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TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion Part 1. Mathematical basis and physical assumptions

R.K.S. Hankin [a,1], R.E. Britter [b,*]

[a] Health and Safety Laboratory, Harpur Hill, Buxton, Derbyshire SK17 9JN, UK
[b] Cambridge University Engineering Department, Trumpington Street, Cambridge CB2 1PQ, UK

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Abstract

The Major Hazard Assessment Unit of the Health and Safety Executive (HSE) provides advice to local planning authorities on land use planning in the vicinity of major hazard sites. For sites with the potential for large scale releases of toxic heavy gases such as chlorine this advice is based on risk levels and is informed by use of the computerised risk assessment tool RISKAT [C. Nussey, M. Pantony, R. Smallwood, HSE's risk assessment tool RISKAT, Major Hazards: Onshore and Offshore, October, 1992]. At present RISKAT uses consequence models for heavy gas dispersion that assume flat terrain. This paper is the first part of a three part paper. Part 1 describes the mathematical basis of TWODEE, the Health and Safety Laboratory's shallow layer model for heavy gas dispersion. The shallow layer approach used by TWODEE is a compromise between the complexity of CFD models and the simpler integral models. Motivated by the low aspect ratio of typical heavy gas clouds, shallow layer models use depth-averaged variables to describe the flow behaviour. This approach is particularly well suited to assess the effect of complex terrain because the downslope buoyancy force is easily included. Entrainment may be incorporated into a shallow layer model by the use of empirical formulae. Part 2 of this paper presents the numerical scheme used to solve the TWODEE mathematical model, and validated against theoretical results. Part 3 compares the results of the TWODEE model with the experimental results taken at Thorney Island [J. McQuaid, B. Roebuck, The dispersion of heavier-than-air gas from a fenced enclosure. Final report to the US Coast Guard on contract with the Health and Safety Executive, Technical Report

* Corresponding author.
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1. Introduction

Society benefits considerably from large scale industrial processes. However, these activities can have undesirable side effects which must be adequately controlled. The motivation for this work is risk assessment.

The purpose of risk assessment is to determine the probabilities and consequences of certain undesirable events, and to judge their acceptability to society. Attention usually focuses on quantifying the human suffering or death caused by a specific activity. As large-scale chemical installations have the potential to release large quantities of harmful substances, risk assessment is frequently used to assess the acceptability of such installations.

The Major Hazard Assessment Unit of the Health and Safety Executive (HSE) provides advice to local planning authorities on land use planning in the vicinity of major hazard sites. For sites with the potential for large-scale releases of toxic heavy gases such as chlorine, this advice is based on risk levels and informed by use of the computerised risk assessment tool RISKAT [1]. At present RISKAT uses consequence models for heavy gas dispersion that assume flat terrain. HSE is funding research into heavy gas dispersion over complex terrain and slopes using CFD, shallow layer, and integral models.

The shallow layer approach used by TWODEE is a compromise between the complexity of CFD models and the simpler integral models. [2] Motivated by the low aspect ratio of typical heavy gas clouds, shallow layer models use depth-averaged variables to describe the flow behaviour. This approach is particularly well suited to assess the effect of complex terrain because the downslope buoyancy force is easily included.

Accidentally released gases are often denser than air [3]. This may be due to the high molecular mass of the substance, its low temperature, the formation of an aerosol, or the presence of condensed water vapour. Chemical reactions of the released gas with ambient air may also be significant. This paper will address the problem of the dispersion of heavy gas in the context of risk assessment but considers only inert, monophase, isothermal releases; the possibility of including thermodynamic and chemical effects is discussed below.

Such a heavy gas cloud (i.e., one that is denser than air) will remain closer to the ground than a comparable passive cloud [3], and so the amount inhaled is likely to be

[2] An integral, or 'box', model is one that uses only ordinary (and not partial) differential equations. If the model simulates a continuous release, then the independent variable is typically downwind distance; models for instantaneous releases typically use time.

larger for a heavy gas cloud than an equivalent passive one, increasing the risk to the public.

