

## ТЕХНОГЕННА БЕЗПЕКА ПРОМИСЛОВОСТІ

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*V. Smalii<sup>1,2</sup>, E. Tolok<sup>2</sup>*<sup>1</sup>*Volodymir Dahl East Ukrainian National University*<sup>2</sup>*Scientific Center of Risk Investigation Rizikon*

### MODEL OF A MULTI-COMPONENT LIQUID POOL EVAPORATION FORMED DUE TO ACCIDENTAL SPILLS

Quantitative analysis and assessment of a technogenic risk imply a thorough study of the emergency process at the level of phenomenology. In such of a study, mathematical models of the physical and chemical processes of the hazardous substance formation in the surrounding space are involved. The occurrence and influence of the damaging factors on recipients, such as people, the environment, buildings and equipment, must be assessed. One of the most common scenarios for the formation of a hazardous substance in the environment is spillage of a liquid phase, often of a multicomponent composition, onto the earth's surface. The subsequent evaporation of a hazardous substance is a key factor in the formation of an explosive, flammable or toxic cloud. Therefore, it is extremely important to correctly assess the intensity of the hazardous substance release into the environment.

This study presents a mathematical model for the evaporation of a multicomponent liquid from the surface of an emergency spill. It considers various energy influxes that affect the evaporation process (atmospheric air heat, underlying surface heat, radiation from the sun). The effect of cooling due to evaporation is taken into account. The developed model considers the influence of the liquid phase composition on the evaporation process. A comparative analysis of the simulation results was made using the published experimental data on the mixture of a cryogenic liquid (nitrogen) and liquids under non-boiling conditions such as ethanol and cyclohexane evaporation process. The results of the comparison showed the model's applicability in the field of quantitative risk analysis and assessment. The possibilities of improving the multicomponent liquid pool evaporation mathematical model are presented.

**Keywords:** evaporation, multicomponent mixture, model, phase equilibrium, heat flow, hydrocarbons, cryogenic substance, ethanol

**Problem statement.** Due to the increase in the number of chemical, petrochemical and other hazardous industries, as well as the constant development of technologies, more and more attention is paid to the issues of reducing industrial risks using risk analysis and risk management tools.

The risk-based approach implies not only logic-probabilistic modeling, designed to assess the probability of a certain accident scenario, but also an assessment of all the possible accident scenarios consequences [1 – 2]. The assessment of the consequences is carried out with mathematical modeling of the physical and chemical processes of the damaging factors formation, as they can be a direct threat to people, nature, industrial equipment, buildings and structures.

One of the most common types of accidents at the chemical and petrochemical plants is depressurization of the equipment. It is often followed by the release of a flammable, explosive or toxic liquid, which leads to the formation of a liquid phase spill. The liquid spill consequence is evaporation of the liquid, followed by formation, movement and dispersion of a toxic, flammable or explosive cloud. The evaporation rate of the liquid pool is a key factor in assessing the consequences of a substance release into the environment. It determines the degree of damage to people, flora and fauna as a result of an explosion of a fuel-air mixture, thermal radiation from a fire, or toxic effects [3-6].

Thus, an adequate determination of the evaporation dynamics of the liquid pool is a basic task of the quantitative risk assessment [7-8].

Almost all recommended normative methods are rather simplified and do not consider the possibility of a multicomponent mixture evaporation, the change in the mixture composition over time

and its effect on its physicochemical properties, which affects the modeling accuracy. As an example, the formula for the intensity of evaporation given in the new Ukrainian standard corresponds to the stationary regime, where the intensity of evaporation does not depend on time, composition of the liquid pool or heat fluxes from the environment [2]. No validation using experimental data has been provided, which makes it impossible to evaluate the liquid pool evaporation model's adequacy, as proposed in the standards. This implies certain discrepancy between the real liquid pool evaporation data and the model results.

It is essential to develop a liquid pool evaporation model that accounts the influence of the liquid pool composition, heat flows from ground, air and Sun, to the evaporating rate. The model should be validated using the experimental data available and be applicable for the quantitative risk assessment.

