A HEAVY GAS DISPERSION APPROXIMATE MODEL FROM THE PUFFS COMBINATION – PART 1

Edson Abel dos Santos Chiaramonte
Unipampa, Travessa 45, No 1650, Bairro: Malafaia, Bagé – RS, CEP: 96413-170
edsonchi@portoweb.com.br

Jorge Rodolfo Silva Zabadal
UFRGS, Av. Osvaldo Aranha, 99 - 4º Andar, Bairro: Centro, Porto Alegre – RS, CEP: 90046-900
jorge.zabadal@ufrgs.br

Abstract. *The problem of air pollution has drawn attention in environmental studies. The dense gas releases draw attention due to feather focus at ground level. This paper presents an approximate model to represent these various types of heavy gas releases. The model applies the process of addition and combination of instantaneous releases (so-called model of "puffs") to represent the continuous and intermittent releases. That is, a set of "puffs" are released in series. In the last part of the article, the numerical results obtained with the model are compared with experimental data field of continuous releases of heavy gases from the literature.*

Keywords: *heavy gases, dispersion, puff models*

1. INTRODUCTION

We wish to understand the behavior of accidental releases of heavy gases that have a density value higher than that of air, in the soil level, in the atmosphere. They are toxic or flammable usually. Its gases may be dangerous to people, both in industrial installations and in their neighborhoods. The heavy gas has a scattering behavior in the atmosphere that differs from the light gas. These tend to form releases closer to the ground. Its cloud gases have a much greater width than its height (a large top surface) as described by Tauseef et al. (2011), Mack and Spruijt (2013) and Fay and Zemba (1986).

The heavy gas releases at ground level in the atmosphere can be instantaneous, continuous and intermittent. In this article we present an approximate model, which represents these various types of releases. The continuous and intermittent releases are represented in the model from the sum and combination of several successive instantaneous releases (the model of "puff"). In this article, we show the process of addition and combination of "puffs" to describe a continuous release with constant flow and the numerical results obtained with the model are compared with experimental data obtained in the literature and the DEGADIS model, as Havens and Spicer (1985).

2. THE INSTANTANEOUS RELEASE MODEL

The instantaneous release of heavy gas is a set of ordinary differential equations, which are shown below in equations (1), (2), (3), (4), (5) and (6) respectively for the variables total mass, built-in air mass, velocity, temperature, radius and position of the "puff". The "puff" has the cylindrical shape and has the homogeneous values of the cloud properties of the composition (heavy gas mixture and air), temperature, and speed at any point in its interior ("box model"), as described in Wheatley (1985).

$$m_p = m_{hg} + m_{ar} \tag{1}$$

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

$$\frac{dU}{dt} = \frac{(\bar{U}_{ar} - U)}{m_p}\left(\frac{dm_{ar}}{dt}\right)_l + \frac{(U_{ar} - U)}{m_p}\left(\frac{dm_{ar}}{dt}\right)_t + 1.2\frac{Rh\rho_{ar}[\bar{U}_{ar} - U]^2}{m_p} - 0.0025\frac{\pi\rho U^2 R^2}{m_p} \tag{3}$$

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

$$\frac{dR}{dt} = 1.3\sqrt{gh\frac{(\rho - \rho_{ar})}{\rho}} \quad (5)$$

$$\frac{dX_c}{dt} = U \quad (6)$$

The inlet velocities at the top and side face are determined by empirical relations, respectively:

$$U_e = 0.5\frac{\left(\frac{dR}{dt}\right)_t}{\left(\frac{dR}{dt}\right)_{t=0}} \quad (7)$$

