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AN APPROXIMATE PUFF COMBINATION MODEL FOR HEAVY GAS DISPERSION

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Abstract. *Dense gas releases draw attention due to the plume being concentrated at ground level in leaks. Dense gas leaks pose a major risk in industrial areas, cities, and transportation. Therefore, propagation and dispersion simulation models are important in accident risk assessment processes. The objective of this work is to present a model that makes a rapid assessment of the propagation of dense gases in the atmosphere. In this article, an approximate model is presented to represent the different types of heavy gas releases (instantaneous, continuous, and intermittent). The model applies the process of summing and combining instantaneous releases ("puffs") to represent releases. In other words, instantaneous releases are issued in series. The instant release model is a model of homogeneous properties (box models) in the cylindrical shaped "puff". In the last part of the article, the numerical results obtained with the model are compared with experimental values from the literature.*

Keywords: *heavy gases, dispersion, leakage*

1. INTRODUCTION

Heavy gas has a higher density value than air. The heavy gas has a dispersion behavior in the atmosphere that differs from the neutrally-buoyant gas (It has the same value of the density of the air). These releases tend to form clouds closer to the ground, with a width much greater than their height (a large top surface), as described by (Tauseef et. al. , 2011), (Mack and Spruijt, 2013) and (Fay and Zemba, 1986). Risk analysis during accidental leakage of dense gases into the atmosphere is very important. Therefore, models for evaluating the propagation of these gases are necessary and important. The objective of this article is to show a simulation model for the dispersion of heavy gases that has a fast computational processing time response.

This article presents an approximate model that represents different types of releases. Continuous and intermittent releases are represented in the model based on the sum and combination of several successive instantaneous releases (the "puff" model). The model was developed in FORTRAN programming language, using the free software "FORCE 3.0". In this article, we show the instantaneous release model, the process of adding and combining "puffs" to describe a continuous release with constant flow rate and the numerical results obtained with the model. These are compared with experimental values obtained in the literature. The results obtained showed good agreement with the experimental ones, according to the statistical analysis showed.

2. METHODOLOGY

2.1 The Instantaneous Release model

The instantaneous release of heavy gas is a system of ordinary differential equations, which are shown below in equations (1), (2), (3), (4), (5) and (6), respectively, for the variables total mass "m_p", incorporated air mass "m_{ar}", velocity "U", temperature "T", radius "R" and puff position "X_C". The "puff" has a cylindrical shape and presents the same values of the composition properties of the cloud (mixture of heavy gas and incorporated air), temperature and velocity at any point inside it ("box model"), as described by (Wheatley, 1985).

$$m_p = m_{gp} + m_{ar}, \tag{1}$$

$$m_{ar}^e = \frac{dm_{ar}}{dt} = w_e \pi R^2 \rho_{ar} + U_e 2\pi R h \rho_{ar}, \tag{2}$$

$$\frac{dU}{dt} = \frac{(\bar{U}_{ar} - U) m_{ar}^l + (U_{ar}^t - U) m_{ar}^t + 1{,}2 R h \rho_{ar} (\bar{U}_{ar} - U)^2 - 0{,}0025 \pi \rho U^2 R^2}{m_p}, \tag{3}$$

$$\left(m_{ar} C_{p,ar} + m_{gp} C_{p,gp}\right) \frac{dT}{dt} = \frac{dm_{ar}}{dt} \int_T^{T_{ar}} C_{p,ar} dT + \frac{C_f}{2} U \rho C_{p,p} \pi R^2 (T - T_{ar}), \tag{4}$$

$$\frac{dR}{dt} = 1{,}3 \sqrt{gh \frac{(\rho - \rho_{ar})}{\rho}}, \tag{5}$$

$$\frac{dX_C}{dt} = U, \tag{6}$$

Where m_p is the mass total of the "puff", m_{gp} is the mass of heavy gas released at the source, m_{ar} is the total mass of air incorporated in the "puff", m_{ar}^e is the air mass entering the "puff", t is the time, w_e is the air intake speed through the top of the "puff", R is the radius of the "puff", ρ_{ar} is the air density, U_e is the air intake speed from the side of the puff, h is the puff height, U is the puff speed, $\bar{U}_{ar}$ is the average air speed, m_{ar}^l is the air mass entering from the side, U_{ar}^t is the air speed at the top of the puff, m_{ar}^t is the air mass entering from the top, ρ is the puff density, $C_{p,ar}$ is the specific heat of air at constant pressure, $C_{p,gp}$ is the specific heat of heavy gas at constant pressure, T is the puff temperature, T_{ar} is the air temperature, C_f is the coefficient of friction of the puff with the ground, $C_{p,p}$ is the specific heat of the puff at constant pressure, and X_C is the puff center position.