This tendency to form a low-lying configuration suggests a method of modelling known as shallow layer. A shallow *water* model is a particular type of shallow layer model that solves the shallow water equations [4]. Formally, a shallow layer model describes the cloud as a function of time and (two-dimensional) ground position. At any position and time, the cloud is characterized by four variables: cloud depth, two components of velocity, and cloud concentration. Real clouds do not have an exact depth as they have no definite upper surface and so cloud depth has to be defined in terms of the vertical concentration distribution. The other variables are averaged, in a sense to be made precise, over the depth of the cloud. The shallow layer variables are thus often referred to as depth-averaged.

Shallow layer models lend themselves particularly well to the adoption of the shallow water approximations. The shallow water approximations state that the pressure distribution is hydrostatic within the main body of the cloud; dispensation is usually made for the special processes occurring at the leading edge.

Many workers have called for a shallow layer model to be developed; at least six review articles [3,5–9] specifically state that shallow layer models have been comparatively neglected and would be appropriate for the prediction of heavy gas dispersion, particularly when complex terrain is considered. The advent of cheaper computational power has made this practical.

1.1. Thermal effects in TWODEE

Many dense gas releases of industrial interest involve thermodynamic processes such as condensation, and the low temperature of the cloud may contribute to its negative buoyancy. These effects are not included in TWODEE at present, but further work could account for them. A practical approach would be to reformulate TWODEE in terms of conserved variables that would include mass of contaminant gas, mass of water and air, and enthalpy. Assuming the system to be in homogeneous equilibrium [10] would be reasonable, although some further work would be required to specify vertical distribution of temperature and the different phases present [11]. The TWODEE solver described in part 2 of this paper would have no difficulty with this.

2. Heavy gas dispersion and depth averaged quantities

Heavy gas clouds do not have a uniform vertical distribution of either density or velocity. In general, density ρ, and the two horizontal components of velocity u and v will be functions of altitude z. Depth averaged values of these quantities must therefore be defined in terms of their vertical distributions.

The shallow water equations will be developed and then generalized to account for hydraulic jumps, surface stress, and the effects of non-uniform vertical density profiles caused by entrainment of ambient fluid.

2.1. The shallow water equations

Many fluid systems are composed of a layer of dense fluid under an expanse of lighter fluid, and if typical depth scales are small compared to typical horizontal scales the fluid is known as shallow. This section will begin with a statement of the shallow water equations and will progress to the full case of the generalized shallow water equations over non-uniform terrain. In all of the following, the Reynolds number will be assumed to be sufficiently high for the effects of a small change of kinematic viscosity to be immaterial.

If fluid of constant density ρ and depth $h=h(x,y,t)$ moves with velocity $\boldsymbol{u}(x,y,t)=(u,v)$ over a rigid horizontal surface and under ambient fluid of density ρ_a, the equations of motion are well-known [12]. If surface stresses are neglected they are:

$$\frac{\partial h}{\partial t}+\frac{\partial hu}{\partial x}+\frac{\partial hv}{\partial y}=0 \tag{1}$$

$$\frac{\partial h\rho u}{\partial t}+\frac{\partial h\rho u^2}{\partial x}+\frac{\partial h\rho uv}{\partial y}+\frac{\partial}{\partial x}\left(\frac{1}{2}g(\rho-\rho_a)h^2\right)=0 \tag{2}$$

$$\frac{\partial h\rho v}{\partial t}+\frac{\partial h\rho uv}{\partial x}+\frac{\partial h\rho v^2}{\partial y}+\frac{\partial}{\partial y}\left(\frac{1}{2}g(\rho-\rho_a)h^2\right)=0. \tag{3}$$

Eq. (1) expresses conservation of volume of dense fluid (or mass, as the density is constant); Eqs. (2) and (3) are the vertically integrated Euler equations under the assumption of a hydrostatic pressure distribution. An extra equation is required (expressing conservation of mass) if the density ρ is also allowed to be a function of space and time:

$$\frac{\partial h\rho}{\partial t}+\frac{\partial h\rho u}{\partial x}+\frac{\partial h\rho v}{\partial y}=0. \tag{4}$$

Note that Eqs. (2) and (3) are still true when the restriction of constant ρ is relaxed. Eqs. (1)–(4) will be referred to as the shallow water equations.