**Methods and materials.** The model below takes into account the following:

- 1)  $h_0 \ll d$ , where  $h_0$ ,  $d$  [m] are the initial liquid pool thickness and diameter;
- 2) energy fluxes affecting the evaporation process - heat flux from the atmospheric air, from the soil (underlying surface), radiation flux from the Sun (completely absorbed by the liquid phase);
- 3) heat exchange between the liquid pool and the environment through the lateral surface of the pool is neglected (due to 1);
- 4) the liquid temperature is uniform and throughout the entire liquid layer, which corresponds to complete and rapid mixing (due to 1);
- 5) the mathematical model treats the time dependence of the liquid phase composition and the mixture properties, as a result of the evaporation process;
- 6) the model considers the temperature dependence of the mixture components physical properties. The mixture components physical properties were determined in accordance with [9]. The physical properties of the mixture were determined as follows.

Molecular weight [kg/mol]:

$$M_{mix} = \sum_{i=0}^N x_i M_i \quad (1)$$

The heat capacity at constant pressure [J/(mol·K)]:

$$C_{pL\_mix} = \sum_{i=0}^N x_i C_{pL}^i \quad (2)$$

Density [kg/m<sup>3</sup>]:

$$\rho_{L\_mix} = \frac{M_{mix}}{\sum_{i=0}^N \frac{x_i M_i}{\rho_i}} \quad (3)$$

The latent heat of evaporation [J/mol]:

$$L_{v\_mix} = \sum_{i=0}^N x_i L_v^i \quad (4)$$

Saturated vapor pressure [Pa]:

$$P_{sv\_mix} = \sum_{i=0}^N x_i P_{sv}^i \quad (5)$$

The diffusion coefficient of vapor into air [m<sup>2</sup>/s]:

$$D_{v\_mix} = \sum_{i=0}^N x_i D_v^i \quad (6)$$

where:  $x_i$  is the mole fraction of the  $i$ -th component of the mixture [mol/mol];  $(N+1)$  is the number of components of the mixture.

#### **Mathematical description of the conservation equations**

For simplicity, the mix index is omitted for the liquid mixture physical parameters (i.e.  $D_{v\_mix} \rightarrow D_v$ ).

Heat balance and mass balance equations are described below [3]:

$$\frac{d(h \cdot \rho_L \cdot C_{pL} \cdot T)}{dt} = H_s + H_a + H_{sr} - q_{v_m} \cdot L_v \quad (7)$$

$$\frac{dh}{dt} = -\frac{q_v}{\rho_L} \quad (8)$$

where:  $h$  – thickness of the liquid pool [m];  $C_{pL}$  – heat capacity of the liquid mixture [J/(kg·K)];  $\rho_L$  – density [kg/m<sup>3</sup>];  $L_v$  – latent heat of evaporation [J/kg];  $T$  – temperature [K];  $H_s$  – ground-liquid heat flux [J/(m<sup>2</sup>·s)];  $H_a$  – air-liquid heat flux [J/(m<sup>2</sup>·s)];  $H_{sr}$  – heat flux of solar radiation [J/(m<sup>2</sup>·s)];  $q_{v_m}$  – mass evaporation rate [kg/(m<sup>2</sup>·s)].

Molar rate of evaporation:

$$\frac{dN_{mol}}{dt} = -q_{v_{mol}} \cdot S \quad (9)$$

where:  $N_{mol}$  – amount of substance [mol];  $t$  – time [s];  $q_{v_{mol}}$  – pool surface evaporation rate [mol/(m<sup>2</sup>·s)].

Mass balance for  $i$ -th component:

$$\frac{d(N_{mol} \cdot x_i)}{dt} = -q_{v_{mol}} \cdot S \cdot y_i \quad (10)$$

where:  $x_i$  – molar part of  $i$ -th component in liquid phase (LP);  $y_i$  – molar part of  $i$ -th component in gas phase (GP).

Let's rewrite an equation (10):

$$N_{mol} \frac{dx_i}{dt} + x_i \frac{dN_{mol}}{dt} = -q_{v_{mol}} \cdot S \cdot y_i \quad (11)$$

Substitution of (9) in (11) gives:

$$\frac{dx_i}{d\tau} = \frac{q_{v_{mol}} \cdot S}{N_{mol}} \cdot (x_i - y_i) = \frac{q_{vm}}{h \cdot \rho_L} \cdot (x_i - y_i) \quad (12)$$

According to Rault's law (gas/liquid equilibrium is considered) [11]:

$$P_i(T) = P_{sv}^i(T) \cdot x_i \quad (13)$$

where:  $T$  – temperature [K];  $P_i(T)$  –  $i$ -th component partial pressure [Pa];  $P_{sv}^i(T)$  – pressure [Pa] of the  $i$ -th component saturated vapor.

