

## Disaster Simulation in Chemical Plants Considering Diffusion of Gas and Heat Radiation from Tank Fire

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## ABSTRACT :

We have developed a computer simulation program in order to make clear effects of storage's outflow, evaporation, diffusion of gas, tank fire and extinguishments in chemical plants. The trigger of disaster is the outflow of the storage subjects in a tank. The occurrence of the outflow is classified into three modes: little, middle and large leakage. In case of middle leakage mode, we have developed the simulation program for the concentration of gas considering combination of the flash evaporation and the evaporation by temperature of ground. When the tank fire occurs in a plant, the heat radiation from flame to affected tanks is calculated with Monte Carlo method in order to consider the climate, the location and the shape of tanks. The spread of tank fire is judged by the increase of temperature of the heat affected tank. As the prevention of the disaster progress, the effect of extinguishment with sprinklers is also taken into account. Furthermore, GIS (Geographical Information Systems) is very effective, because it is very easy to get the situation immediately of the occurrence of disaster for a plant. The disaster simulation is connected with GIS, and the dangerous zone caused by tank fire can be estimated. When the tank fire occurs in an actual plant model in Kawasaki area in Japan, the dangerous heat affected zone for a human body and the increase of inner temperature of heat affected tanks can be indicated on digital map by using the proposed system.

KEYWORDS: Simulation, Chemical plants, Diffusion of Gas, Heat Radiation, GIS

## **1. INTRODUCTION**

If a big earthquake attacks a chemical plant and tanks are broken, the disaster will extend due to heat radiation from fire and explosion pressure. Recently, tank fires and explosion phenomena often occurred at chemical plants in Japan. So, the estimation of the dangerous area caused by disaster is very important for the safety and reliability of chemical plants. However, it is very difficult to estimate the dangerous area caused by the disaster due to complex phenomena, such as ignition, heat radiation from fire, explosion pressure and so on. If the affected area caused by disaster can be estimated with numerical simulation, it will become a very useful tool for safety and reliability of chemical plants.

In the previous study, we had developed the computer simulation program in order to estimate the spread of fire, and proposed a probabilistic estimation approach of the risk based on the developed simulation [1]. In this study, we have developed the computer simulation program in order to make clear the effects of storage's outflow, evaporation, diffusion of gas, tank fire and extinguishments. Heat radiation from flame to affected tanks is calculated with Monte Carlo method in order to consider the climate, the location and the shape of tanks. The spread of tank fire is judged by the increase of the temperature and pressure of the heat affected tank. As the prevention of the disaster progress, the effect of extinguishment with sprinklers is also considered.

Furthermore, Geographical Information Systems (GIS) is very effective to get the situation immediately of the occurrence of disaster for a plant. The disaster simulation system connects to GIS, and the dangerous zone caused by fire and gas diffusion can be indicated in actual geographical area. The detail is described in this paper.

### 2. CLASSIFICATION OF DISASTER IN CHEMICAL PLANTS

The trigger of a tank fire or an explosion is the outflow of the combustibility storage subjects in a tank. Simulating the behavior of outflow and gas diffusion is useful for the safety and reliability for chemical plants.



The High Pressure Gas Safety Institution of Japan had established the estimation procedure of the gas diffusion in a plant based on the guide of KHK-E-007 [2]. In the guide, the estimation methods for gas diffusion considering the amount of leakages have been presented. As the case of most severe incident, when the tank are destroyed by the earthquake and all amount of contents in the tank is flowed inside the oil dike, the contents is evaporated by the heat exchange on the surface of the ground instantaneously. And the concentration of gas is calculated as the instantaneous two dimensional area sources. On the other hand, if the amount of the leakage is very small such as an outflow from a micro crack in a pipe, a phenomenon of flash evaporation, which means the radical vaporization caused by the difference of pressure and does not occur the heat exchange on the

surface of the ground, may appear. And the concentration of gas is calculated as the continuous source. However, a phenomenon of middle amount of leakage, which induces both evaporations, occurs frequently. In the KHK guide, the combination effects of both evaporations have not been taken into account.

The occurrence of outflow is classified into three modes: little, middle and large leakage. Figure 1 shows the classification of the disaster scenario. In case of middle leakage mode, we propose the calculational method of the gas concentration by the combination of flash evaporation and evaporation by temperature of ground. Furthermore, the heat effects when the tank fire occurs are also estimated with Monte Carlo method.



