APPLICATION OF ARTIFICIAL NEURAL NETWORKS FOR ESTIMATION OF LIQUID EVAPORATED MASS IN CASE OF ACCIDENTAL SPILLS

Kuptsov A. I., Galeev A. D. and Gimranov F. M.

1Department of Industrial Safety, Kazan National Research Technological University, Kazan
2Department of Machines and Apparatus of Chemical Production, Kazan National Research Technological University, Kazan
E-Mail: artpb@yandex.ru

ABSTRACT

The ability of using an artificial neural network to determine the mass of evaporated liquid in emergency spills is considered. The data from numerical experiments by computational fluid dynamics model (CFD model) on the evaporation of hexane at different wind speeds and pool sizes were used to form a training set for the artificial neural network model. In the present work, the K-fold cross-validation method was used to evaluate the model and its behavior on the independent data set. The selection of parameters of artificial neural network was carried out using successive approximation method. The advantage of the proposed method is ability to obtain acceptable results (the average deviation from CFD calculations is 14.17%) for a relatively small computational time.

Keywords: liquid spill, pool evaporation, artificial neural networks.

INTRODUCTION

Industrial accidents involving releases of flammable or toxic substances may generate extremely serious consequences. A correct prediction of the consequences of hypothetical accident scenarios is essential for the development and implementation of appropriate protective measures. To solve this problem, it is required to apply the reliable mathematical models describing the release of toxic or explosive substances into the atmosphere and their subsequent dispersion. The complete model of an adverse event (accident scenario) can be divided into three parts: the source model, the dispersion model and the impact model. There is a lot of work concerning the modeling of hazardous substances dispersion in the environment, whereas little attention has been given to source term modeling. In emergency spills of stable liquids (when the temperature of the liquid in the apparatus does not exceed the boiling point at atmospheric pressure), the input of hazardous substances into the environment is the result of evaporation from the pool surface. The accurate estimation of evaporation rate from the pool is of primary importance for evaluation of flammable or toxic zones.

Generally, there are two main types of mathematical models to evaluate the evaporation rate from a pool: semi-empirical and computational fluid dynamics (CFD) models. In the area of hazard analysis of accidental chemical spills, many investigators and hazard reference books have applied Mackay and Matsugu mass transfer equation (Kawamura and Mackay, 1987; Mackay and Matsugu, 1973). In the model (Kapias & Griffths, 1999) the mass transfer coefficient is calculated using Brighton’s theory (Brighton, 1987). This analytical model takes into account the effects of surface roughness, friction velocity of the airflow, and the effect of high vapor pressure on the mass transfer process. Khajehnejad et al. (2011) used Churchill’s equation (Churchill, 1976) where the Nusselt number is determined for the complete range of Re and Pr covering laminar, transition and turbulent regimes. This equation is based on experimental data for forced convection from isothermal flat plates. The Churchill’s equation is applied to mass transfer calculation substituting the Sh and Sc for the Nu and Pr.

Because evaporation is the nonlinear, complex, and unsteady process, it is difficult to derive an accurate formula to represent all the physical processes involved. The abovementioned semi-empirical models are derived from the assumption that the evaporating component is passive, i.e. it does not affect the structure of the vapor-air flow above the pool surface. This assumption may be incorrect when the evaporating component has a molecular weight exceeding the molecular weight of air [Galeev, 2014; Galeev, 2015]. In the work [Galeev, 2014], it was shown that the dynamics of evaporation of volatile liquid can be strongly influenced by the presence of the fence around the pool. In the work [Galeev, 2015], it was found out by numerical simulation that at low wind speeds the intensity of hexane evaporation depends essentially on the size of the pool due to buoyancy effects. The using of CFD models makes it possible to overcome the limitations of existing semi-empirical models. This approach is based on the numerical solution of the three-dimensional equations of conservation of mass, momentum, and energy, and takes into account the complex mutual influence of processes of evaporation from the pool and the vapor dispersion in the atmosphere. However, the numerical simulation requires a large amount of computational resources. The computation of a single case can take from several hours to several days, which is not compatible with operational needs of emergency response or risk assessment. Currently to reduce the computational time when solving environmental and industrial safety problems, an alternative approach is used, including a combination of CFD models with artificial neural networks. So, in the work [Lauret et al., 2016] the Cellular Automata with an Artificial Neural Network (CA-ANN) are developed to calculate the atmospheric dispersion of methane. In this work a CFD simulations database is created to provide variables for the artificial neural network (ANN).
In the present paper, the ability of using an artificial neural network to determine the mass of evaporated liquid in emergency spills is considered. To the best knowledge of the authors, no work has been reported in the literature that addresses the application of ANN to evaporation estimation in case of accidental spills of volatile liquids. Numerous researchers have used the neural networks to predict the water evaporation rate [Sudheer et al., 2002; Moghaddamnia et al., 2009; Lu et al., 2014]. However, the evaporation rate of water is much lower than that of volatile liquids such as acetone or hexane, which determines the difference in the dynamics of their evaporation, depending on the meteorological conditions, the pool size and the presence of obstructions in the pool area.