The pressure of saturated vapor at a given temperature is determined by the Antoine equation, which is a common practice.

The Dalton equation [11]:

$$P_i(T) = P_{tot}(T) \cdot y_i \quad (14)$$

where:  $P_{tot}(T)$  – total pressure [Pa] of the GP.

The total pressure [Pa] of the GP:

$$P_{tot}(T) = \sum_{i=0}^N P_i(T) \quad (15)$$

where:  $P_i(T)$  –  $i$ -th component partial pressure [Pa].

Equations (14) and (15) imply that [12]:

$$y_i = \frac{P_i(T)}{\sum_{i=0}^N P_i(T)} \quad (16)$$

Equations (13) and (16) imply that:

$$y_i = \frac{P_{sv}^i(T)}{\sum_{i=0}^N (P_{sv}^i(T) \cdot x_i)} \cdot x_i = k_i(T) \cdot x_i \quad (17)$$

where:  $k_i(T)$  – is the distribution coefficient of the substance between GP and LP.

From (12), considering (17), follows, that:

$$\frac{dx_i}{dt} = \frac{q_{v_{mol}}}{N_{mol}} \cdot (x_i - k_i(T) \cdot x_i) = \frac{q_{vm}}{h \cdot \rho_L} \cdot (x_i - k_i(T) \cdot x_i) \quad (18)$$

In the order to correctly choose the evaporation rate formula it is important to check the presence of the boiling process of the mixture every moment of the modeling time.

It is known that boiling is an intense process of evaporation, which occurs if evaporating mixture's saturated vapors' pressure is equal or exceeds atmospheric pressure [3].

The boiling point  $T_b$  [K] of a mixture at atmospheric pressure could be determined from:

$$P_a = \sum_{i=0}^N x_i P_{sv}^i(T_b) \quad (19)$$

### **Heat flux from the ground**

The heat influx  $H_s$  [J/(m<sup>2</sup>·s)] from the soil can be determined as follows.

Consider the one-dimensional problem of heat conduction:

$$\frac{\partial T}{\partial t} = a_s \frac{\partial^2 T}{\partial x^2} \quad (20)$$

where:  $T(x, t)$  – soil temperature [K] at a certain depth  $x$  [m] and time  $t$  [s];  $a_s$  – soil coefficient of thermal diffusivity.

Initial conditions:

$$T(x, 0) = T_s \text{ для } \forall x \in [0; L_s) \quad (21)$$

Boundary conditions:

$$T(0, t) = T_p; T(L_s, t) = T_s \text{ для } \forall t \in [0; +\infty) \quad (22)$$

where:  $T_s$  – soil temperature [K] at the depth  $L_s$  [m];  $T_p$  – temperature [K] of the evaporating pool;  $L_s$  – soil depth [m] where the temperature remains constant.

Consider  $L_s = 10h_0$ , where  $h_0$  is the evaporating pool initial depth [m].

The heat influx from the soil to the pool:

$$q(t) = \lambda_s \cdot \frac{\partial T(0, t)}{\partial x} \quad (23)$$

The heat flux  $H_a$  [W/m<sup>2</sup>] from the atmosphere is determined by the formulas [3]:

$$Pr_a = \frac{\nu_a}{\alpha_a} \quad (24)$$

$$Re = \frac{u_a d}{\nu_a} \quad (25)$$

$$Nu = 0.037 \cdot Pr_a^{\frac{1}{3}} \cdot Re^{0.8} \quad (26)$$

$$k_a = Nu \cdot \frac{\lambda_a}{d} \quad (27)$$

$$H_a = k_a(T_a - T) \quad (28)$$

where:  $\nu_a$  – air kinematic viscosity [m<sup>2</sup>/s];  $\alpha_a$  – air thermal diffusivity [m<sup>2</sup>/s];  $u_a$  – wind speed [m/s] at 10 m height;  $d$  – pool diameter [m];  $\lambda_a$  – air thermal conductivity [W/(m·K)];  $k_a$  – heat transfer coefficient [W/(m<sup>2</sup>·K)];  $T_a$  – air temperature [K];  $T$  – evaporating pool temperature [K];  $Pr_a$  – air Prandtl number;  $Re$  – air Reynolds number;  $Nu$  – air Nusselt number.