Figure 1 Classification of disaster scenario

### **3. ESTIMATION OF DANGEROUS AREA CAUSED BY TANK FIRE**

#### 3.1 Estimation Method of Heat Radiation by KHK and TNO

A pool fire is one of the conflagration phenomena with a great deal of flames and heat. The shape of the flame can not be determined clearly, however, it is reasonable to treat the shape as cylindrical model. The heat radiation energy from a cylindrical fire can be evaluated as follows;

$$E = \phi \cdot \varepsilon \cdot \sigma \cdot T^4 = \phi \cdot R_D \tag{3.1}$$

where *E* is heat radiation energy,  $\varepsilon$  is emissivity of a flame,  $\sigma$  is Stefan Boltzmann's constant, *T* is the flame temperature, and  $\phi$  is the configuration factor indicating heat transfer rate from a flame to a heat affected surface. Based on the equation, the heat radiation can be evaluated by using two parameters  $\phi$  and  $R_D$ . Parameter  $R_D$  means the heat radiant emittance and the value is constant dependent on the kind of fuel. The key point is how to estimate the configuration factor  $\phi$ .

In the KHK guide [2], the estimation procedure of the dangerous zone caused by heat radiation from tank fire is described. The shape of a tank fire is treated as a cylindrical model, and the estimation of configuration factor  $\phi$  is adopted by the Hamilton's equation [2]. However, there are some problem in the guideline, i.e., the heat radiation considering the inclination of flame due to the wind had not been estimated because of the difficulty for solving the integral equation of heat radiation.

In TNO (The Netherlands Organization of Applied Scientific Research), the 'Yellow Book' report is published [3]. The report provides the methods for the calculation of physical effects due to the release of hazardous liquids and gases, and the estimation procedure of heat radiation is also described. In the Yellow Book method, an effect of wind on heat radiation is considered, and the method is generally applied to estimate the heat radiation from tank fire. However, the interruption of heat radiation by oil dikes or other tanks and equipments in plants had not been considered.



#### 3.2 Estimation of Heat Radiation based on Monte Carlo Method

In order to solve the above difficulty, the configuration factor  $\phi$  considering the effect of wind is calculated with Monte Carlo method. The calculational procedure for heat transfer from fire to the affected surface with Monte Carlo method is as follows. Heat from fire is radiated by the independent particles, and the radiant behavior of each particle is simulated with random number. Figure 2 shows the geometric coordinate and the starting point of a particle on the surface of flame cylinder. The shape of flame is treated as the shape as cylindrical model.



Figure 2 Geometrical coordinate and a radiant particle.

The starting point  $(x_i, y_i, z_i)$  of a particle is given as follows;

$$x_{i} = x_{c} + R_{1} \cdot h_{f} \cdot \sin \theta_{v} \cos \xi + r_{f} \cdot \cos \tau$$

$$y_{i} = y_{c} + R_{1} \cdot h_{f} \cdot \cos \theta_{v}$$

$$z_{i} = z_{c} + R_{1} \cdot h_{f} \cdot \sin \theta_{v} \sin \xi + r_{f} \cdot \sin \tau$$
(3.2)

where  $(x_c, y_c, z_c)$  means the coordinate of the center of flame cylinder on the ground surface. Symbol  $h_f$  is the height of flame cylinder,  $r_f$  is radius of flame cylinder,  $\xi$  is the orientation of wind direction, and  $\tau = (\pi/2)(2R_2-1)$ .  $R_1$ ,  $R_2$  are random numbers. Radiant direction of a particle is given by Lambert's cosine law. The directional cosine  $(\alpha, \beta, \gamma)$  is calculated as follows;

$$\begin{cases} \alpha \\ \beta \\ \gamma \end{cases} = \begin{cases} \cos\varphi \cdot \cos\tau - \sin\varphi \cdot \sin\omega \cdot \sin\tau \\ \sin\varphi \cdot \cos\omega \\ \cos\varphi \cdot \sin\tau + \sin\varphi \cdot \sin\omega \cdot \cos\tau \end{cases}$$
(3.3)

The distance from a starting point of a radiant particle to receiving surface is calculated with the directional cosine. The achievement to the affected tank surface of the particle is judged, and the arrived particles are accumulated at each position on the receiving surface. The heat transfer rate, i.e., configuration factor, is obtained from the number of accumulated particles.