**CFD MODEL FOR POOL EVAPORATION**

To form the training set we used the CFD model, which included the conjugate solution of the equations for the emission of vapor from the pool surface and its dispersion in the atmosphere by wind flow and turbulent diffusion.

\[ \Delta B = \frac{1}{\kappa} \ln \left( \frac{K_i^+ - 2.25}{87.75} + C_s \cdot K_s^+ \right) \cdot \sin \left( 0.4258 \cdot \left( \ln K_i^+ - 0.811 \right) \right) \]

\[ K_i^+ = \frac{\rho \cdot K_i \cdot C_{\mu}^{0.25} k_p^{0.5}}{\mu} \]

\[ P_c = 9.24 \left[ \left( \frac{S_{y^+}}{S_c} \right)^{3/4} - 1 \right] \left[ 1 + 0.28 \exp \left( -0.007 S_{y^+}/S_c \right) \right] \]

\[ K = \frac{\ln \left( \left( 1 - Y_{g,s} \right) / \left( 1 - Y_{g,p} \right) \right)}{Y_{g,s} - Y_{g,p}}. \]

where \( \Delta B \) is the roughness function; \( C_i \) is the roughness constant; \( C_{\mu} \) is the coefficient in the turbulence model; \( J_{g,s} \) is the mass flux of vapor from the pool surface due to evaporation, kg/(m²·s); \( K_i \) is the roughness height, m; \( K_s^+ \) is the turbulent kinetic energy in the centroid of the wall-adjacent cell, m²/s²; \( P_c \) is a function which takes into account the resistance of the diffusion sublayer to mass transfer; \( S_c \) and \( S_{y^+} \) are the molecular and turbulent Schmidt numbers, respectively; \( u^+ \) is the non-dimensional velocity; \( Y_{g,p} \) and \( Y_{g,s} \) are the mass fractions of the evaporating component in the wall-adjacent cell and gas phase, respectively; \( Y^+ \) is the non-dimensional mass-fraction; \( y^+ \) is the non-dimensional distance; \( y_C^+ \) is the non-dimensional distance from the pool surface to the neighboring node of the computational grid, m.

The change in the local liquid temperature was determined from equation:

\[ \frac{\partial T_{liq}}{\partial t} = \frac{q_s + q_{grd} + q_s - q_p + q_{at} - J_{g,s} \cdot \Delta H_s}{C_{P,liq} \cdot m_{liq}} \]

where \( q_s \) is the heat flux from the atmosphere, W/m²; \( q_{grd} \) is the heat flux from the ground to the pool, W/m²; \( q_s \) is the heat flux from solar radiation, W/m²; \( q_p \) is the heat flux emitted by the pool, W/m²; \( q_{at} \) is the heat flux absorbed by the pool, W/m²; \( \Delta H \) is the latent heat, J/kg; \( C_{P,liq} \) is the specific heat of liquid, J/(kg K); \( m_{liq} \) is the mass of the liquid per unit surface area of the pool, kg/m².

