusion coefficient (eq. (16))	$k_0$	1,035 m <sup>2</sup> /s

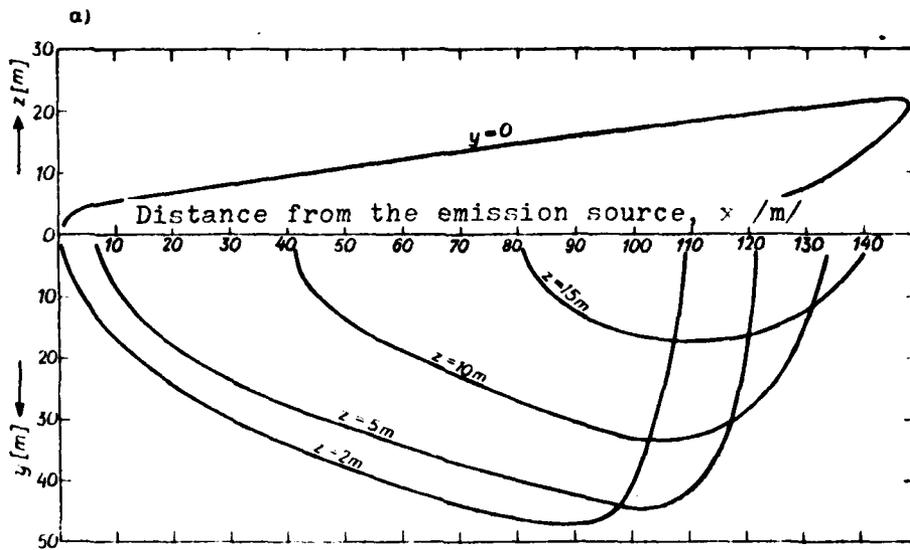


Fig. 2a. Vertical-section  $XZ$  and cross-section  $XY$  of a chlorine cloud for the inversion at the end time of source emission

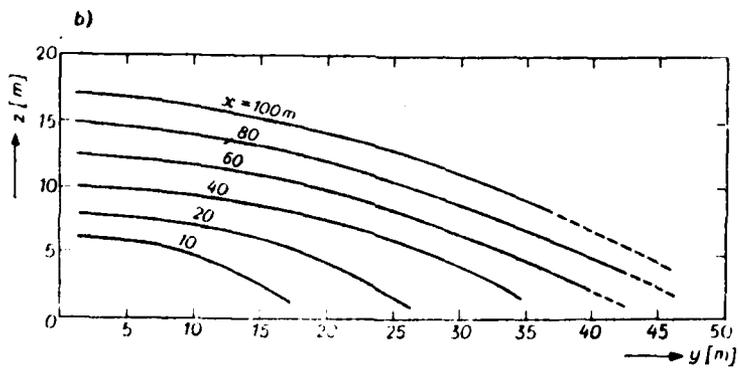


Fig. 2b. Vertical-sections  $FZ$  of a chlorine cloud for the inversion at the end time of source emission

$$m = 1, 2, c_a = 0,10 \cdot 10^{-2} \text{ g/m}^3, Q = 1000 \text{ kg}, d = 10 \text{ m}, u_2 = 4 \text{ m/s}, \tau_p = 27 \text{ s}$$

The cloud section at the moment of the evaporation termination in the  $z=2$  m plane has the shape close to the isosceles triangle. Two triangles were found. On their sides there are the known  $c_1$  and  $c_2$  concentration. The areas of these triangles' surfaces have been calculated. After that the radius of the circles whose area is equal to the triangles' areas have been found. For calculations the following concentrations have been accepted:  $c_1 = .001 \text{ mg/dm}^3$ ;  $c_2 = .200 \text{ mg/dm}^3$ . The obtained radiuses were:  $R_1 = 43.50 \text{ m}$ ;  $R_2 = 42.12 \text{ m}$ . Using formula /2/ as a basis and assuming that  $\tilde{v}_u = 0$ , it was obtained a specific radius of the cloud -  $r = 17.75 \text{ m}$ .