$$w_e = \frac{3.5}{5.83+Ri_*}v_t \quad (8)$$

Where m_p, m_{hg}, m_{ar} are the "puff" mass (the mixture of the heavy gas and air), heavy gas mass released in the source, the air mass inside at the "puff", respectively. The variables R, h, $C_{P.p}$, U, T, X_c and ρ are the radius, height, gas specific heat, velocity, temperature, center position and density of the "puff" mixture, respectively. The variables ρ_{ar}, $\overline{U}_{ar}$, U_{ar}, $C_{P,ar}$, T_{ar}, are the density, average velocity in the puff height, velocity, specific heat and temperature of the air. And, the variables $\left(\frac{dm_{ar}}{dt}\right)_l$, $\left(\frac{dm_{ar}}{dt}\right)_t$, $\frac{dm_{ar}}{dt}$, w_e, U_e, v_t, Ri_*, C_f and g are the rate of the entrainment of the air (lateral, top and total), air entrainment velocity on the puff top, air entrainment velocity on the puff lateral, turbulent velocity at the top, Richardson number, friction coefficient (adopted the value of the 0.0025) and gravity acceleration.

The system of differential equations (2), (3), (4), (5) and (6) are solved by the Runge-Kutta fourth order method, as Leal and Chiaramonte (1998) and Eidsvik (1980).

3. THE SUM OF "PUFFS" METHOD TO REPRESENT A CONTINUOUS HEAVY GASES RELEASES

A heavy gas release may be considered to be instantaneous, or may have a wide range of time to leave the source. The release with wide range of duration may have different behaviors, such as the flow is continuous and steady, or continuous and decrease exponentially with the release time, or an intermittent source. The purpose of this section is to show a method of representation of these various forms of releases made from the sum of several independent instantaneous releases ("puffs"). The model to represent a continuous source with constant flow will be described below.

The model used to represent a continuous constant rate source will be described in this work. Other kinds of the sources would follow a similar procedure. The heavy gas dispersion and transport system is constituted by two models. The puff combination model is used for heavy gases, and the Gaussian plume model to describe the neutrally-buoyant gas dispersion. This model performs the change from the puff model to the Gaussian plume model. The system used to represent the heavy gas plume through a sum of puffs is show in Figs. (1) and (2) and follows the procedures described next.

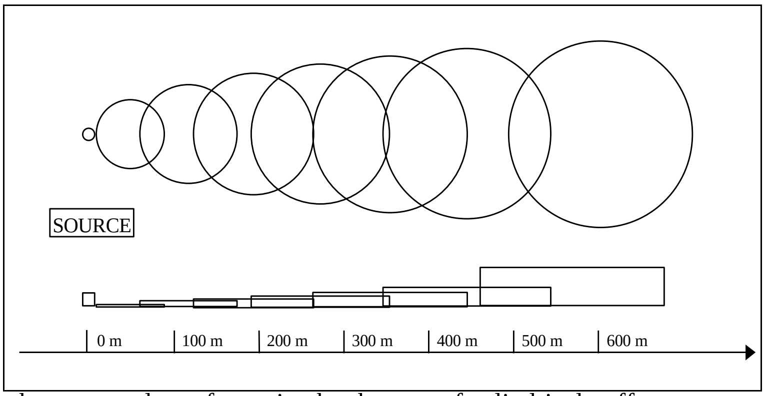

Figure 1- Diagram showing heavy gas plume formation by the sum of cylindrical puffs.

3.1.The puff source release model

Each heavy gas puff has a formation time on the source, as shown in Fig. (3). All puffs have the same formation time. The adopted formation time is equal to the time the puff takes to leave the release source border, as shown in Fig. (3). This time is obtained through a search and trial procedure. The puff initial diameter is equal to the source diameter.

3.2 The puffs combination system

The system to perform the sum and combination of puffs is composed of:

a) Heavy gas puffs flow and dispersion - the set of puffs follows the model shown in section 2 in each period of formation time, each puff being independent;

b) Heavy gas puffs combination process - the puffs that form the plume have common regions among them, as can be seen in the diagram of Fig. (1). The mass, temperature and velocity properties are combined for each period of formation time in these regions. The procedure performs mass, energy and momentum equilibrium balances in the puff and common regions with other puffs.

The combination system also reduces the air inlet area for every "puff" due to the cylindrical base regions and tests if the "puff" has passed for more dilute neutral gas dispersion condition using empirical criteria adopted by Fryer and Kayser (1978) and Melhen and Little (1992).

