MODELS OF BUOYANT PLUMES REVISITED FOR SIMULATION

Pablo Ripollés Iturralde
Departamento de Matemática Aplicada y Estadística
E.T.S.I. Aeronáuticos, U.P.M.
Madrid, Spain
email: ripolles@gmail.com
date: August, 2007

ABSTRACT
In this paper the models of weakly and strongly buoyant plumes are revisited and compactly rewritten with a systematic and unifying approach. Clearly casting the physical problem into the mathematical one is essential prior to any simulation to be carried out properly. In the process it was found that earlier traditional assumptions might be no longer necessary. A simulation based on these models with real world data was carried out successfully.

KEY WORDS
Simulation, Atmospheric Modeling, Power Plants Modeling, Buoyant Plumes.

1 Introduction

The main purpose of this work is to present a *simulation* of the aero-thermodynamical effects produced by the gas emissions that come out from industrial stacks, generating either flue gases or gas flares, in a dry calm environment. The simulation was carried out with real data from a propane dehydrogenation (PDH) plant that BASF ESPAÑOLA S.A. wanted to build in Tarragona (Spain). All the necessary constants and initial conditions were extracted from that data. The PDH plant would have flue gas stacks as well as gas flare ones. The motivation for this simulation was the concern about the height reached by the plumes and their induced velocities. The PDH plant was to be located near an airport.

The secondary purpose of this work is to *model* both plumes with a systematic and unifying approach. Provided that an acceptable model accuracy and simplicity are expected, it seems necessary to model both plumes separately. This seems partly so due to the intrinsic physical differences existing between them. From direct observation it is easy to see that these industrial stacks eject buoyant gases into the atmosphere. However, the flue gas stack produces weak buoyancy forces, whereas the gas flare stack produces strong buoyancy forces. The motivation for this approach was the need to have the associated physical and mathematical problems clearly written prior to their implementation. While looking for these clean written forms, none of the found ones were satisfactory.

In the turbulent buoyant convection from small area sources, vertical motions are produced under gravity by the temperature (density) differences between the ejected gases and their local environment, thus generating buoyancy forces [1], [2], [3]. For the case of *flue gas plumes* the temperature (density) differences are *moderated* and therefore *the buoyancy is weak*. For the case of *gas flare plumes* the temperature (density) differences are *extreme* and therefore *the buoyancy is strong*. The terms *weakly buoyant plume* and *strongly buoyant plume* [2] are used to abstractly refer to each one of the produced phenomena.

In the turbulent plumes there exists a clear-cut separation between the buoyant turbulent gas system quickly evolving upwards and its local environment [3]. This gas system grows in size essentially due to the *entrainment* process by taking air into the plume from its local environment. The entrainment process is augmented by the formation of large eddies in the mixing layer.

In the turbulent radiant plumes the *thermal radiation* is due to the turbulent combustion taking place in the lowest part of the plume [2]. The temperatures are extreme, so radiation is important. The flux of radiation from the hot plume gases depends on the composition of these gases; where two limiting cases are the plume behaving either transparent or opaque to radiation.

The theory employed to model the strongly buoyant plumes is based on the one employed to model the weakly buoyant. However, it becomes necessary [2] to include certain modifications which take into account large variations in temperature (density), the different levels of air entrainment and the presence of thermal radiation, all occurring at the lower end of the plume.

From a *mechanical* point of view, the main difference is due to the *entrainment into the plume* effect. The flue gas and gas flare plumes both have contributions of this effect. However, the entrainment into the plume is larger for the flue gas one than for the gas flare one. This difference is even larger at the lower end of the plume [2].

From a *thermal* point of view, the main difference is due to the absence/presence of *thermal radiation* effects. The flue gas plume is generated as a consequence of conveying the combustion exhaust gas produced somewhere in the industrial plant. The gas flare plume is generated as a consequence of an intense turbulent combustion taking place on the burner at the stack's exit. Hence, the gas flare plume is the only one that might contribute to the thermal radiation.

In the indicated early literature where these simple models were first derived, a common assumption was the *Boussinesq approximation* [1], [2], [3]. This assumption is physically justified for the weakly buoyant plumes but not for the strongly buoyant [4], [5]. Another common assumption was the omission of the *thermal radiation* effects [2], [6]. This assumption is not physically justified, however it was common because of the lack of simplicity of the above referenced thermal phenomenon.