Note: the coefficients  $\nu_a$ ,  $D_v$ ,  $\lambda_a$ ,  $k_a$ ,  $Pr_a$ ,  $Re$ ,  $Nu$  are calculated for the average temperature  $T_{mid} = 0.5 \cdot (T_a + T)$  [13].

### Evaporation rate

The evaporation mass rate [kg/(m<sup>2</sup>·s)] is determined by the formulas [3]:

$$k_m = C_m \cdot u_a^{0.78} \cdot d^{-0.11} \cdot Sc^{-0.67} \quad (29)$$

$$Sc = \frac{\nu_a}{D_v} \quad (30)$$

$$q_{vm} = k_m \cdot \frac{P_{sv} M}{RT} \quad (31)$$

where:  $C_m = 0.004786$  – constant;  $u_a$  – wind speed [m/s] at 10 m height;  $d$  – evaporating pool diameter [m];  $Sc$  – Schmidt number;  $P_{sv}$  – evaporating substance saturated vapor pressure [Pa];  $M$  – evaporating substance molecular weight [kg/mol];  $R = 8.314$  – gas constant [J/(mol·K)];  $T$  – evaporating pool temperature [K].

The evaporation mass rate [kg/(m<sup>2</sup>·s)] for a boiling liquid is determined by the formula [3]:

$$q_{vm} = \frac{H_s(T_b) + H_a(T_b) + H_{sr}}{L_v(T_b)} \quad (32)$$

The molar evaporation rate:

$$q_{vmol} = \frac{q_{vm}}{M} \quad (33)$$

The molar evaporation rate of the  $i$ -th component:

$$q_{vmol}^i = X_i \cdot q_{vmol} \quad (34)$$

The evaporation molar rate of the  $i$ -th component from the total surface of liquid pool:

$$q_{v_{mol_s}}^i = S \cdot X_i \cdot q_{v_{mol}} \quad (35)$$

where:  $S$  – evaporating surface area [ $\text{m}^2$ ] of the pool.

**Results and discussion.** To validate the model, 2 series of computational experiments have been performed. The first series – evaporation of a cryogenic liquid (liquid nitrogen) in boiling regime. The second series – evaporation of organic substances such as ethanol and cyclohexane in non-boiling regime.

**Evaporation of the liquefied nitrogen.** To check the adequacy of the considered numerical model, the simulation results were compared with the experimental data for cryogenic boiling liquid presented in [13].

The experiment was carried out with liquid nitrogen (LN2) spilled on the polystyrene. The inner size of the box was 0.48 m x 0.48 m x 0.1 m [13]. The thickness of the walls and base is 0.15 m. The box was completely made of polystyrene, so the heat loss throughout the walls is neglectable due to small thermal conductivity of the polystyrene. The base and walls of box were equipped with built-in thermocouples. To supply LN2 into the polystyrene box an outlet pipe was used. Analysis started after the filling was stopped. The box itself was positioned in a wind tunnel 2.04 m wide, 0.855 m high and 12 m long, which was specially designed to isolate the box from natural wind and provide a controlled and stable airflow. The initial data of the evaporation of liquid nitrogen experiment are presented below (Table).