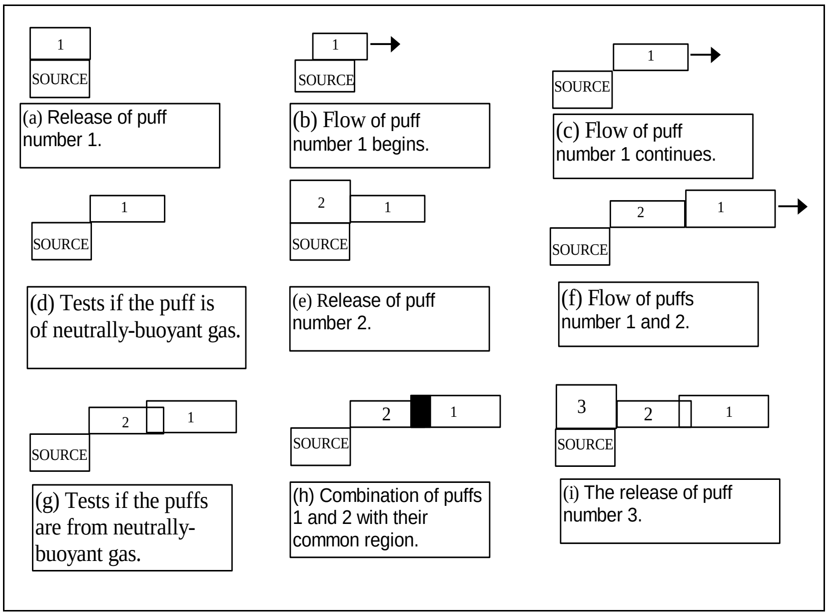

Figure 2- System of release and combination of heavy gas puffs.

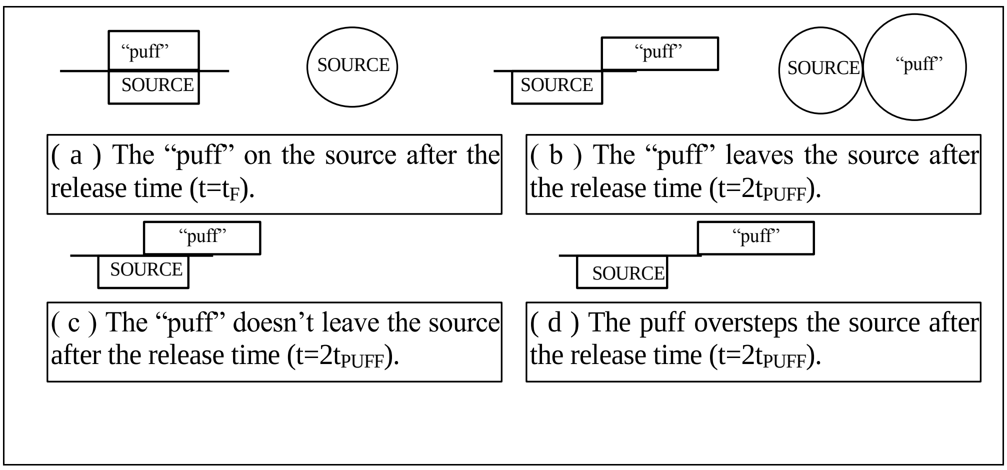

Figure 3- The formation time of the puff in the source.

4. THE CHANGE TO THE NEUTRALLY-BUOYANT GAS DISPERSION MODEL

In the continuous Gaussian plume model for a neutrally-buoyant gas the concentration is obtained by:

$$\rho(x,y,z) = \frac{Q}{2\pi\bar{u}\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right)+\exp\left(\frac{-(z+h)^2}{2\sigma_z^2}+\right)\right] \quad (9)$$

Where ρ, Q, $\bar{u}$, σ_y, σ_z, x, y, z and h are the plume concentration at coordinates (x,y,z), the rate of mass release of the source, the average wind velocity, the horizontal atmospheric dispersion parameter, the atmospheric vertical dispersion parameter, the gas emission source distance in the downwind direction, transversal distance to the wind from the plume center, vertical distance measured from the ground and the source height, respectively.