2.2. The shallow water equations with entrainment

Eqs. (1)–(4) may easily be modified to account for entrainment of the ambient fluid. This was done by Wheatley and Webber [12], although the approach used here differs slightly.

The right hand sides of Eqs. (1)–(4) must account for the volume, mass, and momentum of the entrained fluid. If the entrainment rate is u_{ent}, which may be a function of time and space, the shallow water equations for an entraining system are

$$\frac{\partial h}{\partial t}+\frac{\partial hu}{\partial x}+\frac{\partial hv}{\partial y}=u_{ent} \tag{5}$$

$$\frac{\partial h\rho}{\partial t}+\frac{\partial h\rho u}{\partial x}+\frac{\partial h\rho v}{\partial y}=u_{ent}\,\rho_a \tag{6}$$

$$\frac{\partial h\rho u}{\partial t}+\frac{\partial h\rho u^2}{\partial x}+\frac{\partial h\rho uv}{\partial y}+\frac{\partial}{\partial x}\left(\frac{1}{2}g(\rho-\rho_a)h^2\right)=u_{ent}\,\rho_a\boldsymbol{u}_a \tag{7}$$

$$\frac{\partial h\rho v}{\partial t}+\frac{\partial h\rho uv}{\partial x}+\frac{\partial h\rho v^2}{\partial y}+\frac{\partial}{\partial y}\left(\frac{1}{2}g(\rho-\rho_a)h^2\right)=u_{ent}\,\rho_a v_a, \tag{8}$$

where $\boldsymbol{u}_a=(u_a, v_a)$ is the velocity of the ambient fluid. Expressions for u_{ent} will be given below.

2.3. Turbulent stress

The equations above apply to a layer with uniform vertical profiles. In such a layer, it is clear that the velocity of fluid in a dense layer varies from the shallow layer velocity [3] by a fluctuating amount, due to the turbulent nature of the flow. These fluctuations are potentially important in hydraulic jumps as turbulent stresses may be generated. Several workers [13–15] consider such stresses in the context of tidal flow fields in estuaries. Although the turbulence in tidal flows is different from that in density currents (stable density gradients are generally absent in these flows), it is reasonable to adopt a similar term to model the turbulent shear stress, possibly with different constants. Note that the shape parameter S_1 (Eq. (17)) is not included in this analysis.

If the dense layer moves with depth averaged velocity $\boldsymbol{u}=(u, v)$, the result of turbulent shear stress is to exert a force $\boldsymbol{V}=(V_x, V_y)$ per unit area on the dense fluid, where $\boldsymbol{V}=\zeta h\rho\nabla(\lambda\nabla\boldsymbol{u})$. Here ζ is a small constant of proportionality and λ is a quantity that measures turbulent interaction between adjacent fluid elements. Dimensionally, λ must be of the form m^2/s in SI and a common choice is $\lambda=h|\boldsymbol{u}|$; this is used in TWODEE.

The effects of a non-zero ζ are mostly apparent at hydraulic jumps because only there do the second derivatives used to calculate $\boldsymbol{V}$ become large. Hydraulic jumps were anticipated in heavy gas dispersion by Webber et al. [16] (although this study was confined to the non-entraining case) and must therefore be simulated accurately. Turbulent shear does not strongly affect the leading edge under the depth-averaged approach adopted here [4].

Typical heavy gas releases travel over rough ground, and it is clear that a drag on the dense layer will be exerted. Although the surface shear stress is a function of the stratification of the dense layer as reported by Kantha et al. [17], this effect will be ignored.

The shallow water approximations require a hydrostatic pressure distribution within the dense layer. It is clear that any fluid with significant vertical Lagrangian acceleration will invalidate this approximation. As system-averaged vertical accelerations are $\sim g'(h/L)^2$, where L is the horizontal length scale, [4] the hydrostatic approximation is well

[3] Shallow layer variables are implicitly averaged on the timescale for a particle to move from the top of the layer to the bottom; because velocities are $\mathcal{O}(g'h)^{1/2}$, this timescale is $h/(g'h)^{1/2}=(h/g')^{1/2}$.