Table

**Initial data of experimental evaporation of cryogenic liquid (nitrogen)**

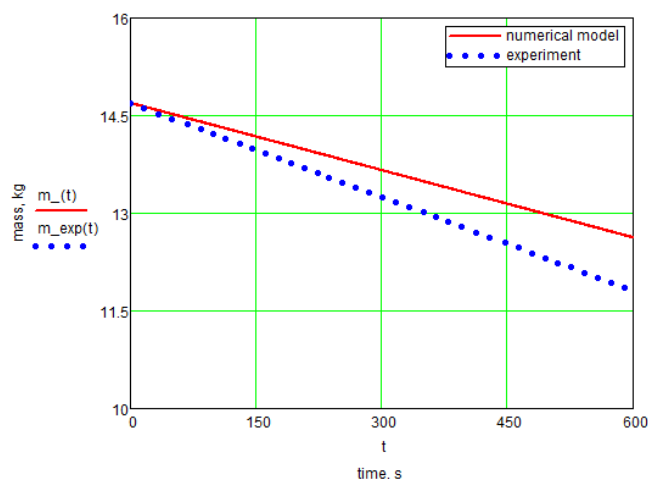
Parameter	Symbol and Dimension	Value
Air temperature	$T_a$ , [K]	309
Atmospheric pressure	$P_a$ , [Pa]	101325
Wind speed at 10 m height	$u_a$ , [m/sec]	6.2
Kinematic viscosity of air at defined air temperature	$\nu_a$ , [ $\text{m}^2/\text{sec}$ ]	$1.638 \cdot 10^{-5}$
Heat conductivity of air	$\lambda_a$ , [W/(K·m)]	0.027
Insolation flux	$H_{sr}$ , [W/ $\text{m}^2$ ]	0
Heat conductivity of the ground	$\lambda_s$ , [W/(m·K)]	No heat exchange with ground
Thermal diffusivity of the ground	$a_s$ , [ $\text{m}^2/\text{sec}$ ]	No heat exchange with ground
Temperature of the ground	$T_s$ , [K]	No heat exchange with ground
Area of liquid spill	$S$ , [ $\text{m}^2$ ]	0.23
Initial temperature of liquid pool	$T_0$ , [K]	boiling temperature of nitrogen at atmospheric pressure
Initial thickness of liquid pool	$h_0$ , [m]	0.08
Liquid pool composition	$X_0$ , [molar parts]	(100% nitrogen)
Duration of experiment	$t_N$ , [sec]	600

Next considerations and preparations have been made:

- in the model, the heat flux from the underlying surface  $H_s = 0$  due to the use of the heat-insulating material of evaporating box during the experimental study;
- the wind speed at the height  $h = 10$  m has been obtained via calculation using experimental value of the wind speed  $u_a = 2.99$  m/s at a height  $h = 0.305$  m. The method presented in [14] has been used;
- the initial thickness of the pool has been obtained using initial mass in the pool  $m_0 = 14.69$  kg and evaporating pool geometry;
- the nitrogen coefficient of diffusion into the air has been obtained for the mixture "nitrogen - oxygen" according to [15].

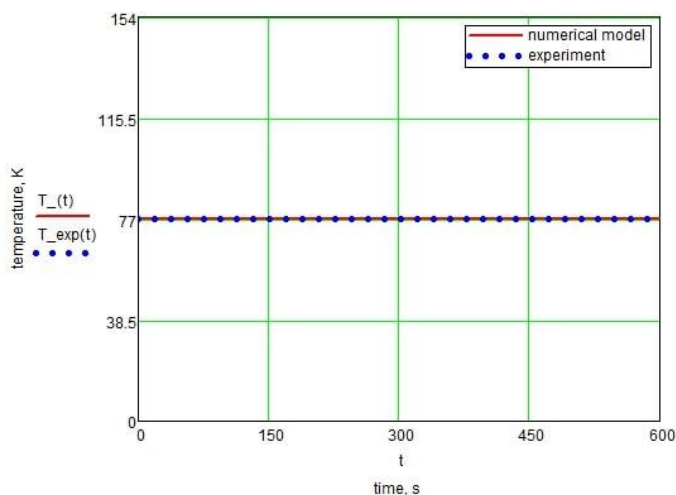
The model slightly underestimates the evaporation rate for a cryogenic liquid during boiling process (see Fig. 1). After 600 seconds, the amount of nitrogen evaporated was 2.88 kg, while the model predicted 2.066 kg of evaporated nitrogen. The evaporation rate according to the model is approximately 1.39 times less than the evaporation rate according to the experiment. In this case, evaporation model

should be applied for risk assessment with caution. Possible underestimation of evaporation rate should be taken into account.



**Fig.1. Time dependence of liquid pool mass ( $m(t)$  – simulation data,  $m_{exp}(t)$  – experimental data)**

The temperature of the pool, calculated according to the model, is in full agreement with the temperature of the pool, measured during the experiment (see Fig. 2). Both of the temperatures are equal to the boiling point of pure nitrogen at atmospheric pressure.



