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MATHEMATICAL MODELLING AND SIMULATION OF HEAT DISPERSION DUE TO FIRE AND EXPLOSION

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Abstract. Fire and explosion are among the commonly occurring major hazards in the operation of chemical plants. In this paper, a mathematical model for heat dispersion in the event of an industrial fire and explosion is presented. The model is simulated numerically within MATLAB environment to provide both the time and space dependence of the heat flux and temperature using a finite difference method. Three classes of fire were considered. These are pool fire, flash fire and fireball following the event of Boiling Liquid Expanding Vapour (BLEVE). The simulation program that has been developed is employed to study the impact of the three types of fire hazard on a LPG storage facility at the Chemical Engineering Pilot Plant in the Universiti Teknologi Malaysia. The results obtained highlights the various hazard condition for all the three events, with fireball imposing the most severe condition by having safety distance of 300 meters away from the source of release, within which fatalities are expected.

Key words: Fire, heat transfer model, simulation, temperature and heat flux distribution, finite difference

Abstrak. Kebakaran dan letupan adalah antara bahaya yang kerap berlaku dalam operasi loji kimia. Dalam kertas kerja ini, perbincangan ditumpukan terhadap model matematik serakan haba yang berpunca daripada kebakaran dan letupan. Model yang diselaku berasaskan MATLAB ini menggunakan kaedah perbezaan terhingga bagi menyelesaikan masalah yang berkaitan dengan fluks haba dan suhu. Tiga kelas kebakaran telah dipertimbangkan, iaitu kebakaran kolam, kebakaran kilat dan bebola api yang berkait dengan Cecair Didih mengembangkan Wap (BLEVE). Program penyelakuan ini digunakan untuk mengkaji kesan ketiga-tiga bahaya kebakaran tersebut yang diandaikan berlaku di kemudahan storan LPG, Loji Pandu Kejuruteraan Kimia, Universiti Teknologi Malaysia. Keputusan penyelakuan menunjukkan bahawa bebola api menyebabkan berlakunya mala petaka yang paling serius dengan kematian mencapai sehingga jarak 300 meter.

Kata kunci: kebakaran, model pemindahan haba, penyelakuan, pengagihan fluks haba dan suhu.

1.0 INTRODUCTION

Safety is one of the most important factor in chemical process plants. All operations and processes must be carried out under safe conditions in order to protect the environment. Among the commonly occurring major accidents in chemical process plant are fire and explosions. Fire occurs when a source of heat comes into contact with a combustible material, in which combustion is started, while explosion is a

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sudden and violent release of energy. Usually, human errors and failure of equi pment during operation are the main causes of these incidents.

The occurrence of fire and explosion would release a large amount of heat. Most of the heat is transferred by convection and radiation. Heat flux from flame can cause serious injury, fatality and damage. This research has been carried out to determine the temperature and heat flux distribution from fire and explosion. Thus, the effects and safe distance related to the particular incident can be examined. These predictive results can be used as guidance for the authority to arrange precautionary measures in order to minimise injury, fatality and damage during accident.

Some issues pertinent to this class of industrial hazard had been addressed by several researchers [1,2,3]. They had classified the fire and explosion incidents occur in the chemical process plant into several categories. Those commonly happen are pool fire, fireball and BLEVEs, flash fire and vapour cloud explosion. The definitions for these fire and explosions are listed as below [2]:

(i) pool fire occurs when a flammable liquid spills onto the ground and is ignited. Fire in a liquid storage tank is also a form of pool fire.
(ii) flash fire occurs when a vapour cloud formed from a leak is ignited. If the vapour cloud is formed with overpressure, the event is a vapour cloud explosion.
(iii) BLEVEs occur when a pressure vessel containing a flammable liquid is exposed to fire and ruptures. Usually, any incident of BLEVE will generate fireball.