[4] Typical velocities are $\sim(g'h)^{1/2}$; the vertical component will be $\sim(g'h)^{1/2}(h/L)$ if $h/L\leq 1$; transport timescales are $\sim L/(g'h)^{1/2}$ and thus vertical accelerations will be $\sim g'(h/L)^2$.

suited to systems of low aspect ratio, as here. However, vertical acceleration occurs at dense flow phenomena such as leading edges or hydraulic jumps. It is well known [18,19] that it is important to simulate these features accurately as they may exert a profound effect on the overall structure of the flow.

The surface shear stress τ at the ground is taken to be $\tau = 1/2 \rho C_D \boldsymbol{u}|\boldsymbol{u}|$, where C_D is a skin friction coefficient which depends on ground roughness. In TWODEE, C_D may be a function of position, thus allowing some account of the effect of surface roughness variations to be made.

2.4. Depth averaging in heavy gas dispersion

Extension of Eqs. (5)–(8) to cases with nonuniform vertical profiles is now carried out. Full details are given by Hankin [4].

When considering dense flows whose vertical structure may be ignored, four quantities are needed for shallow water modelling. These are: the depth-averaged density $\bar{\rho}$; two components of depth averaged velocity, $\bar{u}$ and $\bar{v}$; and the depth of the layer, h. The approach adopted in TWODEE is to define the four depth averaged quantities in such a way as to make the treatment of buoyancy simple. The buoyancy b per unit volume of fluid of density ρ is $g(\rho - \rho_a)$; and it is the case that the continuity equation $\partial b/\partial t + \nabla(b\boldsymbol{u}) = 0$ is satisfied in a uniform gravitational field.

With these comments in mind, it is convenient to use the following relations for *definition* of the four depth averaged quantities h, $\bar{\rho}$, $\bar{u}$, and $\bar{v}$:

$$h(\bar{\rho} - \rho_a) = \int_{z=0}^{\infty} (\rho(z) - \rho_a) \mathrm{d}z \tag{9}$$

$$h(\bar{\rho} - \rho_a)\bar{u} = \int_{z=0}^{\infty} (\rho(z) - \rho_a) u(z) \mathrm{d}z \tag{10}$$

$$h(\bar{\rho} - \rho_a)\bar{v} = \int_{z=0}^{\infty} (\rho(z) - \rho_a) v(z) \mathrm{d}z \tag{11}$$

where $\rho = \rho(z)$ is the density of the layer at height z, and $u(z)$, $v(z)$ are the two horizontal components of velocity. This set of definitions requires another relation to close the system. The definitions used in TWODEE are partially in response to risk assessors who require a definition of cloud height h related in a simple and direct way to the vertical density profile. The definition for h that will be used is that h is the height below which some fraction α of the buoyancy is located: [5]

$$\int_{z=0}^{h} (\rho(z) - \rho_a) \mathrm{d}z = \alpha \int_{z=0}^{\infty} (\rho(z) - \rho_a) \mathrm{d}z. \tag{12}$$

The choice of α is clearly arbitrary, but necessary. Useful values for α might be 0.90 or 0.95. Note that $\alpha = 1$ is not always meaningful if the vertical distribution has no upper limit, as for $\rho(z) = \rho_a + \rho_0 \exp(z/h)$.

[5] A good alternative is to define $1/2(\bar{\rho}\text{-}\rho_a)h^2 = \int_{z=0}^{\infty} (\rho(z) - \rho_a) z \,\mathrm{d}z$. However, such a definition is not well-defined for many vertical distributions such as $\rho(z) = \rho_a + \rho_0 (z/h_0)^2$; and this approach makes it difficult to state precisely the approximations inherent in shallow water equations [4].