#### 3.3 Numerical Results of Configuration Factor

To investigate the accuracy of configuration factor calculated with the proposed Monte Carlo method, the numerical results are compared with the conventional method of KHK and TNO. Figure 3 shows the numerical results of the configuration factors. The horizontal axis means the calculation point which has the distance from center of tank fire. The configuration factor is estimated under the wind velocity 0 (m/s). In the Monte Carlo



method, the number of generated particles is 50 million. As the results, the proposed Monte Carlo method has good agreements with both methods. The proposed Monte Carlo method is very effective in case that the wind conditions and the interruption of heat radiation by oil dike and other equipments have to be considered.



#### 3.4 Simulation method for spread of tank fire

The spread of tank fire in a plant is simulated with the developed system. The procedure is as follows; the data on contents and shape of tanks are inputted at first. The tanks affected by fire are referred. Temperature on the surface of the heat affected tank increases by the effect of heat radiation. The calory at the surface is calculated as follows;

$$Q = S \cdot E \cdot t \tag{3.4}$$

where S is the sectional area of tank, and t is time. As prevention of disaster progress, the effect of extinguishment with sprinklers was estimated [5]. The calory at the surface of heat affected tank with extinguishment is calculated as follows;

$$Q = S \cdot (E \cdot \Pi - E_v) \cdot t \tag{3.5}$$

where  $\Pi$  is transmission rate of radiation through water curtain of sprinkler, and  $E_v$  is latent heat of vaporization as follows. Finally, temperature on inner surface of the wall of the heat affected tank is calculated as follows;

$$T = \frac{Q - Q_i}{A \cdot \delta \cdot \rho \cdot \kappa} + T_0 \tag{3.6}$$

where A is surface area of tank.  $\delta$  is average thickness,  $\rho$  is density, and  $\kappa$  is specific heat of tank wall.  $T_0$  is atmospheric temperature, and  $Q_i$  is calory due to thermal conduction from fire to contents in heat affected tank through the wall.

#### 3.5 Numerical example of spread of tank fire

Based on the Monte Carlo method on the heat radiation, the disaster simulation for chemical plants considering spread of tank fire has been developed in Figure 4. Firstly, the data on fuel of tanks, shape of tanks, and initial burning tanks are inputted at first. And, the tanks affected by initial burning tanks are referred. Temperature on the surface of the heat affected tank can be calculated by Eq.(3.6). As the most dangerous case, when the



temperature exceeds the ignition point of contents, the tank explodes and the occurrence of the sequential disaster is judged.



Figure 4 Estimation of spread of tank fire by developed simulation

## 4. ESTIMATION OF SPREAD OF DAMAGES BY SIMULATION WITH GIS

### 4.1 Geographical Information System (GIS)

In order to get the situation of the occurrence of disaster for a plant, Geographical Information System (GIS) will be very effective. Therefore, the disaster simulation system is connected with GIS. Figure 5 shows the scheme of developed disaster simulation system with GIS. The procedure of calculation is as follows; the data on tanks entries and the database on material properties for contents of tanks is prepared. By these input data, heat affected zone for a human body caused by tank fire and the damage states of tanks are calculated with the developed system. The results of simulation, which are the heat affected zone, damage states of tanks, etc., are indicated on the GIS. In this study, we have used the GIS program developed by NIED (National research Institute for Earth science and Disaster prevention, Japan).

### 4.2 Numerical Results of spread of tank fire by simulation with GIS

As an application of the simulation on GIS, the dangerous zone caused by tank fire can be estimated in an actual geographical area as shown in Figure 6. The location of plants is a place at Kawasaki in Japan and the area consisted of four parts. Petroleum tanks are accumulated in plant 2 zone and several LPG tanks are located in a zone of Plant 4.

When an initial fire occurs at No.3 tank, which the shape is a cylinder and the contents is petroleum, the heat affected zone for a human body is indicated as shown in Figure 7. Wind speed is 4.7m/s and wind direction is shown in the figure.  $\Delta T$  means the increase of inner temperature of a heat affected tank.

From the numerical results, the fire extends inside of plant 2 zone. In case of 30(min.), the dangerous area for human body is only appeared at the surrounding part of initial burning tank in Figure 7(a). On the other hand, the sequential fire appeared at the neighbor tank (contents: petroleum), and the tank fire spreads because the heat radiation from fire accelerates due to the inclination of the shape of fire by wind in Figure 7(b).

Figure 8 shows the numerical result considering an effect of extinguishment with sprinklers. Suppose the total amount of water distributed to tanks is 20,000(l/min.), the occurrence of sequential burning tank can be prevented. By using the developed system, we can estimate an optimum amount of water.