Various types of model describing the fire and explosions incidents have been compiled and discussed by the pioneer researchers in this field [2]. Besides, the Centre for Chemical Process Safety of the American Institutes of Chemical Engineers (CCPS/AIChE) has also given some information and guidance to examine the behaviour of vapour cloud explosions, flash fire and BLEVEs.

For the determination of heat flux distribution from a heat source or a flame, The CCPS/AIChE has introduced two relevant methods, which are point source model and solid-flame model [3]. In the case of thermal radiation from pool fire and tank fire, three models have been recommended [4]. These models are point source model, solid-flame model and equivalent radiator model. However, these models only consider the heat transfer by radiation in one dimension. Some factors such as heat transfer by convection, wind and boundary conditions have been neglected.

This paper compiles mathematical models describing various form of industrial fire and explosion, and develops a three dimensional model that describes the heat flow from a heat source. A simulation program is developed to simulate the heat transfer model using finite difference method. Lastly, a case study involving an accidental release from an LPG storage tank at Chemical Engineering Pilot Plant, UTM is presented.

2.0 DEVELOPMENT OF HEAT TRANSFER MODEL

In this project, heat transfer modelling from a heat source is done in free space without blockage. The media involved in the heat transfer process is air. Heat released from a flame or a heat source is transferred by conduction, convection, radiation and shear stress between air molecules. This is a three dimensional model and the derivation is based on transport phenomena [5].

According to Fourier's law, heat transfer by conduction in y-axis can be described by Equation (1), while the energy balance without heat generation is presented by Equation (2).

$$q_{c,y} = -k\frac{dT}{dy} \tag{1}$$

$$\text{Rate of heat accumulation} = \text{rate of heat in} - \text{rate of heat out} \tag{2}$$

Thus, the balance equation for heat transfer by conduction is:

$$\begin{aligned}(\Delta x\Delta y\Delta z)\frac{\delta}{\delta t}\left(\rho C_p T\right)\Big|_{cond} &= \left[-k\left(\frac{\delta T}{\delta x}\right)_x + k\left(\frac{\delta T}{\delta x}\right)_{x+\Delta x}\right]\Delta y\Delta z \\ &+ \left[-k\left(\frac{\delta T}{\delta y}\right)_y + k\left(\frac{\delta T}{\delta y}\right)_{y+\Delta y}\right]\Delta x\Delta z \\ &+ \left[-k\left(\frac{\delta T}{\delta z}\right)_z + k\left(\frac{\delta T}{\delta z}\right)_{z+\Delta z}\right]\Delta x\Delta y\end{aligned} \tag{3}$$

In this case, ρ and C_p are assumed to be constant and are independent of temperature. This equation can be differentiated, rearranged and simplified into Equation (4), which is in the terms of temperature.

$$\rho C_p\frac{\delta T}{\delta t}\Big|_{cond} = k\left(\frac{\delta^2 T}{\delta x^2} + \frac{\delta^2 T}{\delta y^2} + \frac{\delta^2 T}{\delta z^2}\right) \tag{4}$$

Equations for heat transfer by convection and shear stress of air molecules can also be derived by referring to the equation of motion [5]. Similar with Equation (3), ρ and C_p are assumed to be constant and are independent of temperature. In addition, the velocity of flow (v_x, v_y and v_z) at free space is also assumed to be constant. After derivation and rearrangement, equation of heat transfer by convection and shear stress among air molecules are described by Equation (5) and Equation (6), respectively.

$$\rho C_p\frac{\delta T}{\delta t}\Big|_{conv} = -\left[\rho C_p\left(v_x\frac{\delta T}{\delta x} + v_y\frac{\delta T}{\delta y} + v_z\frac{\delta T}{\delta z}\right)\right] \tag{5}$$

$$\rho C_p \left.\frac{\delta T}{\delta t}\right|_{shear} = -\left[v_x \left(\frac{\delta \tau_{xx}}{\delta x} + \frac{\delta \tau_{yx}}{\delta y} + \frac{\delta \tau_{zx}}{\delta z} \right) + v_y \left(\frac{\delta \tau_{xy}}{\delta x} + \frac{\delta \tau_{yy}}{\delta y} + \frac{\delta \tau_{zy}}{\delta z} \right) + v_z \left(\frac{\delta \tau_{xz}}{\delta x} + \frac{\delta \tau_{yz}}{\delta y} + \frac{\delta \tau_{zz}}{\delta z} \right) \right] \quad (6)$$