2.4.1. The generalized shallow water equations with groundslope

Because the shallow water Eqs. (5)–(8) include nonlinear terms, the quantities defined in Eqs. (9)–(11) (together with Eq. (12)) may not be substituted for the uniform-profile variables h, ρ, u and v. However, Hankin [4] argues that it is reasonable to do so provided certain, generally reasonable, caveats are made. If the ground elevation is $e = e(x,y)$, entrainment rate is u_{ent}, and the ambient fluid moves at speed $\boldsymbol{u}_a = (u_a, v_a)$, then:

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} + \frac{\partial h\bar{v}}{\partial y} = u_{ent} \tag{13}$$

$$\frac{\partial h(\bar{\rho} - \rho_a)}{\partial t} + \frac{\partial h(\bar{\rho} - \rho_a)\bar{u}}{\partial x} + \frac{\partial h(\bar{\rho} - \rho_a)\bar{v}}{\partial y} = 0 \tag{14}$$

$$\frac{\partial h\bar{\rho}\bar{u}}{\partial t} + \frac{\partial h\bar{\rho}\bar{u}^2}{\partial x} + \frac{\partial h\bar{\rho}\bar{u}\bar{v}}{\partial y} + S_1\frac{\partial \frac{1}{2} g(\bar{\rho} - \rho_a)h^2}{\partial x} + S_1 g(\bar{\rho} - \rho_a)h\frac{\partial e}{\partial x} = u_{ent}\,\rho_a u_a \tag{15}$$

$$\frac{\partial h\bar{\rho}\bar{v}}{\partial t} + \frac{\partial h\bar{\rho}\bar{u}\bar{v}}{\partial x} + \frac{\partial h\bar{\rho}\bar{v}^2}{\partial y} + S_1\frac{\partial \frac{1}{2} g(\bar{\rho} - \rho_a)h^2}{\partial y} + S_1 g(\bar{\rho} - \rho_a)h\frac{\partial e}{\partial y} = u_{ent}\,\rho_a v_a. \tag{16}$$

Here, S_1 is a shape parameter defined as

$$\int_{z=0}^{h} g[\rho(z) - \rho_a]z\,dz + h\int_{z=h}^{\infty} g(\rho(z) - \rho_a)dz = S_1\frac{1}{2}gh^2(\bar{\rho} - \rho_a). \tag{17}$$

This definition for S_1 ensures that momentum Eqs. (15) and (16) include the hydrostatic force acting on an infinitesimal fluid element of height h. Note that S_1 as determined from Eq. (17) agrees closely with the value determined from $1/2(\bar{\rho} - \rho_a)h^2 = \int_{z=0}^{\infty} (\rho(z) - \rho_a)z\,dz$ [20] if α is close to 1.

3. The shallow water equations and heavy gas dispersion

This section discusses how the shallow water equations discussed above may be altered to account for the interaction between the dense layer and the ambient fluid. Because the densities of the two fluids are similar, the ambient fluid may influence the behaviour of the dense layer significantly.

3.1. Bores and hydraulic jumps

In shallow water flow, a bore is a near-discontinuity in fluid depth that moves in the same direction as the deeper fluid.

A bore is equivalent to a hydraulic jump for the case when the density of the upper fluid ρ_a is small compared to that of the lower, ρ; a bore is a hydraulic jump moving with respect to the coordinate system chosen. The equivalence is lost if $\rho \gg \rho_a$, as then the upper fluid, if moving relative to the jump, may exert a significant net force on the fluid of the jump by virtue of its velocity.

It is convenient to define a hydraulic jump as a special case of a bore in which the relative speed of jump and upper fluid is zero. A leading edge is thus a special case of a bore in which the upstream fluid depth is zero.

Such flow features are particularly important to shallow water flow. The leading edge, in particular, may control the flow behind it and thus may exert an important effect on the global flow structure; also, bores may control regions of the flow, as reported by Wood and Simpson [21].

A unified method by which both these phenomena may be simulated in a shallow water model is presented below.

3.2. The effect of the ambient fluid on a dense layer

The shallow water equations as developed above assume that the ambient fluid has a pressure distribution that is hydrostatic. It is clear that this is not true for the ambient fluid close to a leading edge, as this fluid undergoes considerable acceleration as it is displaced by the oncoming dense current.