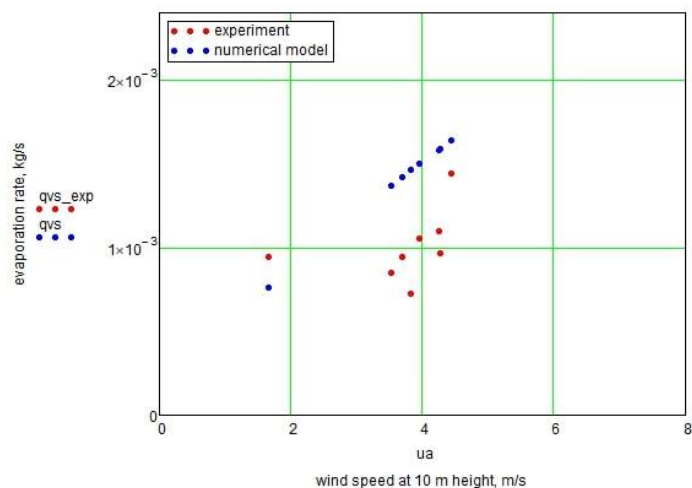
**Fig. 2. Time dependence of liquid pool temperature ( $T(t)$  – simulation data,  $T_{exp}(t)$  – experimental data)**

**Evaporation of the ethanol and cyclohexane in non-boiling regime.** To validate the model in the case of organic substances evaporation in non-boiling regime, the comparison with experimental data has been made [7].

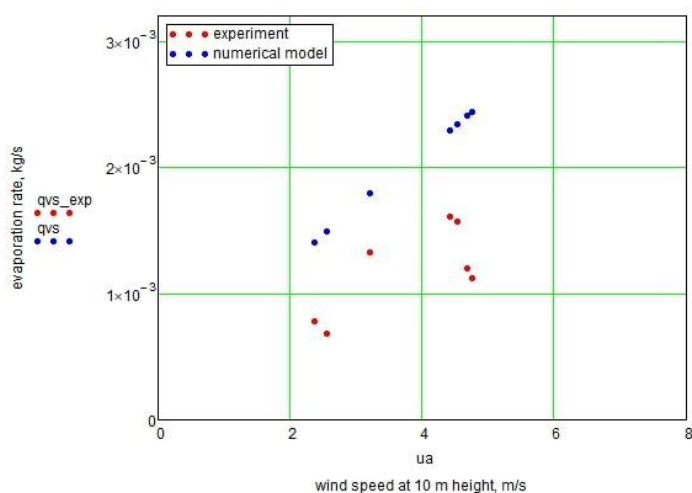
Evaporation experiments with ethanol and cyclohexane in basin were carried out. The diameter of basin is 0.74 m. An open-air non-built-up environment were investigated. The basin was heated up via a water-heated heating coil and the evaporating mass flow was determined by weighing the liquid content before and after the experiment in correlation to the duration of the experiment. Two K-type thermocouples were placed in the liquid, one near the interphase and one at the bottom of the basin. The average of both temperatures was used as the liquid temperature [7].

The wind speed at 10 m height were provided by the German meteorological services from a measuring station on the site [7].

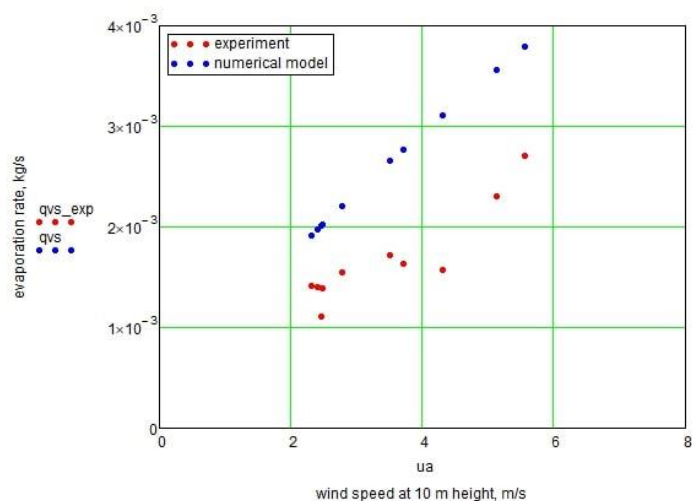
The results of the comparison of developed model and experimental data for ethanol evaporation at different temperatures and wind speeds are presented on figures 3, 4, 5.