For heat transfer by radiation, the basic equation for thermal radiation can be used. This relationshi ps, in the form of solid flame equation is also recommended by CCPs/ AIChE (Equation (7)).

$$q_r = F \varepsilon \tau_a \sigma T^4 \quad (7)$$

In three dimensional form, the equation of heat transfer by radiation can be written as follows:

$$\rho C_p \left.\frac{\delta T}{\delta t}\right|_{rad} = -\left[F \varepsilon \tau_a \sigma \left(\frac{\delta T^4}{\delta x} + \frac{\delta T^4}{\delta y} + \frac{\delta T^4}{\delta z} \right) \right] \quad (8)$$

Having all the individual equations representing the various heat transfer mechanism, a model for heat transfer from a flame in free space can be developed. Here, the equations for conduction, convection, shear stress among air molecules and radiation are combined to form the comprehensive solutions. Some reasonable assumptions have been made, which are (i) the density of air is constant, (ii) thermal conductivity (k) for air is negligible, and (iii) heat transfer by shear stress among air molecules is negligible. Based on these assumption, Equation (4), (5), (6) and (8) can be combined, rearranged and simplified to obtain a heat transfer model in three dimensions given by Equation (9) and (10). Note that due to the above assumptions, the models are limited to certain operating conditions. For example, constant density for air indicates that the equation will only be valid if the temperature does not change very much.

$$\rho C_p \frac{\delta T}{\delta t} = -\underbrace{\left[\rho C_p \left(v_x \frac{\delta T}{\delta x} + v_y \frac{\delta T}{\delta y} + v_z \frac{\delta T}{\delta z} \right) \right]}_{\text{Convection}} - \underbrace{\left[F \varepsilon \tau_a \sigma \left(\frac{\delta T^4}{\delta x} + \frac{\delta T^4}{\delta y} + \frac{\delta T^4}{\delta z} \right) \right]}_{\text{Radiation}} \quad (9)$$

$$\rho C_p \frac{\delta T}{\delta t} = -\underbrace{\left[\rho C_p \left(v_x \frac{\delta T}{\delta x} + v_y \frac{\delta T}{\delta y} + v_z \frac{\delta T}{\delta z} \right) \right]}_{\text{Convection}} - \underbrace{\left(\frac{\delta q_{r,x}}{\delta x} + \frac{\delta q_{r,y}}{\delta y} + \frac{\delta q_{r,z}}{\delta z} \right)}_{\text{Radiation}} \quad (10)$$

Equation (9) and (10) show the heat transfer equation in terms of temperature and heat flux, respectively. Note that these equations have neglected the conduction and shear stress components of heat transfer. This is a reasonable simplification because both the thermal conductivity and viscosity of air are small. The direction of the heat flow from a heat source is illustrated in Figure 1.