A gravity current such as a heavy gas release may be modelled as a shallow water flow, with additional terms that are applied close to the leading edge. These additional terms encompass the strong interaction between dense fluid of the leading edge and the ambient fluid. For the purposes of identifying closeness to the leading edge, a 'front parameter' will be defined that is large close to a leading edge and small everywhere else. These comments may apply equally to a bore as a bore can control the flow behind it [21].

3.3. The leading edge in a two-dimensional gravity current

Fig. 1 shows a schematic cross-section of a gravity current advancing along a horizontal lower boundary into an expanse of lighter fluid. This type of flow is known as two-dimensional as the vertical structure is also important. The depth averaged density of the current is ρ and that of the ambient fluid ρ_a. The leading edge is viewed in a coordinate system that brings it to rest. Motion will be assumed to be steady, following Britter and Simpson [22].

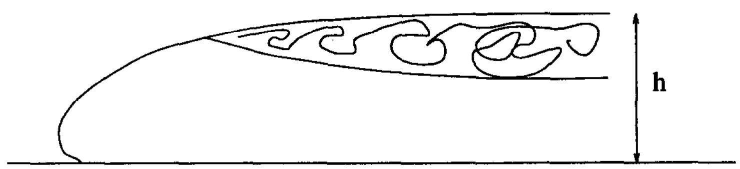

Fig. 1. Schematic view of gravity a one-dimensional gravity current.

The velocity U_f of the gravity current is determined by the quantities ρ, ρ_a, h, and g; thus $U_f = f(\rho, \rho_a, h, g)$. Introduction of the Boussinesq approximation reduces the independent variables to h and the reduced gravity $g' = g(\rho - \rho_a)/\rho_a$. A simple dimensional analysis [23] shows that the densimetric Froude number $\mathrm{Fr} = U_f/\sqrt{g'h}$ is constant; several workers [16,18,19,24] have carried out simulations on the supposition of constant densimetric front Froude numbers, and this work follows those cited.

A slight rearrangement of the equation expressing the fact that the densimetric front Froude number is constant gives

$$\frac{1}{2} S_1 g(\rho - \rho_a) h^2 = kh\rho_a (U_f)^2, \tag{18}$$

where S_1 is the shape parameter introduced on page 8, and k is another constant.

The generalized shallow water equations do not simulate the behaviour of a gravity current, because they predict that a net force acts on the dense fluid of the leading edge, thereby accelerating it. This is clearly not the case, as gravity currents such as illustrated in Fig. 1 advance at a constant speed over level ground, if the buoyancy flux at the head is constant.

The shallow water equations give erroneous results for the leading edge of a dense layer as they assume that the pressure distribution at $z = h$ is hydrostatic; this is untrue in the vicinity of a leading edge as the ambient fluid has a stagnation point close to the frontmost part of the head. The pressure there thus exceeds that far upstream at the same level by $1/2 \rho_a U_f^2$.

Eq. (18) suggests a simple method by which the leading edge of a gravity current may control the following flow in a depth-averaged model.

(1) The shallow water equations will be applied to the whole of the dense layer, including the leading edge where they are not applicable. The shallow water equations predict that a net force is exerted on the fluid of the leading edge whose magnitude per unit width is the left hand side of Eq. (18).

(2) A force equal to the right hand side of Eq. (18) per unit width will be applied to the fluid of the leading edge, accounting for the non-hydrostatic pressure distribution found at $z = h$.

The result of steps 1 and 2 above is to simulate the leading edge insofar as it controls the following flow, although the detailed structure of the leading edge is not simulated. This must be the case as the shallow water approximations are violated in this region.

Forces of the same form as the right-hand-side of Eq. (18) are commonly encountered when considering the form drag exerted on bluff bodies moving through a fluid [25]. Rearranging Eq. (18) gives

$$k = 2/(S_1 \mathrm{Fr}^2). \tag{19}$$

This relation furnishes (by virtue of defining k) a method for simulating shallow water flow with a leading edge moving at a fixed front Froude number.

The force corresponding to the right hand side of Eq. (18) affects the dense layer at the leading edge. However, this force acts upon an extended region of the dense layer and methods of accounting for this force are discussed below.