Figure 5 Scheme of disaster simulation connected with GIS

### Figure 6 A plant model on GIS



(a) After 30(min.) (b) After 180(min.) Figure 7 Numerical results when an initial fire appeared at a petroleum tank



Figure 8 Numerical results considering an effect of extinguishments



Figure 9 Numerical results when an initial fire appeared at a LPG tank after 60(min.)



As other case of the simulation, the results of dangerous zone when an initial fire occurred at No.25 LPG tank in plant 4 area are shown in Figure 9. The heat affected zone is propagated in plant 4 area. From these results, it is recognized that the sequence of disaster is quite different due to the contents of tanks and the location of initial disaster, and the difference can be estimated by the proposed simulation.

#### 5. ESTIMATION OF DIFFSUION GAS CAUSED BY LEAKAGE

#### 5.1 Calculation of gas diffusion in the middle amount of leakage

In the case of middle amount of leakage, the storage's outflow, flash evaporation, and evaporation by the environment may occur as shown in Figure 10. The combination effect of both evaporations can be evaluated as follows [4].



Figure 10 Outflow of storage subjects, an evaporation and a diffusion

$$\frac{dL}{dt} = (1 - f)\frac{dQ}{dt} - \frac{dV}{dt}$$
(5.1)

where L is the amount of leakage, f is coefficient of flash evaporation, Q is the amount of outflow from a tank, and V is the amount of evaporation by the ground. The emitting amount of gas  $q_i$  is calculated as follows.

$$q_i = \left( f \frac{dQ}{dt} + \frac{dV}{dt} \right) / S \tag{5.2}$$

where *S* is the area of the leakage or the inside area of the dike. The concentration of gas is calculated as follows. The equation is obtained by the solution of the differential equation of Fick's low in case of instantaneous two dimensional sources [2].

$$C(X,Y,Z,t) = \frac{q_i}{4U} \frac{\exp(-Z/B)}{B}$$

$$\cdot \left[ erf\left(\frac{Y+M/2}{A}\right) - erf\left(\frac{Y-M/2}{A}\right) \right]$$

$$\cdot \left[ erf\left(\frac{X-U\cdot t+M/2}{A}\right) - erf\left(\frac{X-U\cdot t-M/2}{A}\right) \right]$$
(5.3)

where C is the concentration of gas, U is the velocity of wind, t is time, X, Y, and Z are coordinates of the calculational point. We take X-axis along the wind direction, Z-axis vertically from the ground, and Y-axis perpendicularly to them. M is a equivalent diameter of the leakage area. A, and B are coefficients dependent on the climate condition. The key point of the above equations is how to calculate the emitting amount of gas  $q_i$ . In the conventional method by KHK,  $q_i$  is all amounts of tank contents in order to estimate the large amount of



leakage. On the other hand, the change with time of  $q_i$  is taken into account by solving Eqs.(5.1),(5.2), and (5.3). The procedure induces that the combination effect of both evaporations in the case of middle amount of leakage can be estimated.

#### 5.2 Numerical example of gas diffusion with GIS

As the numerical example, we suppose that the shape of damaged tank is sphere, and the content is ammonia. The diameter and capacity are 22.3m, 6000kl, respectively. The tank is connected with the pipeline which height is 1.0m. The crack hole, which diameter is 100mm, is appeared on the pipe, and the diffusion of gas is calculated. Figure 11 shows the concentration zone of 700 ppm at height 1.0m and 10m after 10minutes. From the results, we can estimate the diffused zone clearly by using GIS.



Figure 11 Dangerous zone displayed by GIS

### 6. CONCLUSION

The computer simulation system to make clear the effects of storage's outflow, evaporation, diffusion of gas, tank fire and extinguishments had been developed and the numerical procedures were described. As numerical examples, the gas concentration in case of middle amount of leakage can be calculated by considering of the combination of flash evaporation and evaporation by temperature of ground. When the tank fire occurs in a plant, the heat radiation from flame to affected tanks is calculated with Monte Carlo method to consider the climate condition, and the spread of fire is judged by the increase of temperature of the heat affected tank. Furthermore, when the tank fire occurs in an actual plant model in Kawasaki area, the dangerous heat affected zone for a human body and the increase of inner temperature of heat affected tanks can be indicated on GIS. From these results, it is recognized that the developed simulation system can be applied the evaluation of the safety and the reliability for plants.

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