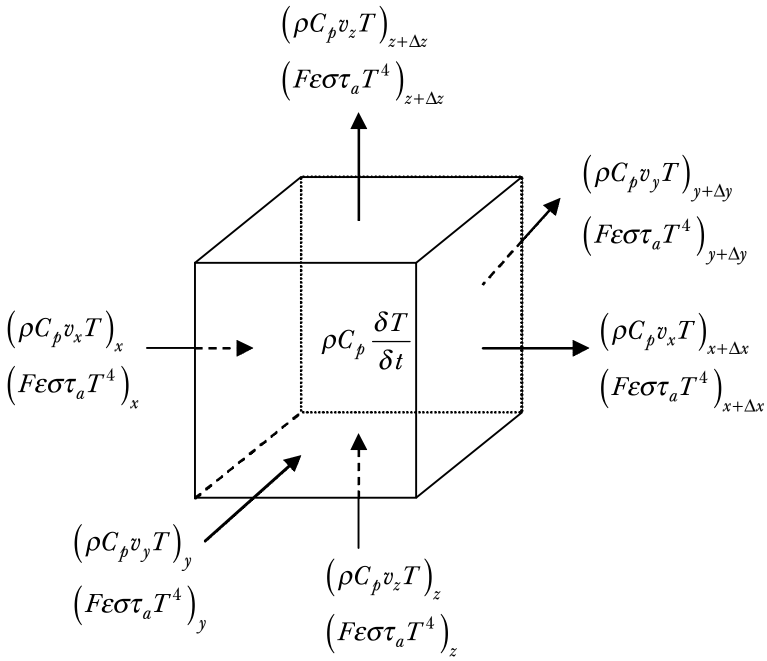

Figure 1 Heat flow in three dimension

3.0 NUMERICAL SOLUTION FOR HEAT TRANSFER MODEL

The heat transfer model, which is developed in the earlier section, is in the forms of partial differential equation. Both of the Equation (9) and (10) must be solved by suitable numerical methods such as finite element and finite difference methods. In this work, finite difference method is chosen as it can provide sufficient accuracy for the case under consideration despite its simplicity compared to the finite element method. Using finite difference method, the set of partial differential equations for a boundary-value problem is solved using a grid system. In this case, an equal size system grid has been used. Figure 2 shows the grid system at a particular node for two dimensional space. Here, n is the number of iteration of time, and both i and j represent the x and y axis.

Relevant techniques to rearrange the heat transfer model into the forms of finite difference equation can be found [6]. In this study, an explicit method with both forward

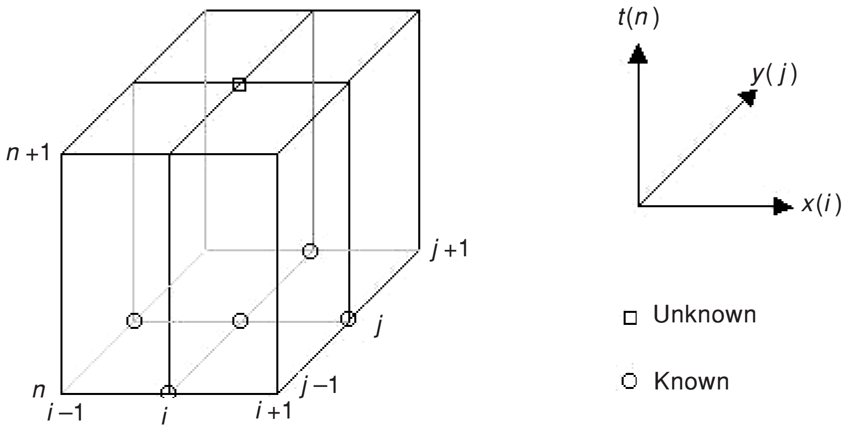

Figure 2 The grid system for two dimensional space

and backward difference to solve this model. After rearrangement, Equation (9) and (10) are expressed in the finite difference equation as below:

(i) Heat transfer equation in terms of temperature
Forward difference

$$T_{i,j,k}^{n+1} = T_{i,j,k}^{n}\left(1 - v_x P - v_y P - v_z P - 3EP\left(T_{i,j,k}^{n}\right)^3\right) + T_{i+1,j,k}^{n}\left(v_x P + EP\left(T_{i+1,j,k}^{n}\right)^3\right)$$
$$+ T_{i,j+1,k}^{n}\left(v_y P + EP\left(T_{i,j+1,k}^{n}\right)^3\right) + T_{i,j,k+1}^{n}\left(v_z P + EP\left(T_{i,j,k+1}^{n}\right)^3\right) \quad (11)$$