Because shock-smearing techniques are constrained to use only shallow water variables (that is, the depth, density, and speed of the flow) some way must be found to distribute the force $F = k\rho_a h(U_f)^2$ amongst the dense fluid 'near' the front and this is done by isolating a parameter P of the flow which is large near the front and small everywhere else. The resisting force F may then be applied to the fluid in proportion to P and as long as $\int_{x=0}^{\infty} P\,dx = F$, the total resistive force applied will be as indicated in Eq. (18). This scheme allows the simulation of a gravity current front moving at a constant front Froude number.

3.4. Choice of P

The choice of P will have to account for both leading edges and hydraulic jumps. Also, to preserve the shallow water equations' accuracy, P must be small everywhere except close to a leading edge or a bore.

There is only one simple choice of P that is Galilean invariant, and correctly predicts the force exerted by moving ambient fluid on a dense layer for both leading edges and hydraulic jumps. This is

$$P = -k\rho_a\left[\frac{\partial h(u-u_a)}{\partial t} + u_a\frac{\partial h(u-u_a)}{\partial x}\right]. \tag{20}$$

One interpretation of P is the volume rate of displacement of ambient fluid per unit area per unit width, as measured by an observer at rest relative to the ambient fluid. In two dimensions, the front parameter P becomes the vector quantity $\boldsymbol{P}$, where

$$\boldsymbol{P} = -k\rho_a\left[\frac{\partial[h(\boldsymbol{u}-\boldsymbol{u}_a)]}{\partial t} + (\boldsymbol{u}_a\nabla)[h(\boldsymbol{u}-\boldsymbol{u}_a)]\right]. \tag{21}$$

This formula for the front resistance per unit area is the one used by TWODEE. The resisted shallow water equations in two dimensions become

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} + \frac{\partial h\bar{v}}{\partial y} = u_{\text{ent}} \tag{22}$$

$$\frac{\partial h(\bar{\rho}-\rho_a)}{\partial t} + \frac{\partial h(\bar{\rho}-\rho_a)\bar{u}}{\partial x} + \frac{\partial h(\bar{\rho}-\rho_a)\bar{v}}{\partial y} = 0 \tag{23}$$

$$\frac{\partial h\bar{\rho}\bar{u}}{\partial t} + \frac{\partial h\bar{\rho}\bar{u}^2}{\partial x} + \frac{\partial h\bar{\rho}\bar{u}\bar{v}}{\partial y} + S_1\frac{\partial\frac{1}{2}g(\bar{\rho}-\rho_a)h^2}{\partial x} + S_1 g(\bar{\rho}-\rho_a)h\frac{\partial e}{\partial x}$$
$$+\frac{1}{2}\bar{\rho}C_D\bar{u}|\bar{\mathbf{u}}| + V_x + k\rho_a\left[\frac{\partial}{\partial t} + u_a\frac{\partial}{\partial x} + v_a\frac{\partial}{\partial y}\right]h(\bar{u}-u_a) = u_{\text{ent}}\,\rho_a u_a \tag{24}$$

$$\frac{\partial h\bar{\rho}\bar{v}}{\partial t}+\frac{\partial h\bar{\rho}\bar{u}\bar{v}}{\partial x}+\frac{\partial h\bar{\rho}\bar{v}^2}{\partial y}+S_1\frac{\partial\frac{1}{2}g(\bar{\rho}-\rho_a)h^2}{\partial y}+S_1 g(\bar{\rho}-\rho_a)h\frac{\partial e}{\partial y}$$
$$+\frac{1}{2}\bar{\rho}C_D\bar{v}|\bar{\mathbf{u}}|+V_y+k\rho_a\left[\frac{\partial}{\partial t}+u_a\frac{\partial}{\partial x}+v_a\frac{\partial}{\partial y}\right]h(\bar{v}-v_a)=u_{ent}\,\rho_a v_a, \qquad (25)$$

where all variables are as previously described. Eqs. (22)–(25) are the mathematical basis of the TWODEE model.

4. Entrainment in a shallow layer model

Eqs. (22)–(25) use u_{ent} as the entrainment velocity. The approach adopted here is to use empirical formulations for u_{ent} and these are discussed below.