The gaseous cloud section in the  $y=0$  vertical section has also (it is possible to assume in approximation) the triangle shape. Two triangles corresponding the  $c_1$  and  $c_2$  concentrations have been found. Their surface areas have been determined and then one obtained the circle sections having the same areas and chords being equal to the  $2R_1$  and  $2R_2$  diameters. The calculated arrows of these sections amount to  $z_1 = 27.50 \text{ m}$  and  $z_2 = 14.55 \text{ m}$ . Applying these data it has been obtained from equation /21/ with the condition that  $\tilde{v} = 0$  that the h-specific height is equal to  $3.03 \text{ m}$ .

Knowing  $r$  and  $h$  which are specific parameters of the cloud, one calculated on the basis of equation (24) the radiuses and the following areas of the horizontal sections of the cloud in the  $z=2 \text{ m}$  plane after different  $\tau_u$  time for two concentration values of the chlorine in the air, that is for the permissible concentration ( $.001 \text{ mg/dm}^3$ ) and the concentration which is beyond endurance of the human being even for short-lasting exposure. This concentration is evaluated as  $.012 \text{ mg/dm}^3$  /7/ and called "toxic" and designated as  $c_t$ . The next step was to find out the triangles with the areas being equal to the area of the horizontal sections of the cloud. These triangles are similar to the triangular appearing at the  $\tau_p$  time. These triangles represent approximative dimensions and shape of the chlorine cloud at the moment of its diffusion. They are shown on Fig. 3. It is natural that the gaseous cloud having the shape approximating the triangle does not possess its sharply outlined elements, especially vertexes. It is exemplified on the picture by means of likening the shape of the diffusing cloud to the  $z=2 \text{ m}$  section on Fig. 2.

The change of the cloud dimensions at the moment of its diffusion when the emission is over is represented in a continuous way on Fig 4 as the change of its front width.

The essential values enabling to conduct the evaluation of the threat in a specified distance from the emission source are the following ones: the time after which the cloud front will reach this place; the time, during which this place will remain within the cloud. The dependence of these times on the distance from the emission source is shown on Fig.5.