Differential equations (2), (3), (4), (5), and (6) are solved by the 4th order Runge-Kutta method, with a choice of integration step in time for the convergence of the dependent variables . The densities of the heavy gas cloud and air are determined by an equation of state. The instant release model can be seen in detail in the works of (Leal and Chiaramonte, 1998) and (Eidsvik, 1980).

The 4th order Runge-Kutta method is applied to solve the system of equations, for example, for the variable air inlet mass (m_{ar}) for the "puff", evaluated by the differential equation shown in Eq. (2), we are left with the relationship

$$m_{ar}(t + h_t) = m_{ar}(t) + \frac{(K_{ar,0} + 2K_{ar,1} + 2K_{ar,2} + K_{ar,3})}{6}, \tag{7}$$

Where "$m_{ar}(t + h_t)$" is the mass of air in the "puff" at time "$t + h_t$", "$m_{ar}(t)$" is the mass of air at time "t", e "h_t" is the step advance in time of the Runge-Kutta method. The constant "$K_{ar,0}$" is determined by the relationship on the right of Eq. (2) estimated at time "t", that is, the variables air entry speed at the top of the "puff" "w_e", the radius "R", the air entry speed on the side "U_e", and height "h" are estimated with the time values "t". The constant "$K_{ar,1}$" is determined by the relationship on the right of Eq. (2) estimated at time "$t + \frac{h_t}{2}$", that is, the variables "w_e", "U_e", and "h" are estimated with the time values "$t + \frac{h_t}{2}$", and the radius "R" estimated in "$R(t) + \frac{K_{R,0}}{2}$". The constant "$K_{ar,2}$" is determined by the relationship on the right of Eq. (2) estimated at time "$t + \frac{h_t}{2}$", that is, the variables "w_e", "U_e", and "h" are estimated with the time values "$t + \frac{h_t}{2}$", and the radius "R" estimated in "$R(t) + \frac{K_{R,1}}{2}$". The constant "$K_{ar,3}$" is determined by the relationship on the right of Eq. (2) estimated at time "$t + h_t$", that is, the variables "w_e", "U_e", and "h" with the time values "$t + h_t$", and the radius "R" estimated in "$R(t) + K_{R,2}$".

The Runge-Kutta method is applied to the variable displacement speed "U(t)" by the relation

$$U(t + h_t) = U(t) + \frac{(K_{U,0} + 2K_{U,1} + 2K_{U,2} + K_{U,3})}{6}, \tag{8}$$

Where $U(t + h_t)$ is the speed of the "puff" at time "$t + h_t$", $U(t)$ is the speed at time "t". The constant "$K_{U,0}$" is determined by the right-hand relationship of Eq. (3) estimated at time "t". The constant "$K_{U,1}$" is determined by the right-hand relationship of Eq. (3) estimated at time "$t + \frac{h_t}{2}$" and the dependent variables of the differential equations at "$V_i + \frac{K_{V_i,0}}{2}$". The constant "$K_{U,2}$" is determined by the relationship on the right of Eq. (3) estimated at time "$t + \frac{h_t}{2}$" and the dependent variables of the differential equations in "$V_i + \frac{K_{V_i,1}}{2}$". The constant "$K_{U,3}$" is determined by the right-hand relationship of Eq. (3) estimated at time "$t + h_t$" and the dependent variables of the differential equations at "$V_i + K_{V_i,2}$". The 4th Order Runge-Kutta method is also applied to the "puff" variables: the temperature "T" in Eq. (4), the radius "R" in Eq. (5) and the position of the center "X_C" in Eq. (6).