The heat flux from the underlying layer to the pool, \( q_{grd} = \lambda_{grd}(\partial T_{g,grd}/\partial y)\big|_{y=0} \), is calculated from the numerical solution of the three-dimensional nonstationary heat conduction equation for the substrate. The heat flux from the atmosphere \( q_s \) is calculated using standard wall functions (ANSYS Fluent Theory Guide):

\[ \text{The change in liquid mass is determined by equation:} \]
\[
\frac{\partial m_{\text{vap}}}{\partial t} = -J_{g,s}.
\]  

(11)

The equations (10) and (11) were integrated into the CFD code ANSYS FLUENT as the user-defined scalar transport equations without convective and diffusion terms.

The mass flux \( J_{g,s} \) was set as a source term in the pool area in the dispersion model. The dispersion of vapor in the atmosphere was calculated by three-dimensional nonstationary Reynolds-averaged Navier-Stokes equations, the energy conservation equation and the species conservation equations, which are closed by the realizalbe \( k-e \) turbulence model.

A more detailed description of the used dispersion and evaporation models can be found in [Galeev, 2013] and [Galeev, 2015] respectively.

In the work [Galeev, 2015] the above model was used to examine the effect of wind velocity and pool sizes on the evaporation rate of hexane. The pools with sizes of 10 m\( \times \)10 m, 30 m\( \times \)30 m, 60 m\( \times \)60 m and 100 m\( \times \)100 m was considered. The numerical study included the series of calculations at wind velocities of 1, 2.5 and 5 m/s at height of 10 m for each of pool sizes. The initial liquid layer height was equal to 0.05 m. The temperature of ambient air and pool substrate was 303K. Based on the numerical simulation, the data on the change in the specific evaporated mass and the volume-averaged liquid temperature depending on the pool size and the wind speed were obtained. The results of the computational experiments were used to generate a data set for training the neural network.

METHOD / ANN DESIGN

Database creation

The first step of designing ANN calculations is getting trustful database. It is possible to get data from real size experiments, small-scale physical simulations in wind tunnel or CFD modeling. As the database must contain numerous examples of various configurations, which are impossible to obtain in actual configurations, CFD calculations were used to build the database as they enabled to get numerous data in various scenarios [Lauret et. al., 2016]. Description of the CFD model for pool evaporation is given above. The database included input data (wind speed, pool sizes, time) and output data (specific evaporated mass).

Cross-validation

In the article, the K-fold cross-validation method was used. The original data set was divided into K blocks of the same size. One of the K blocks remained for testing the model, and the remaining K-1 blocks served as a training set. The process was repeated K times, and each of the blocks was used once as a test set. The advantage over random sub sampling is that all observations are used for training and testing the model, and each observation is used for one-time testing only.

Figure-1. Method of K-fold cross-validation.

ANN architecture

The task of predicting values of specific evaporated mass from the surface of the pool \( m_{\text{vap}} \) (kg/m\(^2\)) is related to regression problems (predicting a continuous-valued attribute associated with an object). Our structure of the neural network corresponds to a Multi-Layer Perceptron regressor (MLPR).

ANN used the following parameters in calculations: \( m_{\text{vap}} \), normalization of input data was linear - (X-min)/(max-min); the normalization parameters depended on the minimum and maximum values of the input data; activation function for the hidden layer - logistic; the logistic sigmoid function, returns \( f(x) = 1 / (1 + \exp(-x)) \); sigmoid parameter – 0.8; hidden layer sizes = (5, 5, 10), where the I-th element represents the number of neurons in the I-th hidden layer. To train the neural network, 80% of the sample was used. Learning speed - 0.1, moment – 0.9.

ANN carried out selection of the above parameters by the method of successive approximation, based on the mean and maximum errors on training and test samples obtained in the learning process.
RESULTS AND DISCUSSIONS

In the final analysis, the calculation of $m_{vap}$ values using ANN takes no more than 15 minutes of computer time (AMD A10-8700P Radeon R6), which greatly exceeds the expenditure of computer time using CFD methods.