Although both models are presented here separately, they are treated as similarly as possible, therefore reducing the formal differences to a minimum. This approach has two main implications for both models. One consequence will be dropping the Boussinesq approximation for the weakly buoyant plumes. Another consequence will be ignoring the relevant thermal radiation effects for the strongly buoyant plumes.

2 Dry Calm Environment

Prior to the introduction of the flue gas and gas flare plume models, it is useful to present a simplified model of the dry calm environment where both plumes shall develop. The *fluid statics* basic model for the dry calm atmosphere is integrated analytically. According to the following laws[1]:

$$T_\infty = T_\infty(0) - kh \tag{1}$$

$$\frac{\mathrm{d}p_\infty}{\mathrm{d}h} = -\rho_\infty g \tag{2}$$

$$\frac{p_\infty}{\rho_\infty} = R_\infty T_\infty \tag{3}$$

and for a given known atmosphere, it is easy to see that the closed-forms for p_∞, ρ_∞ and T_∞ in terms of h are:

$$\frac{T_\infty}{T_\infty(0)} = 1 - \frac{k}{T_\infty(0)}h \tag{4}$$

$$\frac{p_\infty}{p_\infty(0)} = \left[1 - \frac{k}{T_\infty(0)}h\right]^{\frac{g}{R_\infty k}} \tag{5}$$

$$\frac{\rho_\infty}{\rho_\infty(0)} = \left[1 - \frac{k}{T_\infty(0)}h\right]^{\frac{g}{R_\infty k}-1} \tag{6}$$

where h is the *true altitude*. It should be noted that the ∞ subscript refers to the atmospheric magnitudes and, wherever they appear, they will be assumed to be known functions of the true altitude.

3 Weakly Buoyant Plumes

In this section, the general assumptions and the model of weakly buoyant plumes are presented. Only the aero-thermodynamical effects of the emission of buoyant gases in a dry calm environment are considered. For this case there are no relevant thermal effects such as the thermal radiation.

As already mentioned, a *flue gas plume* can be considered to be produced by a *small area source* ejecting hot gases at *moderated* high temperatures into the atmosphere. In the absence of wind, the plume generated by such an emission constitutes, essentially, a *convection column*. The *general assumptions* under which the model is developed are the following:

- **Axisymmetric Plume:** The central line of the convection column is a symmetry axis, hence the equations will be written in cylindrical polar coordinates.
- **Similarity of Profiles:** The axial velocity profiles are similar in shape at various heights, this is further simplified commonly by using the *top-hat* profiles formulation [1], [2], [3].
- **Entrainment Function:** The entrainment function is assumed to be *constant* [2]. This essentially means that the entrainment mean radial (local) velocity, defined over the mean exterior (local) boundary of the convection column, is *proportional* to the mean axial (local) velocity, defined over the central line of the convection column.

  $$u_e = E\,w, \quad E = \alpha \tag{7}$$

  For the *top-hat* profiles of velocity, density and temperature, the experimental value of the *proportionality constant*, $\alpha \approx 0.116$, has been proven useful [3].
- The differences of density (temperature) between the convection column and its local environment *might* be important. Therefore, the density (temperature) variations will be taken into account in the equations for the rate of change of mass and momentum, hence they are not neglected in any way. This differs from the traditional treatment of the matter where, due probably to historical reasons, such variations were taken into account only through the resulting buoyancy forces, thus assuming the well-known *Boussinesq approximation* [7].

3.1 Model for the Flue Gas Plume

Starting from the *Navier-Stokes* equations in conservative form and using cylindrical polar coordinates, the following *integral model* is obtained:

- From the *conservation of mass* principle:

  $$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w b^2) = 2b\,u_e \rho_\infty \tag{8}$$

- From the *conservation of momentum* principle:

  $$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w^2 b^2) = -g b^2\,(\rho - \rho_\infty) \tag{9}$$

  $$p_\infty = p \tag{10}$$

[1] The linear dependence of the temperature with the true altitude is valid only within the first 11 000 m.