The time advance step of the Runge-Kutta method "h_t" is chosen by evaluating the dependent variables of the differential equations in the value step "h_t" and with two value steps "$\frac{h_t}{2}$". If the variables obtained in the largest and smallest steps have a relative error smaller than 1×10^{-4} in the largest and smallest steps, time advances. Otherwise the step is reduced to half.

The instant release model was developed and implemented in FORTRAN programming language using the free software "FORCE 3.0".

2.2 The "Puffs" Combination model

The sum model of "puffs" in series to represent a continuous release of heavy gas with constant flow is composed of the release system of a "puff" in the source, the release system of "puffs" in series, the displacement system of the "puffs" series, and the neutral-buoyant gas "puff" model (when the density of the heavy gas puff is equal to that of air). The "puff" release system at the source determines the time for it to leave the source, as shown in Figure 1. The system of displacement and combination of the series of "puffs" follows the dispersion model of section (2.1) and a combination of properties in the common regions, shown in Figures 2 and 3. The combination system also decreases the air intake area for each cylindrical "puff" due to the common regions and tests whether the more diluted "puff" passed to the dispersion condition of neutral-buoyant gas, using the empirical criteria adopted by (Fryer and Kayser, 1978) and (Melhen and Little, 1992).

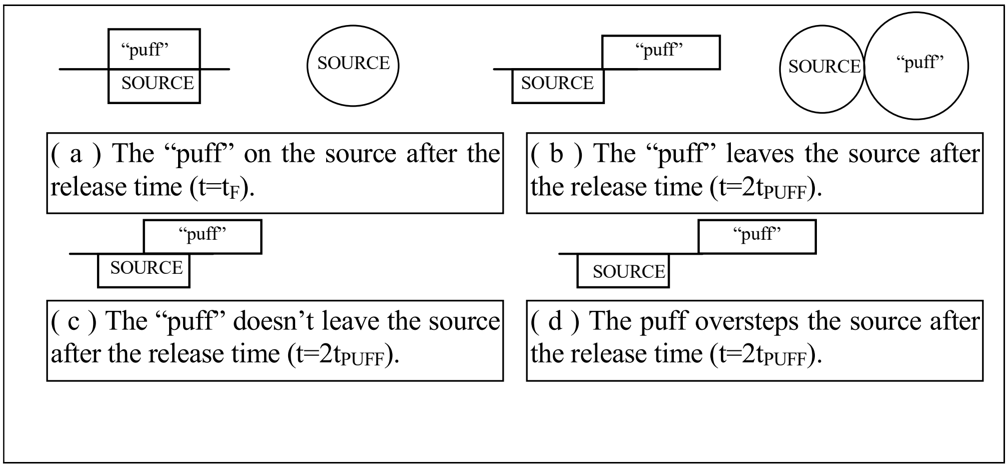

Figure 1. Release system for a "puff" at the source.

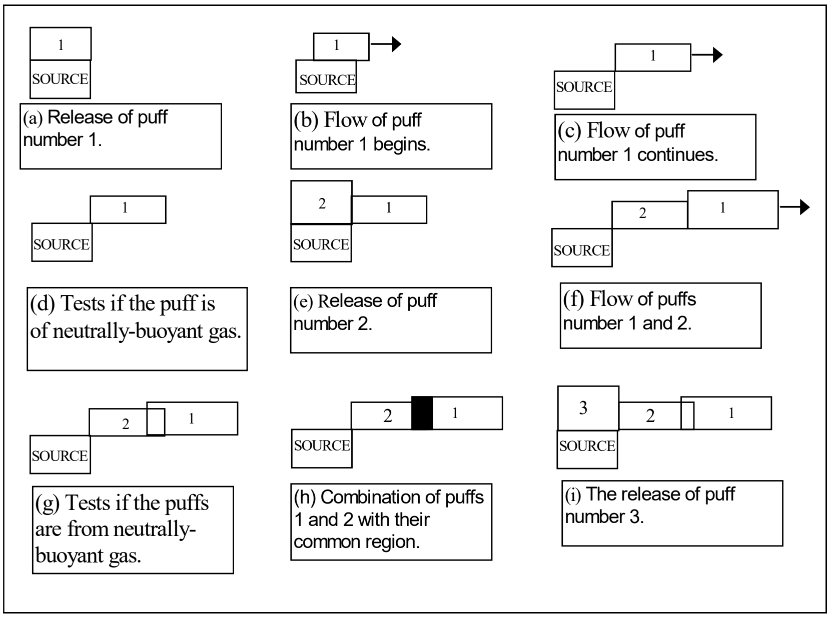

Figure 2. Release system and combination of heavy gas puffs.