Atmospheric dispersion coefficients in horizontal and vertical directions are determined by empirical relationships, shown by van Buijtenen (1979):

$$\sigma_z(x_{vz}) = c(10Z_0)^{0.53x_{vz}^{-0.22}} x_{vz}^{d} \quad (10)$$

Where x_{vy}, x_{vz}, Z_0, a, b, c and d are the virtual distance from a point source in the horizontal direction, the virtual distance in the vertical direction, the length of the ground roughness, and the parameters determined according to the classes of the atmospheric stability of the Pasquill-Gifford.
After moving to the model of Gaussian plume concentration happens to be evaluated considering "puffs" cylindrical approximate radius and height dimensions determined by the relationships (12) and (13), which will be shown below. In these maximum concentration is obtained with the equation (7) on the axis of the plume at ground level (with the horizontal and vertical distances with zero values), and the average concentration obtained with the relation:

$$\bar{\rho}_{plu} = \frac{Q\,\mathrm{erf}(\frac{h}{\sqrt{2}\sigma_z})\,\mathrm{erf}(\frac{R}{\sqrt{2}\sigma_y})}{2URh} \quad (11)$$

Where $\bar{\rho}_{plu}$ is the average concentration of Gaussian plume profile in a cylindrical region and erf(x) is the error function of the argument x.

4.1 The exchange of heavy gas plume dispersion model for the light gas

The heavy gas dispersion models determine the virtual source coordinates in the vertical and horizontal directions, at the moment of transition from the dispersion model from the following relationships:

$$R_t = 2.15\sigma_{yt} \quad (12)$$

$$\frac{h_t}{2} = 2.15\sigma_{zt} \quad (13)$$

Where R_t, H_t, σ_{yt}, and $\sigma_{z\ t}$ are the radius of the "puff", the height of the "puff", the horizontal air scattering coefficient and vertical atmospheric scattering coefficient (at the time of transition).

In this work, we introduced a method for determining the value of the proportionality coefficient between the dimensions of the "puff" heavy gas and dispersion coefficients for the continuous Gaussian plume model keep the mean concentration value at the instant of the transition .

There is a proportionality between the size of the "puff" and dispersion coefficients:

$$R_t = C_t\sigma_{yt} \quad (14)$$

$$\frac{h_t}{2} = C_t \cdot \sigma_{zt} \quad (15)$$

Where C_t is the proportionality coefficient for the instant of heavy gas transition to the light plume.

The proportionality coefficient is determined by the value that satisfies the following equation.

$$\frac{Q_{gp}\cdot[\mathrm{erf}(\frac{C_t}{\sqrt{2}})]^2}{2\cdot U_t\cdot R_t\cdot h_t} - \frac{m_{gp,t}}{(m_{gp,t}+m_{ar,t})}\cdot\rho_{p,t} = 0 \quad (16)$$

Where $\rho_{gp,t}$, $m_{gp,t}$, $m_{ar,t}$, $\rho_{p,t}$ and U_t are the heavy gas concentration of the "puff", the heavy gas mass of the "puff", air mass of the "puff", the total concentration of the "puff" and the heavy gas "puff" velocity (at the time of transition to light plume).

5. RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

The results obtained from the model are compared to Maplin Sands field tests conducted by Shell Oil Company, which are continuous releases of LNG (Liquefied Natural Gas) and LPG (Liquefied Petroleum Gas) on water, as shown by Havens (1992) . The release site was an area of tidal sands in the Thames estuary. The gas handling plant was on shore at the edge of flat farmland. The spill point was 350 m offshore and liquid was delivered along a pipeline from the gas handling plant. A 300m diameter dike was constructed around the spill point to retain water so that the trials could be conducted at low tide. The water level behind the dike varied by 0.75 m. The spill point was a 150 mm diameter pipe directed vertically downward terminating above the water surface..For these releases were obtained the heavy gas concentrations 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.

The figures 4 and 5 shows graphs of the concentration versus the distance from the center to the source Maplin Sands tests 29 and 46, respectively. The experimental field results are represented in the graphs by points asterisk and provide the maximum percentage of the number of moles of the heavy gas mixture at various distances. Results obtained with the model of "puffs" are represented by the solid line in the graphs and obtained with Degadis model by the dashed lines, the points where the continuous line represent the percentage of the number of moles in the distance from the center of each of the "puffs" to form the plume.