- From the *conservation of energy* principle:

$$\frac{\mathrm{d}}{\mathrm{d}z}[\rho w b^2 \, (c_p T - c_{p_\infty} T_\infty)] = \\ -\rho w b^2 \, [\frac{\mathrm{d}}{\mathrm{d}z} \, (c_{p_\infty} T_\infty) + g] \tag{11}$$

- From thermodynamics, the *equation of state*:

$$\frac{p}{\rho} = RT \tag{12}$$

The above equations form a differential-algebraic equation (DAE) system with three non-linear first order ordinary differential equations (ODEs) (8), (9) and (11) plus two algebraic equations (10) and (12). The independent variable, z, is the axial coordinate measured over the central line of the convection column starting at the source. It represents the *height over the stack*. The rest of the variables (b, w, p, ρ, T) are unknown functions of z to be determined. They represent the mean *radius*, the mean *axial velocity*, the mean *pressure*, the mean *density* and the mean *temperature* of the convection column respectively. It should be noted that the atmospheric magnitudes are expressed in terms of the true altitude, whereas the plume magnitudes are expressed in terms of the height over the stack, hence $h = h_0 + z$ is required.

Special mention should be given to two *additional hypothesis* about the specific heat capacity at constant pressure and the gas constant:

1. Due to the *large* entrainment of air into the plume from its local environment, it seems reasonable to assume that $c_p = c_{p_\infty}$ and $R = R_\infty$.
2. In addition, due to the *moderated* gradients of temperature, the c_p is assumed to be a *constant function* of temperature [2].

From now on, the atmospheric specific heat capacity c_{p_∞} will be rewritten as c_p and R_∞ as R.

By coupling system (1)–(3) with system (8)–(12) the following uncoupled DAE subsystem for the weakly buoyant plumes can finally be written as:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w b^2) = 2b \, \alpha w \rho_\infty \tag{13}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w^2 b^2) = -g b^2 \, (\rho - \rho_\infty) \tag{14}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}[\rho w b^2 \, c_p \, (T - T_\infty)] = -\rho w b^2 \, (c_p \frac{\mathrm{d}T_\infty}{\mathrm{d}z} + g) \tag{15}$$

$$\rho T = \rho_\infty T_\infty \tag{16}$$

where the atmospheric magnitudes should be understood as known functions of h such that $h = h_0 + z$; where z is the independent variable and (b, w, ρ, T) are the dependent variables. To properly solve this DAE system three *initial conditions* (at $z = 0\,\mathrm{m}$) for either (b, w, ρ) or (b, w, T) must be specified such that the algebraic constraint (16) is satisfied.

4 Strongly Buoyant Plumes

In this section, the general assumptions and the model of strongly buoyant plumes are presented. Only the aerothermodynamical effects of the emission of buoyant gases in a dry calm environment are considered. For this case there are indeed relevant thermal effects due to the thermal radiation. However, these are not considered to be in the scope of this work. The rationale behind this consideration is rooted in the conservative approach that motivated this research in the first place: the worst case scenario with respect to the height reached by the gas flare plume is obtained by neglecting the thermal radiation effects.

As already mentioned, a *gas flare plume* can be considered to be produced by a *small area source* ejecting hot gases at *extreme* high temperatures into the atmosphere. In the absence of wind, the plume generated by such an emission constitutes, essentially, a *convection column*. The *general assumptions* under which the model is developed are the following:

- **Axisymmetric Plume:** The central line of the convection column is a symmetry axis, hence the equations will be written in cylindrical polar coordinates.

- **Similarity of Profiles:** The axial velocity profiles are similar in shape at various heights, this is further simplified commonly by using the *top-hat* profiles formulation [1], [2], [3].

- **Entrainment Function:** The entrainment function is assumed to be *variable* [2]. This is in way such that the entrainment mean radial (local) velocity, defined over the mean exterior (local) boundary of the convection column, is *proportional* to the mean axial (local) velocity, defined over the central line of the convection column, times the function $\sqrt{\frac{\rho}{\rho_\infty}}$. That is:

  $$u_e = E \, w, \quad E = \alpha \sqrt{\frac{\rho}{\rho_\infty}} \tag{17}$$

  For the *top-hat* profiles of velocity, density and temperature, the experimental value of the *proportionality constant*, $\alpha \approx 0.116$, has proven useful [3].

- The differences of density (temperature) between the convection column and its local environment are important. Therefore, the density (temperature) variations will be taken into account in the equations for the rate of change of mass and momentum, hence they are not neglected in any way.