The results of the predicted $m_{vap}$ values according to the proposed ANN in comparison with those calculated by CFD are presented in graphs (Figure-2).

The table below shows the average deviations (in%) of ANN predictions from CFD results, depending on the size of the pool and wind speed. The results of the forecast are generally satisfactory. Values of specific evaporated mass obtained with ANN have a difference $\sigma$ to CFD results from 0.17% to 59.64% with an average value of 14.17%.

![Figure-2. Comparison of evaporated mass (kg/m²) predicted using the CFD (solid line) and ANN (dashed line) methods.](image-url)
to CFD results from 0.17% to 59.64% with an average value of 14.17%.

**Table-1.** The average deviation of ANN forecasting from CFD results.

<table>
<thead>
<tr>
<th>$S, m^2/V, m/s$</th>
<th>1</th>
<th>2.5</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>26.6%</td>
<td>10.09%</td>
<td>4.40%</td>
</tr>
<tr>
<td>30</td>
<td>12.97%</td>
<td>3.88%</td>
<td>3.05%</td>
</tr>
<tr>
<td>60</td>
<td>22.83%</td>
<td>6.79%</td>
<td>5.03%</td>
</tr>
<tr>
<td>100</td>
<td>45.80%</td>
<td>26.85%</td>
<td>1.76%</td>
</tr>
</tbody>
</table>

An analysis of the results obtained showed that the most difficult scenarios to predict using ANN are hexane evaporation scenarios at a low rate. The accuracy of forecasting increases in proportion to the increase in wind speed regardless of the area of the pool. This is because the values of specific evaporated mass as a function of time with an increase in speed do not change much for different pools. For example, after an hour of evaporation, the maximum change in $m_{\text{vap}}$ values at a wind speed of 5 m/s is only 14.35%, depending on the area of the pool, while at a wind speed of 1 m/s it is already approximately 3.5 times greater.

It is also noticeable that the prediction accuracy of $m_{\text{vap}}$ deteriorates at the extreme values of the size of the pool. This is explained by the peculiarity of applying the K-fold cross-validation method in those cases where the boundary k-block is unknown. The predicted value in this case, as a rule, is limited on the one side by the value of the previous k-block, and on the other side depending on the boundary of the function - either by plus infinity in case of increasing or by minus infinity in case of decreasing (sometimes, by zero, because of the physics of the process). In addition, if we consider any separately specific hexane evaporation scenario, then the accuracy of the forecast is deteriorated (in%), depending on the duration of evaporation, due to the specific application of the K-fold cross-validation method, at the initial and final stages: The boundary K-block remaining for testing is not trained between the values of two or more K-blocks.

To increase the accuracy of forecasting with the parameters considered, it is necessary to conduct additional CFD calculations, increasing the number of K-blocks. However, in this case, the prediction on the new boundary k-blocks will be noticeably worse than in the internal ones.

The disadvantages of this method are the obvious dependence on the parameters obtained during CFD calculations. In addition, it is necessary to note the time costs for cross-validation, as well as the search for satisfactory parameters of the neural network in other similar tasks.

**CONCLUSIONS**

This article considers the possibility of using an artificial neural network to determine the mass of vaporized liquid in emergency pool. To form a training sample, we used the CFD model, which included a conjugate solution of the equation for the flux of vapor from the surface of the pool and its dispersion in the atmosphere by wind flow and turbulent diffusion. The obtained data, as a result of CFD calculations, were used as initial data for the training of an artificial neural network. The method for evaluating the model and its behavior on an independent data set was K-fold cross-validation. ANN parameters are calculated by the method of successive approximation, based on the mean and maximum error values on the training and test samples obtained in the learning process.

The advantage of the proposed method is obtaining acceptable results (mean deviation from CFD calculations: 14.17%) for a rather short estimated time: less than 15 minutes. The drawbacks of this method include the dependence on the parameters of CFD calculations (the initial data for the training of ANN) and the time costs for cross-validation and the search for satisfactory ANN parameters for other similar tasks.

**REFERENCES**