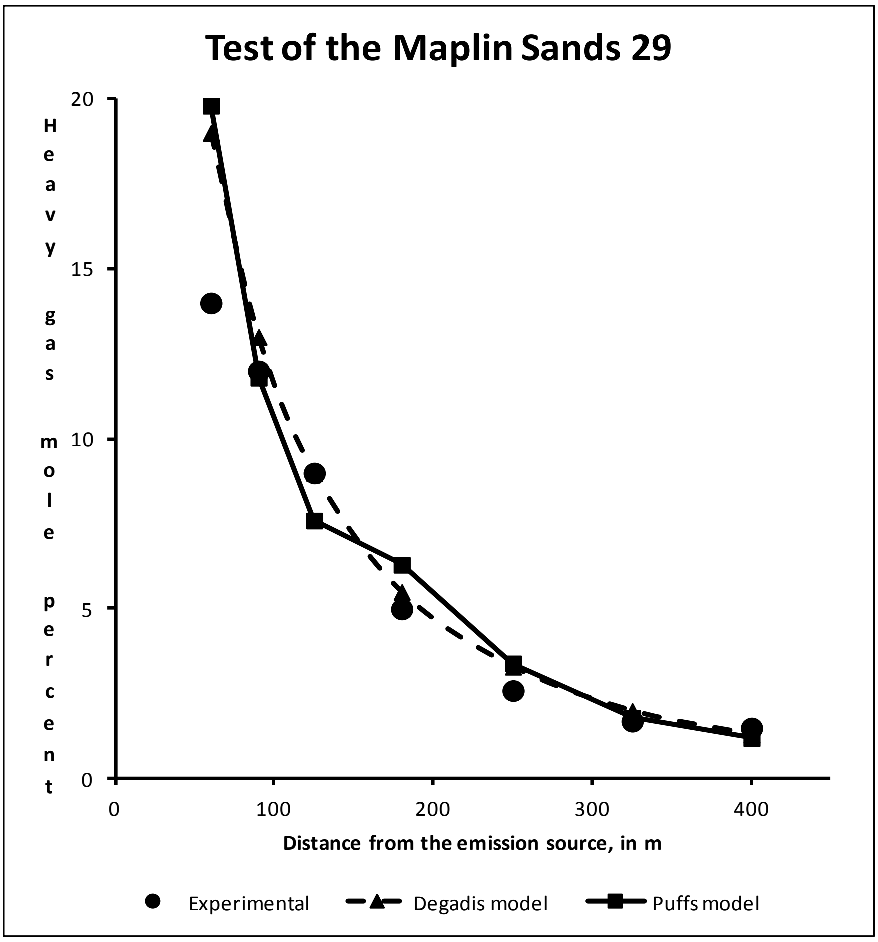

Figure 4. Concentration values obtained for the Maplin Sands 29 test.