Backward difference

$$T_{i,j,k}^{n+1} = T_{i,j,k}^{n}\left(1 - v_x P - v_y P - v_z P - 3EP\left(T_{i,j,k}^{n}\right)^3\right) + T_{i-1,j,k}^{n}\left(v_x P + EP\left(T_{i-1,j,k}^{n}\right)^3\right)$$
$$+ T_{i,j-1,k}^{n}\left(v_y P + EP\left(T_{i,j-1,k}^{n}\right)^3\right) + T_{i,j,k-1}^{n}\left(v_z P + EP\left(T_{i,j,k-1}^{n}\right)^3\right) \quad (12)$$

where $E = \dfrac{F\varepsilon\tau_a\sigma}{\rho C_p}$ and $\dfrac{\Delta t}{\Delta x} + \dfrac{\Delta t}{\Delta y} + \dfrac{\Delta t}{\Delta z} = P$

(ii) Heat transfer equation in terms of heat flux
Forward difference

$$q_{i,j,k}^{n} = \frac{1}{3}\Bigg\{q_{i+1,j,k}^{n} + q_{i,j+1,k}^{n} + q_{i,j,k+1}^{n} - \rho C_p\Bigg[v_x T_{i+1,j,k}^{n} + v_y T_{i,j+1,k}^{n} + v_z T_{i,j,k+1}^{n}$$
$$- \frac{h}{\Delta t}\left(T_{i,j,k}^{n+1}\right) - T_{i,j,k}^{n}\left(v_x + v_y + v_z - \frac{h}{\Delta t}\right)\Bigg]\Bigg\} \quad (13)$$

Backward difference

$$q^{n}_{i,j,k} = \frac{1}{3}\left\{q^{n}_{i-1,j,k} + q^{n}_{i,j-1,k} + q^{n}_{i,j,k-1} - \rho C_p \left[v_x T^{n}_{i-1,j,k} + v_y T^{n}_{i,j-1,k} + v_z T^{n}_{i,j,k-1} - \frac{h}{\Delta t}\left(T^{n+1}_{i,j,k}\right) - T^{n}_{i,j,k}\left(v_x + v_y + v_z - \frac{h}{\Delta t}\right)\right]\right\} \quad (14)$$

where $\Delta x = \Delta y = \Delta z = h$

Solutions to Equation (11), (12), (13) and (14) yield the distribution of temperature and heat flux with respect to time and space. In this work, a simulation program was developed using MATLAB programming language. This program is able to simulate the time and space dependence temperature and heat flux profiles in three dimensions. In addition, the boundary conditions for each case can be fixed during the simulation. The simulation results can be plotted in a three dimensional contour.

In summary, the program developed in this study offers the following:

(i) Temperature and heat flux distribution with respect to time at a fix location
(ii) Temperature and heat flux distribution with respect to all the three dimensions at a specified time.
(iii) The effect of wind can also be accommodated within the model provided that the intended weather data is available.

Since it is based on first principle, reasonable accuracy can be obtained. Further improvements by including temperature dependence relationship for all physical properties can further improve the model.

4.0 CASE STUDY: FIRE SIMULATION ON LPG TANK

As a case study, the LPG storage facility at the chemical engineering pilot plant CEPP, UTM has been chosen. Figure 3 provides the schematic diagram of this facility. The tank with the capacity of 26 kL is located not far from the main building of the CEPP. Analysis of the plausible accident scenario on the tank installation revealed that the LPG storage system is susceptible to pool fire, flash fire and fireball. Relevant data on the design and operation of the tank were gathered. The aim of this investigation is to study the profile of heat dispersion as well as the safety limits of the system. Analyses are based on the data on-site.