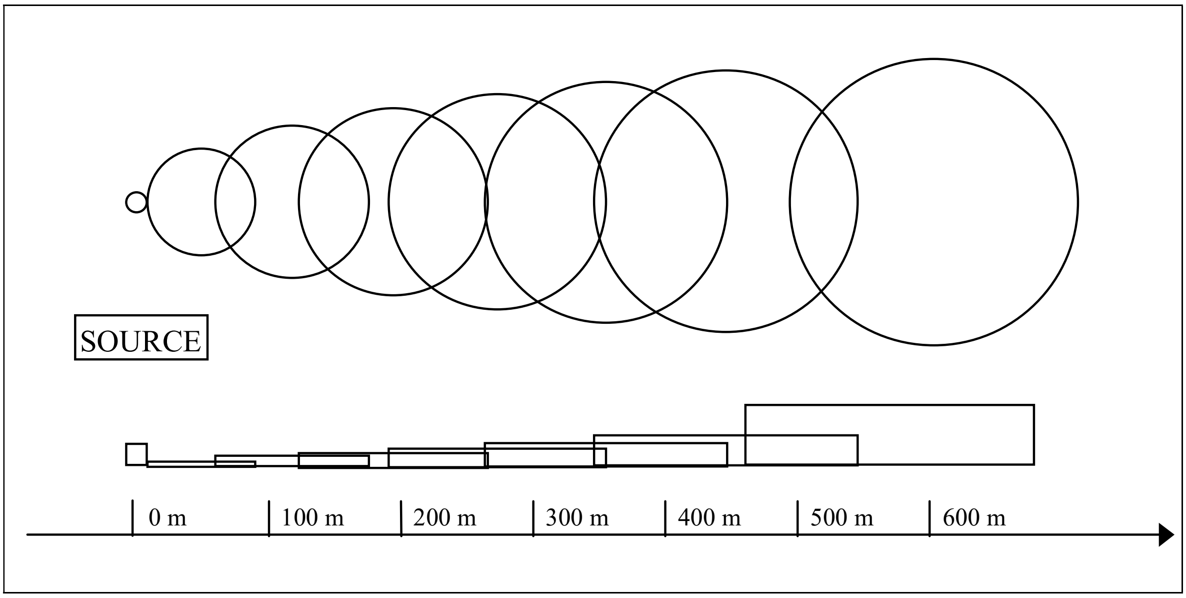

Figure 3. Scheme of formation of the heavy gas plume through the sum of “puffs”.

2.3 The Change for the dispersion for the neutrally-buoyant gas

The heavy gas is losing its density value higher than atmospheric air, due to its incorporation. The gas undergoes a dispersion of neutral-buoyant gas from this point. Therefore, the continuous plume follows the dispersal pattern of the Gaussian plume, when its dispersal regime is dominated by atmospheric turbulence. The concentration of the plume, for the neutral-buoyant gas, is obtained from the relationship

$$\rho_{plu} = \frac{Q}{2\pi U_m \sigma_y \sigma_z} e^{\frac{-y^2}{2\sigma_y^2}} \left[e^{\frac{-(z-h)^2}{2\sigma_z^2}} + e^{\frac{-(z+h)^2}{2\sigma_z^2}} \right], \quad (9)$$

Where ρ_{plu}, Q, U_m, σ_y, σ_z, y, z and h are plume concentration, gas flow at the source, average wind speed, cross dispersion coefficient, vertical dispersion coefficient, cross position, vertical position, and emission height, respectively.