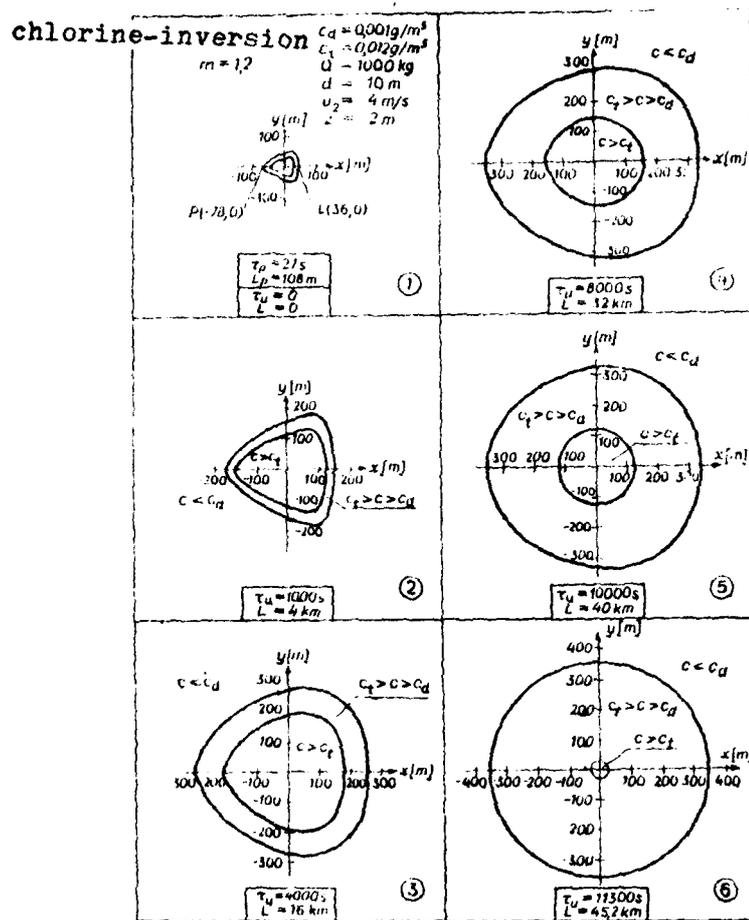


Fig. 3. Zones of chlorine risk

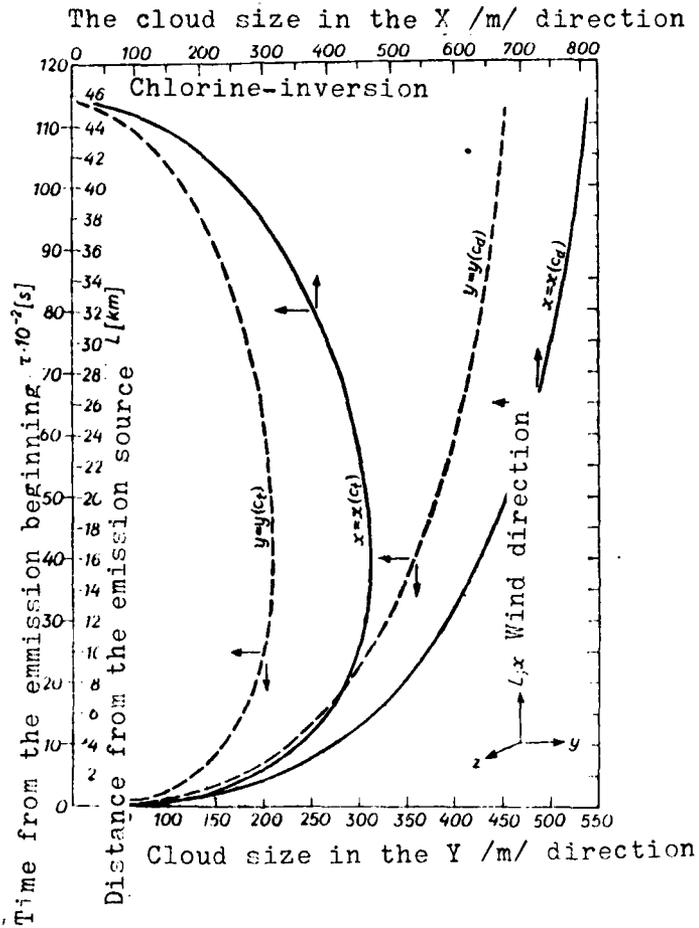


Fig. 4. The change in zones for the allowable and toxic concentration in the vertical direction vs. wind axis during the dispersion of the gaseous chlorine cloud after the end of source emission

$m = 1, 2$ ,  $c_a = 0,001 \text{ g/m}^3$ ,  $c_t = 0,012 \text{ g/m}^3$ ,  $Q = 1000 \text{ kg}$ ,  $d = 10 \text{ m}$ ,  $u_x = 4 \text{ m/s}$ ,  $z = 2 \text{ m}$