In this study, the flame diameter for pool fire, flash fire and fireball are calculated using empirical models available from the literature based on the data obtained on the LPG storage system [2,3]. These empirical models are shown as follows:

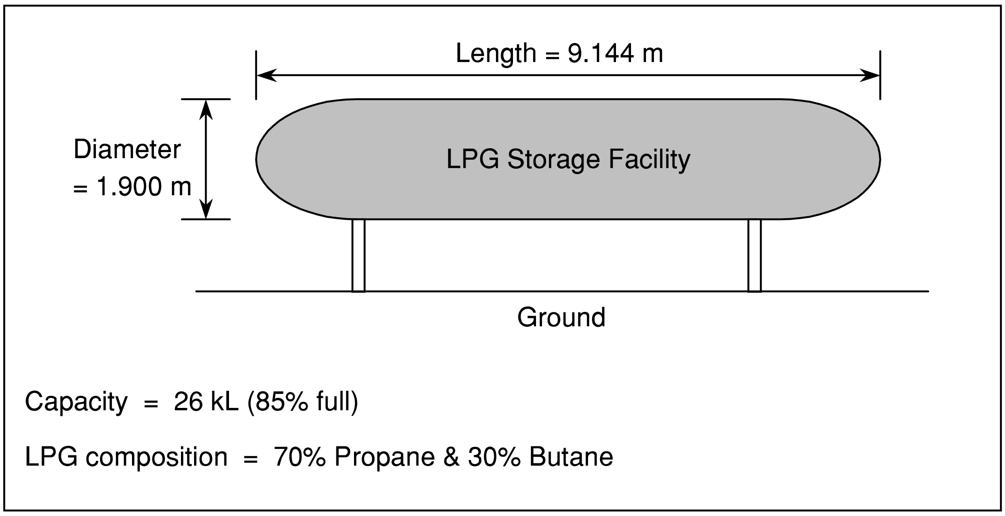

Figure 3 Schematic diagram of an LPG storage facility at CEPP, UTM

(i) *Pool fire*
Visible flame height (H) assumed to be twice the pool diameter (D),

$$H/S \approx 2 \tag{15}$$

(ii) *Flash fire*

$$H = 20d\left[\frac{S^2}{gd}\left(\frac{\rho_0}{\rho}\right)^2 \frac{wr^2}{(1-w)^3}\right]^{1/3} \tag{16}$$

$$\text{where, } w = \frac{\phi - \phi_{st}}{\alpha(1-\phi_{st})} \quad \text{for} \quad \phi > \phi_{st} \tag{17}$$

$$w = 0 \quad \text{for} \quad \phi \le \phi_{st}$$

(iii) *Fireball*

$$D_c = 5.8\, m_f^{1/3} \tag{18}$$

$$\text{and } t_c = 0.45\, m_f^{1/3} \quad \text{for} \quad mf < 30{,}000 \text{ kg} \tag{19}$$

$$t_c = 2.6\, m_f^{1/6} \quad \text{for} \quad mf < 30{,}000 \text{ kg} \tag{20}$$

5.0 RESULTS AND DISCUSSION

These results along with the safe distance obtained from the simulation results are tabulated in Table 1. Note that, a safe distance refers to the limit within which second-degree burn or worse injury will be caused on occasion of fire or explosion.

Table 1 Flame diameter and safe distance for pool fire, flash fire and fireball

Fire	Flame diameter	Safe distance
Pool fire	9.4 meter	30 meter
Flash fire	14.2 meter	35 meter
Fireball	133.3 meter	300 meter

Comparison of the temperature and heat flux distribution for pool fire, flash fire and fireball 100 seconds after release is illustrated in Figure 4 and 5, respectively. As indicated by the profiles displayed, the intensity of the temperature and heat flux is greater for fireball compared to pool and flash fires. This can also be seen from Table 1 where a safe distance for fireball is about 10 times than the other two types of fire.

The results of this study indicated that fireball is the most dangerous incidents if the LPG tank is on fire. Within 150 meters, all buildings and equipments will be badly damaged and the whole population is not expected to survive. Some significant damage and injury still can be observed within 350 meters. However, if pool fire or flash fire happen, the distance that will cause serious damage and fatality is less than 15 meter, and no significant damage and injury are expected outside 35 meters. The damage and injury caused by pool and flash fire are much lesser than fireball incidents.