The atmospheric dispersion coefficients in the vertical “σ_z” and cross “σ_y” directions are determined by empirical relationships, shown by (van Buijtenen, 1979):

$$\sigma_z = c(10 z_0)^{0,53 X_{vz}^{0,22}} X_{vz}^{d}, \quad (10)$$

$$\sigma_y = a X_{vy}^{b}, \quad (11)$$

In this work, it is introduced a method to relate the heavy gas puff dimensions to the atmospheric dispersion model coefficients in such a way that the continuous plume maintains the same puff average concentration at the transition moment, in the cylindrical puff. This proportionality is applied as follows:

$$R_t = C_t \sigma_{yt}, \quad (12)$$

$$\frac{H_t}{2} = C_t \sigma_{zt}, \quad (13)$$

Where R_t, H_t, C_t, σ_{yt} and $\sigma_{z\,t}$ are the puff radius, puff height, proportionality coefficient, horizontal atmospheric dispersion equivalent coefficient and vertical dispersion coefficient in the transition moment, respectively.

The proportionality coefficient for the transition moment in the cylindrical region of the puff, which is the value that satisfies the following equation:

$$\bar{\rho}_{pu} - \bar{\rho}_{plu} = 0, \quad (14)$$

The relations for the average plume and puff concentrations are:

$$\bar{\rho}_{plu} = \frac{Q}{4UR_tH_t} erf\left(\frac{c_t}{\sqrt{2}}\right) \left[erf\left(\frac{c_t}{\sqrt{2}}\right) + erf\left(\frac{3c_t}{\sqrt{2}}\right) \right], \quad (15)$$

$$\bar{\rho}_{pu} = \frac{m_{i,t}^{gp}}{\left(m_{i,t}^{gp} + m_{i,t}^{ar}\right)} \rho_{i,t}, \tag{16}$$

Where R_t, H_t, $m_{i,t}^{gp}$, $m_{i,t}^{ar}$, $\rho_{i,t}$ and are radius of the puff, puff height, heavy gas mass, air mass, and total puff concentration, at the moment of transition, respectively.

3. RESULTS AND DISCUSSION

The results obtained with the model are compared to the Maplin Sands field tests conducted by the Shell Oil Company, which are continuous releases of LNG (Liquefied Natural Gas) and LPG (Liquefied Petroleum Gas) over water, as shown by (Havens, 1992). . For these releases, the heavy gas concentrations were obtained at various distances measured from the center of the emission source, where the concentration is represented by the percentage of the number of moles of the heavy gas mixture released at the source.

In the Figure 4 and 5 shows the graphs of the concentration against the distance from the center of the source for the Maplin 29 and 46 tests, respectively. The field experimental results are represented in the graphs by the points in asterisk and provide the maximum percentage of the number of moles of heavy gas mixture at various distances. The results obtained with the model of "puffs" are represented in the graphs by the continuous line, where the points in the continuous line represent the percentage of the number of moles at the distance from the center of each one of two "puffs" that form the pen. Also shown is an analysis of two results using the statistical parameters of Fractional Deviation (DF) and Normalized Mean Quadratic Error (EQMN) in Table 1, according to (Hanna, 1991).