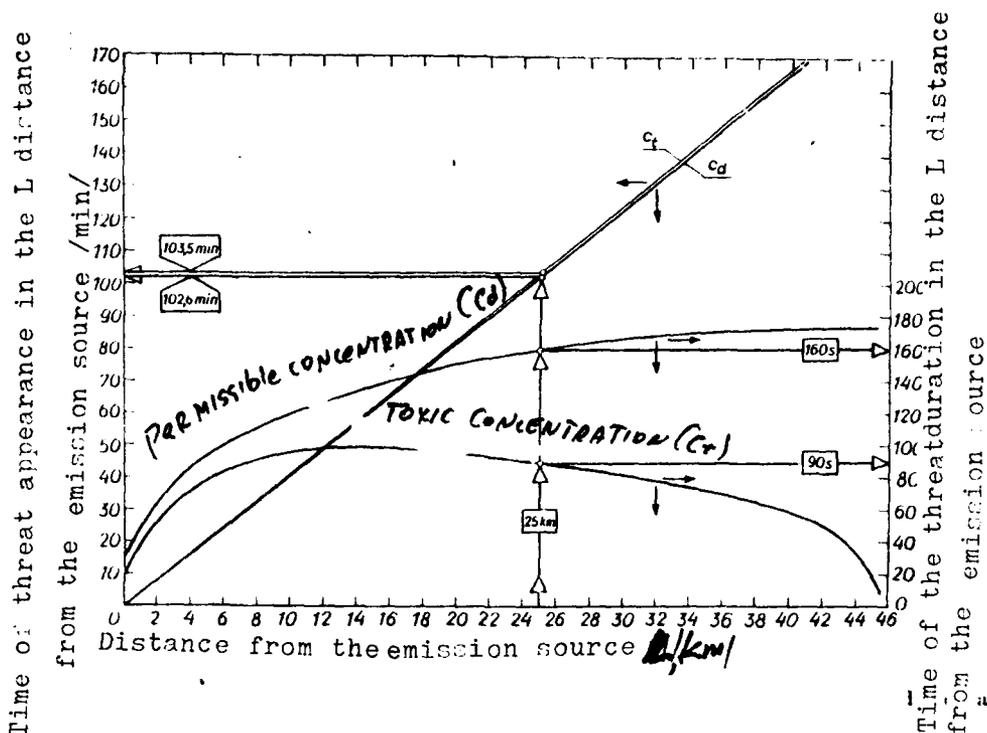


Fig. 5. Start-time and duration of chlorine risk in the wind direction for a given distance from source emission

$$m = 1, 2, c_d = 0,00 \text{ t/g/m}^3, c_t = 0,012 \text{ g/m}^3, Q = 1000 \text{ kg}, d = 10 \text{ m}, u_g = 4 \text{ m/s}, z = 2 \text{ m}$$

## 7. DISCUSSION

The method presented here of calculation of the gas diffusion in the near-Earth layer of the atmosphere is not a perfect method. It has certain faults resulting from the acceptance of numerous simplifying assumptions. Such assumptions are the statements that in the case of damage (e.g. a reservoir) a liquid gas after pouring out compose a blot with permanent thickness; that the surface of the liquid level during the evaporation remains permanent; and that the evaporation speed is a permanent value. In reality, the evaporation speed can undergo significant fluctuations caused not only by a possible change of the evaporated surface but also by the ball absorption, by the wind speed fluctuations, by changes of the thermal conditions. The assumption of the constancy of the evaporation speed was, however, the condition of the solution of equation /19/.

The mathematical model which is represented by formula /19/ is also idealized. It does not take into consideration such factors as the sculpture of the Earth's surface, presence of different regional hindrances, changes of the

atmospheric conditions as well as the fluctuations of the wind speed and direction.

The same remarks are related to the calculations of the gaseous cloud diffusion after the evaporation termination (formula /20/). When introducing this formula it has been assumed that the total gas amount after evaporation is in the atmosphere, whereas a part of the gas is being absorbed by the soil, water reservoirs, forests, etc. It has also been assumed that there is similarity of the gaseous cloud phase during the evaporation, which not always can be realized.

Some of the mentioned simplifying assumptions worsen the results of calculations, others act in a different direction. It is difficult to determine which ones of them will prevail. However, one can assume that these actions can be compensated in certain conditions. Therefore, it is also considered, that this method can be applied to the purpose for which it was adopted, that is for the calculations of the results of damage of the reservoirs with liquid gases and analogous phenomena.

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