Comparisons of the heat flux distribution for these incidents with time at 25 meters from heat source for pool fire and flash fire and 200 meters for fireball also illustrated

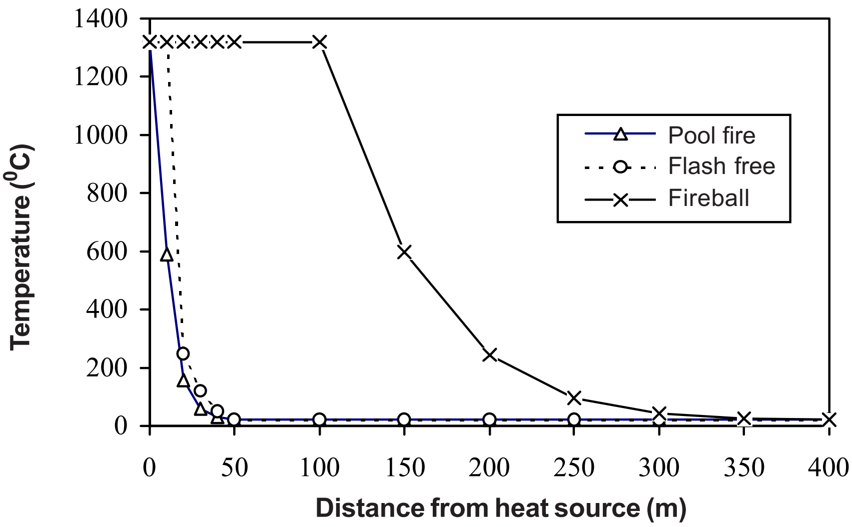

Figure 4 Temperature distribution vs. distance for pool fire, flash fire and fireball at 100 seconds

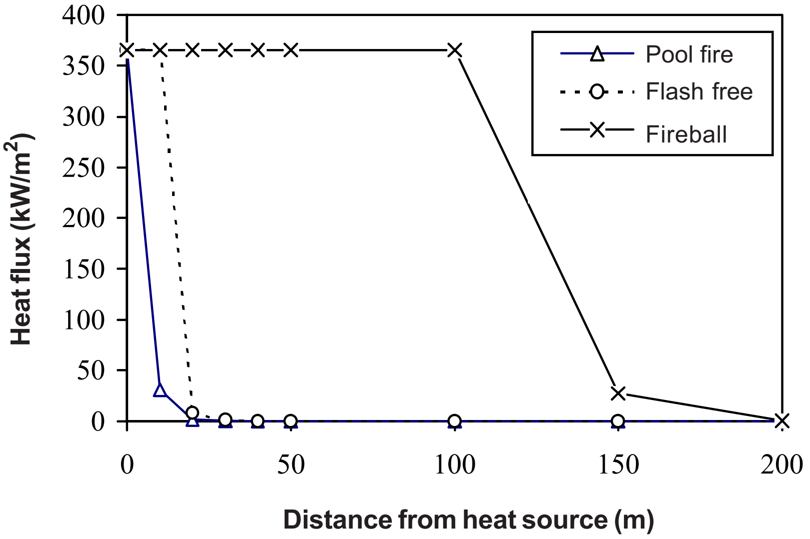

Figure 5 Heat flux distribution vs. distance for pool fire, flash fire and fireball at 100 seconds

in Figure 6. The results show that the heat flux distribution of the pool and flash fires are almost constant after the period of 100 seconds. However, the heat flux distributions at 200 meters from the fireball increase dramatically after 50 seconds. This again highlighted that fireball is the most dangerous incident.