4.1 Model for the Gas Flare Plume

Starting from the *Navier-Stokes* equations in conservative form and using cylindrical polar coordinates, the following *integral model* is obtained:

- From the *conservation of mass* principle:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w a^2) = 2a\, u_e \rho_\infty \tag{18}$$

- From the *conservation of momentum* principle:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w^2 a^2) = -g a^2\,(\rho - \rho_\infty) \tag{19}$$

$$p_\infty = p \tag{20}$$

- From the *conservation of energy* principle:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}z}[\rho w a^2\,(c_p T - c_{p_\infty} T_\infty)] = \\ -\rho w a^2\,[\frac{\mathrm{d}}{\mathrm{d}z}\,(c_{p_\infty} T_\infty) + g]\end{aligned} \tag{21}$$

- From thermodynamics, the *equation of state*:

$$\frac{p}{\rho} = RT \tag{22}$$

The above equations form a differential-algebraic equation (DAE) system with three non-linear first order ordinary differential equations (ODEs) (18), (19) and (21) plus two algebraic equations (20) and (22). The independent variable, z, is the axial coordinate measured over the central line of the convection column starting at the source. It represents the *height over the stack*. The rest of the variables (a, w, p, ρ, T) are unknown functions of z to be determined. They represent the mean *radius*, the mean *axial velocity*, the mean *pressure*, the mean *density* and the mean *temperature* of the convection column respectively. It should be noted that the atmospheric magnitudes are expressed in terms of the true altitude, whereas the plume magnitudes are expressed in terms of the height over the stack, hence $h = h_0 + z$ is required.

Special mention should be given to three *additional hypothesis* about the specific heat capacity at constant pressure and the gas constant:

1. With an acceptable error of about 5% it can be assumed that $c_p \approx c_{p_\infty}$ [2].
2. Due to the *moderated* entrainment of air into the plume from its local environment, it seems reasonable to assume that the effective c_p in the plume is slightly higher than c_{p_∞} [8], however it is assumed that $R \approx R_\infty$.
3. In addition, due to the slower variation rate with temperature of c_p compared to the one of ρ, the c_p is assumed to be a *constant function* of temperature [2].

From now on, the atmospheric specific heat capacity c_{p_∞} will be rewritten as c_p and R_∞ as R.

By coupling system (1)–(3) with system (18)–(22) the following uncoupled DAE subsystem for the strongly buoyant plumes can finally be written as:

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w a^2) = 2a\,\alpha\sqrt{\frac{\rho}{\rho_\infty}}\,w\rho_\infty \tag{23}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}(\rho w^2 a^2) = -g a^2\,(\rho - \rho_\infty) \tag{24}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}[\rho w a^2\, c_p\,(T - T_\infty)] = -\rho w a^2\,(c_p \frac{\mathrm{d}T_\infty}{\mathrm{d}z} + g) \tag{25}$$

$$\rho T = \rho_\infty T_\infty \tag{26}$$

where the atmospheric magnitudes should be understood as known functions of h such that $h = h_0 + z$; where z is the independent variable and (a, w, ρ, T) are the dependent variables. To properly solve this DAE system three *initial conditions* (at $z = 0\,\mathrm{m}$) for either (a, w, ρ) or (a, w, T) must be specified such that the algebraic constraint (26) is satisfied.

5 Results

The simulation of both models has been carried out with the following given data for three *stable stratified environments* characterized by three atmospheric temperature gradients:

- Universal constants:
  - Acceleration due to gravity: $g = 9.81\,\mathrm{m\,s^{-2}}$
  - Entrainment constant: $\alpha \approx 0.116$
- Atmospheric constants:
  - $R = 287.05\,\mathrm{J\,kg^{-1}\,K^{-1}}$
  - $p_\infty(0) = 101\,325\,\mathrm{Pa}$
  - $\rho_\infty(0) = 1.225\,\mathrm{kg\,m^{-3}}$
  - $T_\infty(0) = 288.15\,\mathrm{K}$
  - Three atmospheric types:
    * Inversion: $k = -0.0045\,\mathrm{K\,m^{-1}}$
    * Standard (ISA): $k = 0.0065\,\mathrm{K\,m^{-1}}$
    * Neutral: $k = \frac{g}{c_p}$

Validation of the models would require comparison with experimental data. However, we are not aware of real measured data associated with flue gas and gas flare stacks ejecting gases in a dry calm environment.

5.1 Results for the Flue Gas Plume

The true altitude of the projected flue gas stack's exit is $h_0 = 83\,\mathrm{m}$. The specific heat capacity at constant pressure used is the one of air: $c_p = 1\,000\,\mathrm{J\,kg^{-1}\,K^{-1}}$.