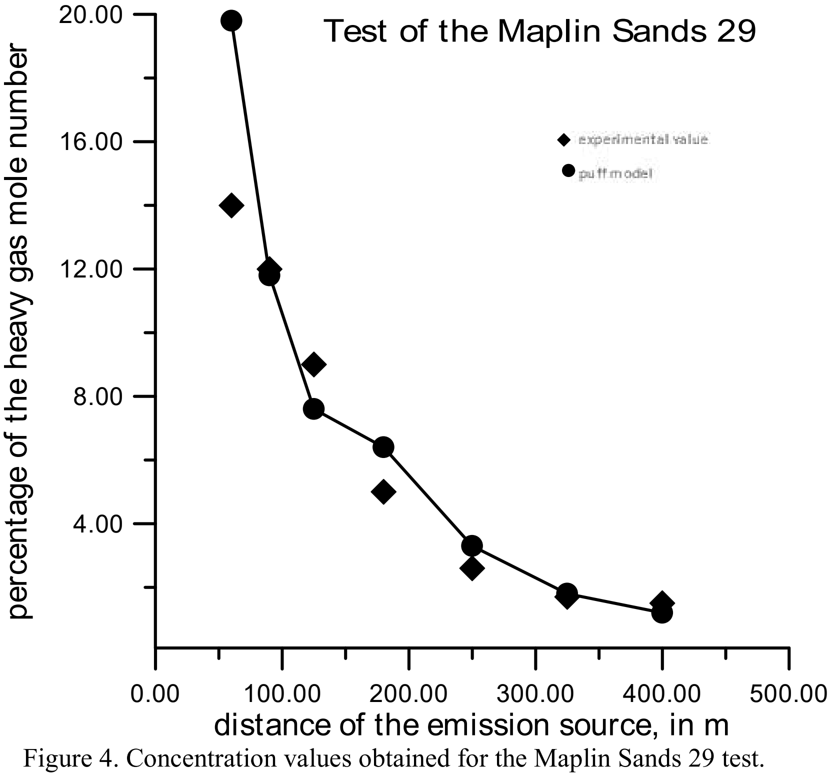

Figure 4. Concentration values obtained for the Maplin Sands 29 test.

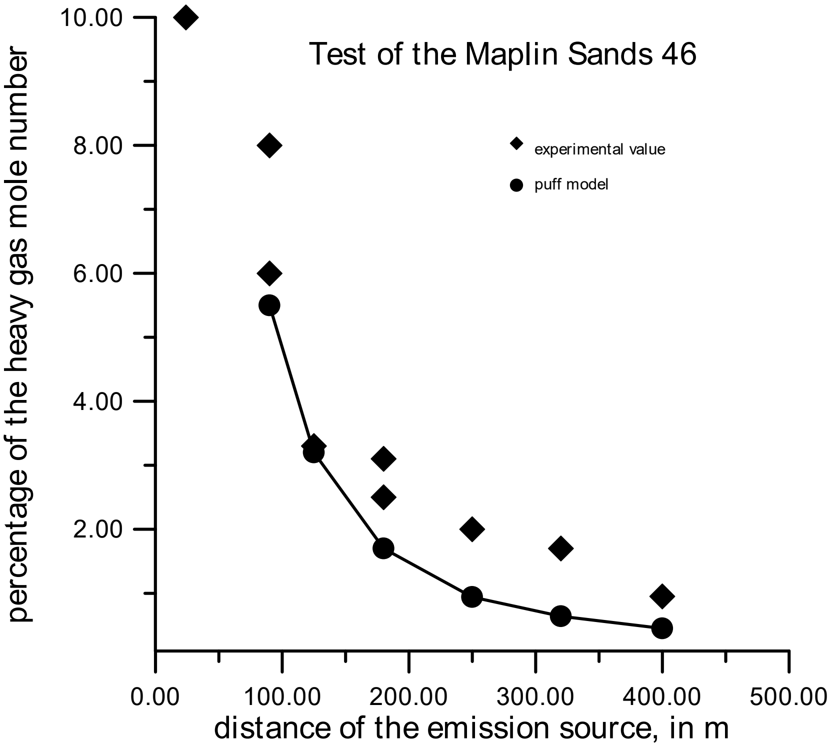

Figure 5. Concentration values obtained for the Maplin Sands 46 test.

Table 1. Statistical parameters obtained with the puff combination model.

Statistical Parameter	Parameter value
Fractional deviation	-0,0372
Normalized Mean Quadratic Error	0,377
Number of positive simple errors obtained as the model	41
Mean of positive errors relative to the measured value	0,576
Number of simple negative errors obtained as the model	57
Mean of negative errors relative to the measured value	-0,349

4. CONCLUSION

The proposed “puff” combination model presented results with adequate error values according to the statistical evaluation presented. And it also has the advantage of being a model with very low computational execution time as it is an approximate model. The model will continue to be developed. The model proved to be suitable for representing continuous releases of heavy gases with constant flow into the atmosphere at ground level. It is worth noting that the model has a quick execution time to evaluate heavy gas leaks.

5. NOMENCLATURE

ar = atmospheric air;
m = mass;
gp = heavy gas;
t = time;
R = radius of the puff;
H = puff height;
w_e= air intake speed through the top of the "puff";
U_e= air intake speed through the side of the "puff";
ρ = density;
C_p= specific heat at constant pressure of the puff;
T= temperature;
X_C= "puff" center position;
C= "puff" concentration;
Q= heavy gas flow released at source;
vz = virtual coordinate of gas release in the vertical direction;
vy = virtual coordinate of gas release in the cross direction;

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