**Fig. 3. Wind speed dependence of evaporation rate (Ethanol, 303K)**

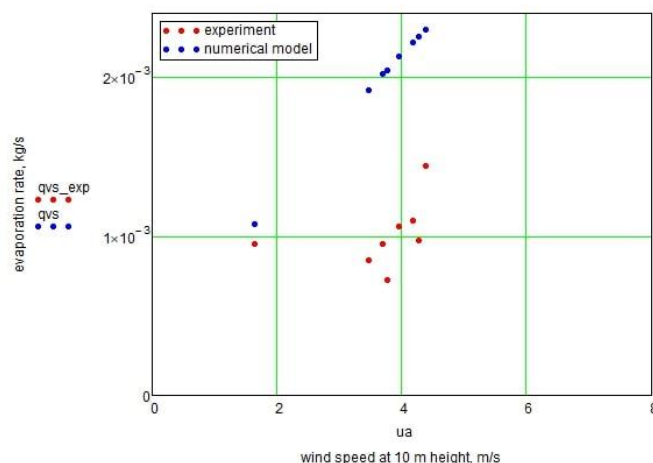


**Fig. 4. Wind speed dependence of evaporation rate (Ethanol, 310K)**

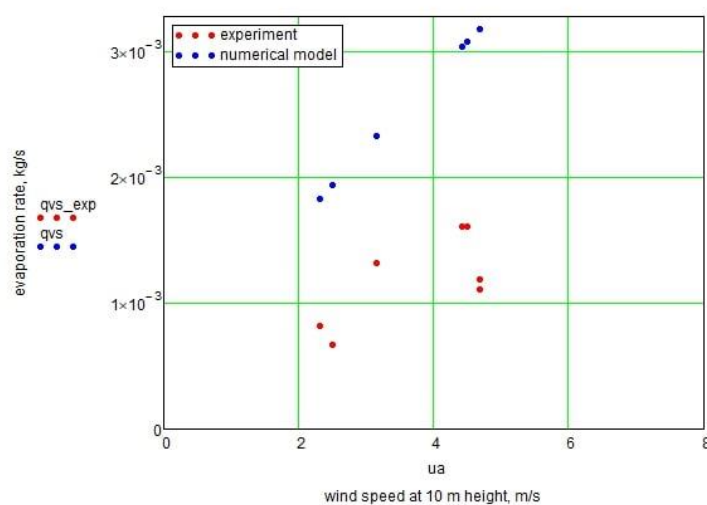


**Fig. 5. Wind speed dependence of evaporation rate (Ethanol, 317K)**

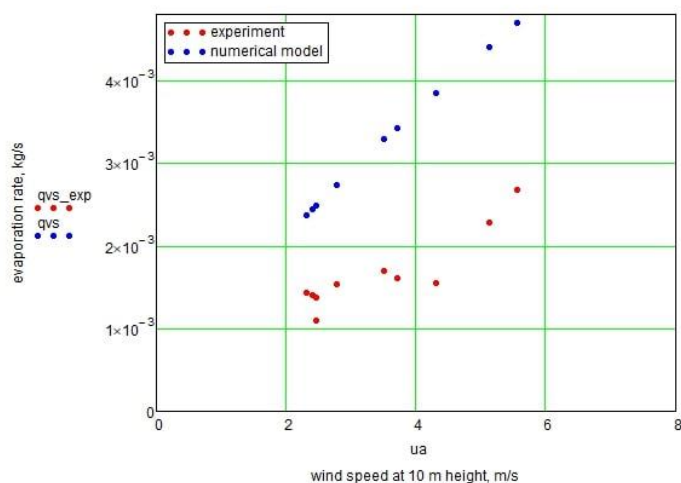
The results of the comparison of developed model and experimental data for cyclohexane evaporation at different temperatures and wind speeds are presented on figures 6, 7, 8.



**Fig. 6. Wind speed dependence of evaporation rate (Cyclohexane, 303K)**



**Fig. 7. Wind speed dependence of evaporation rate (Cyclohexane, 310K)**



**Fig.8. Wind speed dependence of evaporation rate (Cyclohexane, 317K)**

Almost the same declination angle of linear dependence for both experimental and numerical model data (see Fig. 5 and Fig. 8) has been observed.

The model slightly overestimates evaporation rate for both ethanol and cyclohexane which is conservative approach. So the model could be applied in the field of quantitative risk assessment.