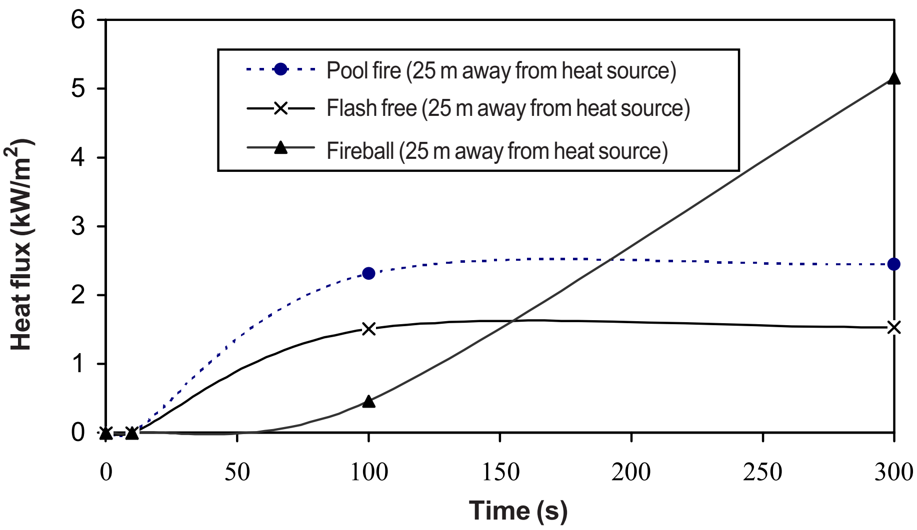

Figure 6 Heat flux distribution respect to time

6.0 CONCLUSIONS

In this study, a mathematical model of heat dispersion in three dimensions has been developed. The model was coded as a MATLAB program and tested by simulating the LPG storage facility at UTM. Some of the results that include time and space dependence of the important properties have been shown in this paper. Based on the results, the following conclusions can be made:

(i) The developed model and simulation software are able to simulate the heat dispersion following the event of fire with specified boundary conditions. In addition, this software is able to simulate a case with wind factor.
(ii) Fireball is the most dangerous incident and the damage and injury caused by this incident is much more serious than pool fire and flash fire.
(iii) The software can predict the hazard of fire and explosion and can be used as guidance for the authority to come up with precaution dry procedures to reduce the possible damage due to fire and explosive of the storege tank.

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NOMENCLATURE

ϕ_{st}	Stoichiometric mixture composition (fuel volume ratio) combustion (typically 8 for hydrocarbons)	[–]
ϕ	Fuel-air mixture composition (fuel volume ratio)	[–]
C_p	Heat capacity at constant pressure	[J/kg.K]
d	Cloud depth	[m]
D	Diameter of pool fire	[m]
D_c	Maximum diameter of fireball (at end of combustion phase)	[m]
F	View factor	[–]
g	Gravitational acceleration	[m/s^2]
H	Visible flame height	[m]
k	Thermal conductivity	[W/m.K]
m_f	Mass of fuel	[kg]
q	Heat flux	[W/m^2]
q_c	Heat flux of convection	[W/m^2]

q_r	Heat flux of radiation	[W/m^2]
r	Stoichiometric mixture air-fuel mass ratio	[–]
S	Burning speed	[m/s]
T	Temperature	[K]
t	Time	[s]
t_c	Combustion duration	[s]
v	Velocity	[m/s]
x, y, z	Distance at x, y and z-axis	[m]
α	Constant pressure expansion ratio for stoichiometric	[–]
ε	Emissivity	[–]
ρ	Density of air	[kg/m^3]
ρ_0	Fuel-air mixture density	[kg/m^3]
σ	Stefan-Boltzmann constant = 5.676×10^{-8} W/m^2·K^4	[W/m^2.K^4]
τ	Shear stress	[kg/m.s^2]
τ_a	Transmissivity	[–]

NOTATION

BLEVEs	Boiling liquid expanding vapour explosions
CCPs/AIChE	Center for Chemical Process Safety of the American Institute of Chemical Engineering
CEPP	Chemical Engineering Pilot Plant
LPG	Liquefied Petroleum Gas

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