With the data from the projected PDH plant it was possible to approximate the initial conditions for the flue gas stack as:

$$b(z{=}0\,\mathrm{m}) = 1.5\,\mathrm{m}$$
$$u(z{=}0\,\mathrm{m}) \approx 15.1\,\mathrm{m\,s^{-1}}$$
$$T(z{=}0\,\mathrm{m}) \approx 460.7\,\mathrm{K}$$

The simulation results related to this case are shown in Figures 1, 3 and 2. It can clearly be seen in Figure 1, that in an environment with a thermal inversion (the most stable case) this plume stratifies at around 300 m over the stack's exit. On the other hand, for a neutrally stable environment the plume does not stratify at all.

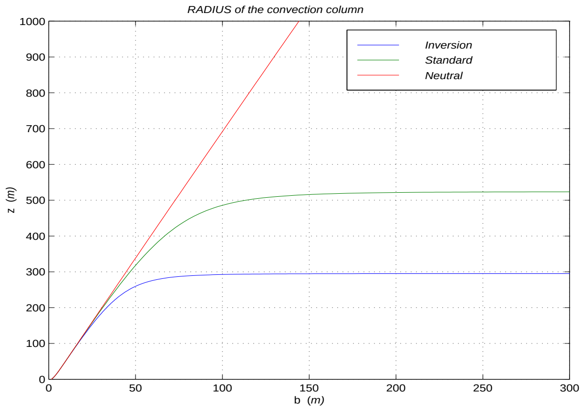

Figure 1. *Radius* of the convection column generated by the *flue gas stack* for each of the three atmospheric types.

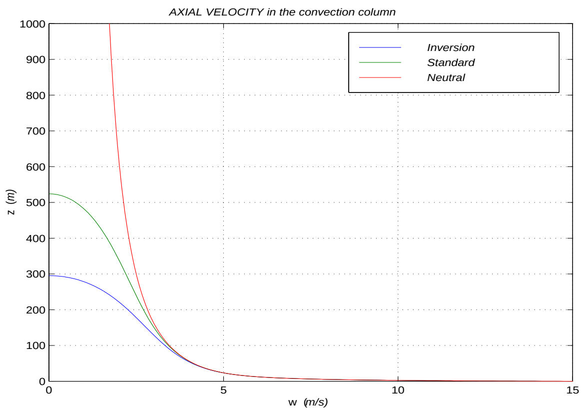

Figure 2. *Axial velocity* in the convection column generated by the *flue gas stack* for the three atmospheric types.

5.2 Results for the Gas Flare Plume

The true altitude of the projected gas flare stack's exit is $h_0 = 153\,\mathrm{m}$. The specific heat capacity at constant pressure used is slightly larger than the one of air: $c_p \approx 1\,200\,\mathrm{J\,kg^{-1}\,K^{-1}}$.

With the data from the projected PDH plant it was possible to approximate the initial conditions for the gas flare stack as:

$$a(z=0\,\mathrm{m}) = 1\,\mathrm{m}$$
$$u(z=0\,\mathrm{m}) \approx 22\,\mathrm{m\,s^{-1}}$$
$$T(z=0\,\mathrm{m}) \approx 1\,800\,\mathrm{K}$$

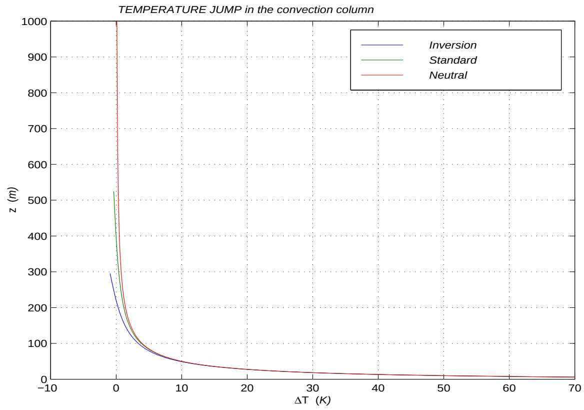

Figure 3. *Temperature jump* between the convection column generated by the *flue gas stack* and the environment for each of the three atmospheric types.

It should be noted that the temperature was unknown, thus a typical adiabatic flame temperature [9] for the propane/propylene was chosen.

The simulation results related to this case are shown in Figures 4, 6 and 5. It can clearly be seen in Figure 4, that in an environment with a thermal inversion (the most stable case) this plume stratifies at around 350 m over the stack's exit. On the other hand, for a neutrally stable environment the plume does not stratify at all.