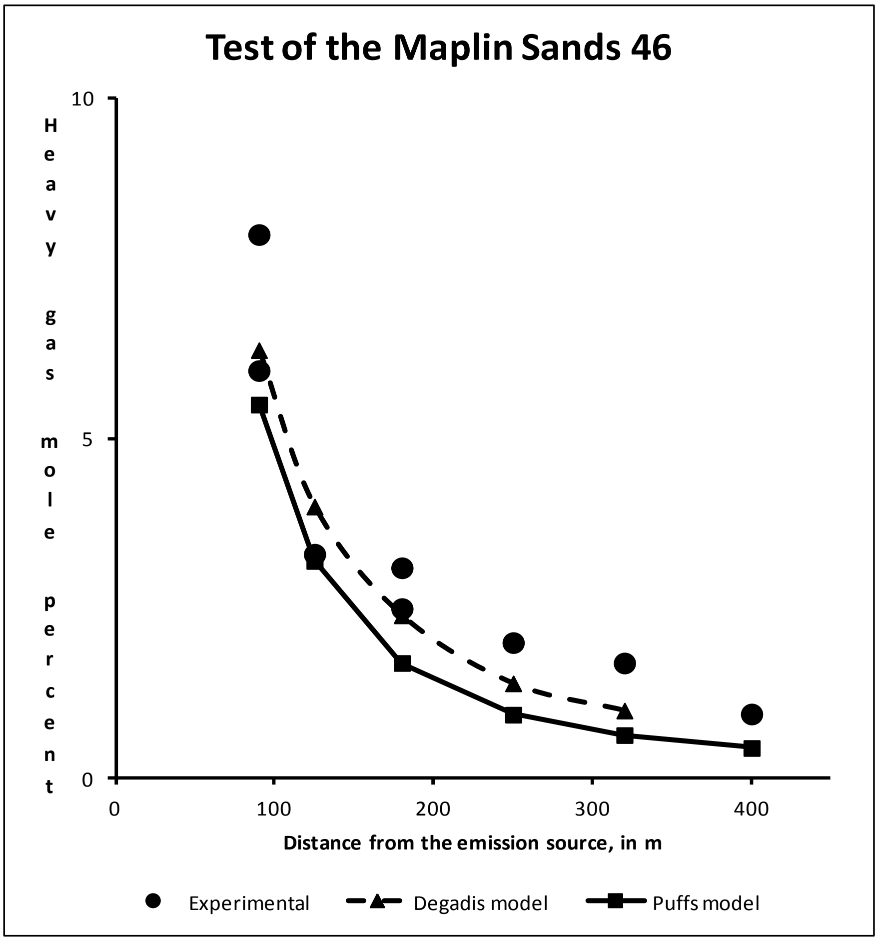

Figure 5. Concentration values obtained for the Maplin Sands 46 test.

6. REFERENCES

Eidsvik, K. J., 1980. "A Model for Heavy Gas Dispersion in the Atmosphere". *Atmospheric Environment*, Vol. 14, p. 769.

Fay, J. A. and Zemba, S. G., 1986. "Integral Model of Dense Gas Plume Dispersion", *Atmospheric Environment*, Vol. 20, p. 1347.

Havens, J. A., Spicer, T. O., 1985. "Development of an Atmospheric Dispersion Model for Heavier-Than-Air Gas Mixtures"(Vol. 1). Report No CG-D-22-85 for the U. S. Coast Guard by the Chem. Eng. Dept. of University of Arkansas, Fayetteville, USA.

Fryer, L. S.; Kaiser, G. D., 1979. "DENZ - A computer program for the calculation of the dispersion of dense toxic or explosive gases in the atmosphere", Technical Report SRD-R152, Safety and Reliability Directorate.

Havens, J., 1992. "Review of dense gas dispersion field experiments", *J. Loss Prev. Process Ind.*, Vol. 5, p. 28.

Leal, C. A.; Chiaramonte, E. A. S., 1998. "Simulação numérica do comportamento de "puffs" para representar a dispersão de gases pesados na atmosfera", In *Proceedings of the 12º Congresso Brasileiro de Engenharia Química*, Porto Alegre.

Mack. A.; Spruijt, M.P.N., 2013, "Validation of Open Foam for heavy gas dispersion applications". *Journal of Hazardous Materials*, Vol. 262, p. 504.

Melhem, G. A.; Little, A. D., 1992. *Advanced Consequence Modeling - Emission, Dispersion, Fires and Explosions*, Van Nostrand Reinhold, New York, 2nd edition.

Tauseef, S. M.; Rashtchian, D.; Abbasi, S. A., 2011. "CFD-based simulation of dense gas dispersion in presence of obstacles". *J. Loss Prev. Process Ind.*. Vol. 24, p. 371.

Van Buijtenen, C. J. P., 2000. *Methods for the calculation of the physical effects of the escape of dangerous material (liquids and gases) Part II, DISPERSION*, Chapter 7, Directorate-General of Labour, Netherlands.

Wheatley, C. J., 1985. *Dispersion of Heavy Gases*, Von Karman Institute for Fluid Dynamics.

7. RESPONSIBILITY NOTICE