Although there are small-scale experimental data, applicable for model validation, there is still no large-scale experimental set-ups close to real liquid spills which occur during industrial accidents. The opinion about possible different behavior large-scale pools evaporation process was also concluded in [7].

The other significant problem is an absence of sufficient experimental data for evaporation of multi-component pools.

**Conclusions.** Quantitative risk analysis and assessment require application of reliable, validated, up-to-date models. One of the most significant accidental processes is liquid pool evaporation formed due to depressurization of factory reactors, vessels, compressors, etc. It is essential to be able to consider multi-component composition of liquid pool as it is most common appearance in practice.

In this work, a model for the evaporation of a spill of a multicomponent liquid phase has been developed. The evaporation process is modeled considering heat exchange of evaporating pool with the Sun, soil and air as well as the effect of cooling due to evaporation. The model considers time dependence of the liquid phase mixture composition during evaporation process. The model is relatively easy to implement by process safety or ecology safety specialists.

A comparative analysis of the model and available published experimental data has been made.

In the first series of tests, the evaporation of a cryogenic liquid (pure nitrogen) has been simulated. The liquid was spilled inside of a heat-insulated box; there was no solar radiation influence; the air temperature and wind speed were known. The evaporation rate according to the model is approximately 1.39 times less than the evaporation rate according to the experiment. Thus careful application of evaporation model for risk assessment of cryogenic liquids is required. Possible underestimation of evaporation rate should be taken into account. The numerical experiment showed excellent agreement between simulated pool temperature and experimental temperature measurements.

In the second series of experimental tests, the evaporation of ethanol and cyclohexane during non-boiling conditions has been simulated. Wind speed dependence of evaporating rate has been obtained. There is similar behavior for both of numerical simulation and experimental data. The best similarity was observed at 317 K for both of ethanol and cyclohexane evaporating pools.

Considering the results of validation made for liquid nitrogen, ethanol and cyclohexane, developed model can be applied in the field of numerical risk assessment taking into account slight underestimation for cryogenic boiling spills.

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**В. В. Смалій<sup>1,2</sup>, Є. В. Толок<sup>2</sup>**

<sup>1</sup>Східноукраїнський національний

університет імені Володимира Даля

<sup>2</sup>Науковий центр дослідження ризиків Ризикон

## МОДЕЛЬ ВИПАРОВУВАННЯ БАГАТОКОМПОНЕНТНОГО РОЗЛИВУ СФОРМОВАНОГО У РЕЗУЛЬТАТІ АВАРІЇ

Кількісний аналіз та оцінка техногенного ризику промислового об'єкта мають на меті обчислення кількісних показників ризику і їх зменшення до прийнятних величин. У процесі такого дослідження залучаються математичні моделі фізико-хімічних процесів формування небезпечної речовини в навколишньому просторі, виникнення та впливу факторів, що вражають, на реципієнтів. Реципієнтами є люди, навколишнє середовище, будівлі та обладнання. Одним із найпоширеніших сценаріїв формування небезпечної речовини у навколишньому середовищі є витік рідкої фази часто багатоконпонентного складу на поверхню землі. Подальше випаровування небезпечної речовини з поверхні розливу спричинює формування вибухонебезпечної, пожежеонебезпечної або токсичної хмари. Тому важливо коректно оцінювати інтенсивність надходження небезпечної речовини у довкілля, враховуючи багатоконпонентний склад суміші розливу.

У даному дослідженні представлена математична модель випаровування багатоконпонентної рідини з поверхні аварійного розливу з урахуванням зовнішніх енергетичних потоків, що впливають на процес випаровування (тепловий потік від атмосферного повітря, тепловий потік від поверхні, що підстиляє, радіаційний потік від сонця). Враховано ефект охолодження за рахунок випаровування. Розроблена модель враховує взаємний вплив компонентного складу рідкої фази та процесу випаровування. Було здійснено порівняльний аналіз результатів моделювання з опублікованими експериментальними даними процесів випаровування розливів азоту, етанолу і циклогексану. Результати порівняння показали можливість застосування моделі випаровування розливу в області аналізу та оцінки ризику, а також виявили шляхи вдосконалення математичної моделі.

**Ключові слова:** випаровування, багатоконпонентна суміш, модель, фазова рівновага, тепловий потік, вуглеводні, кріогенна речовина, етанол

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