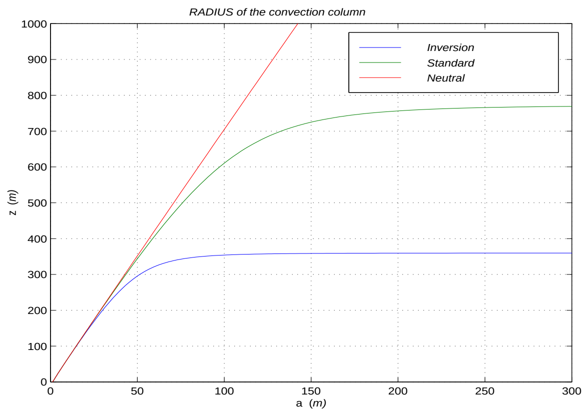

Figure 4. *Radius* of the convection column generated by the *gas flare stack* for each of the three atmospheric types.

6 Conclusion

The classical model of a weakly buoyant plume in a dry calm environment has been reformulated as for a non-Boussinesq buoyant plume; this contrasts with the traditional approach which assumes the *Boussinesq approximation*. The traditional constant entrainment function for this model has been used. Due to the moderated high temperatures associated to this weak buoyancy model, no consideration for thermal radiation has been given.

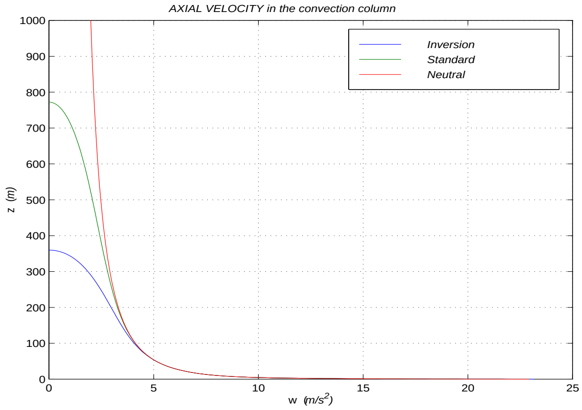

Figure 5. *Axial velocity* in the convection column generated by the *gas flare stack* for the three atmospheric types.

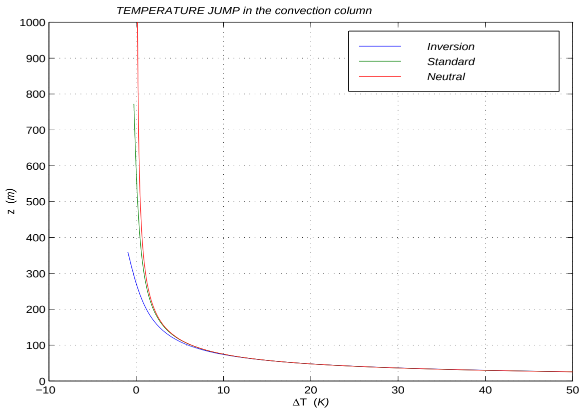

Figure 6. *Temperature jump* between the convection column generated by the *gas flare stack* and the environment for each of the three atmospheric types.

The classical model of a strongly buoyant plume in a dry calm environment has been reformulated as for a non-Boussinesq buoyant plume. The traditional variable entrainment function for this model has been used. Due to the extreme high temperatures associated to this strong buoyancy model, consideration for thermal radiation should be given. However, due to the *conservative approach* of this work it has not been taken into account.

It has been shown that both models may be developed following a similar pattern.

A simulation of the aero-thermodynamical effects produced by the plumes that come out from flue and flare stacks in a dry calm stably stratified environment has been carried out. For this simulation, real world data has been used. Validation of these models would require comparisons with experimental data. However, we are not aware of its existence.

These are simple mathematical models, nevertheless physically useful. Earlier papers are biased towards the analytical simplifications leading to less compact and widely diversified models. Many of these traditional assumptions might be computationally unnecessary. The revision of the classic extensions related to these models —including effects such as *moist calm environment* or *thermal radiation*— is the subject of future work.

Acknowledgements

I would like to thank Prof. Amable Liñan Martínez for his kind patience in explaining to me many of the details and steps needed to understand the derivation of the models. His insight has opened doors for future improvement. Last but not least, I would also like to thank Prof. Ignacio Parra Fabián for inviting me to solve this problem, without him I would not have done this.

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