Although not directly applicable to the shallow layer models, ambient fluid entrainment as implemented by integral models has some desirable features that inspired the present approach.

4.1. Edge entrainment in a shallow water model

Although the terms edge and top entrainment are suggestive of entrainment through the cloud edge and top (as depicted by integral models), this twofold characterization cannot provide any direct insight into where the entrainment actually takes place. Wheatley and Webber [12] consider this and state that

> The edge entrainment term does not necessarily correspond to entrainment through the edge... it may occur over the whole top area of the cloud.

It is clearly necessary to address this problem in TWODEE, as the density is here allowed to vary over the extent of the cloud. Integral models implicitly assume edge entrainment occurs over the whole of the cloud, as the frontal speed is independent of the edge entrainment rate. Characterization of edge entrainment as entrainment that occurs close to the leading edge is thus not necessarily consistent.

With the more sophisticated simulation allowed by a shallow layer approach, entrained air may be incorporated into the heavy gas cloud at a precisely controlled location. Hankin [4] considered several plausible methods of generalizing the concept of edge entrainment as used in integral models to shallow layer models. The conclusion was that edge entrainment was inconsistent with a shallow layer model. [6]

Not all integral models use edge entrainment: the default parameters of the DENZ model [26] set edge entrainment terms to zero. Following this and other models, TWODEE has zero edge entrainment. This approach is not inconsistent with the work of Brighton

[6] For example, consider a simulation in which ambient fluid entrained via edge entrainment was entrained at the point of entrainment (the cloud edge). Such a simulation becomes unstable because positive feedback between leading edge speed and entrainment results in leading edges of very low concentration moving at unrealistically high speeds.

[27], in which top entrainment was shown to be the dominant mechanism; TWODEE top entrainment is most pronounced at the leading edge because the largest shear speeds are found there.

4.2. Top entrainment in a shallow layer

Top entrainment is defined here by analogy with the corresponding terms used in integral models: a volume rate of entrainment that is proportional to the upper surface area of the cloud, and some entrainment velocity that is a function of the local turbulence.

Top entrainment is a process that dilutes the cloud by incorporating eddies of ambient fluid into the body of the cloud. This type of entrainment is driven by three primary sources of turbulent energy: ambient turbulence present in the atmosphere (including any contribution from non-zero w_* [28]); turbulence generated by the shearing motion between air and dense layer; and turbulence generated at the ground by the passage of dense gas across the rough lower boundary of the fluid.

Hankin [4] described some of the previous work that has been done on stratified shear flow in the context of heavy gas dispersion and concluded that a wide range of opinion exists. Fernando, in a review of turbulent mixing in stratified fluids [29], emphasizes the lack of consensus in this field.

The various entrainment formulations developed for integral models are of relevance to TWODEE, but all are necessarily averaged over the extent of the cloud, and not expressible in terms of the shallow water variables at a given point, as is required here. The TWODEE model addresses this problem by using an entrainment formula similar to those used in integral models, but without cloud wide integration.

Motivated by the need to express the rate of entrainment across the top of the cloud, the work of Eidsvik [30] will be used. Eidsvik presented an integral model of heavy gas dispersion with a top entrainment term that was capable of use in a shallow layer model. A brief summary of Eidsvik's entrainment model is given here.

Eidsvik required, as here, a simple model for top entrainment that had only a small number of experimental coefficients. His model incorporated a commonly used [3,31,32] relation

$$w_t = \frac{a}{1 + b\mathrm{Ri}} v \tag{26}$$

where w_t is the top entrainment velocity, a and b experimental coefficients, v a representative velocity scale, and $\mathrm{Ri} = g'h/v^2$ the Richardson number.

Eidsvik noted that as $R_i \to 0$, Eq. (26) reduced to $w_t = av$, which describes the entertainment rate into a passive contaminant in a neutral boundary layer; Tennekes and Lumley [33] discuss the problem of passive dispersion in this context.

The best definition of v, the representative velocity, was argued by Eidsvik to be quadratically weighted sum of the friction velocity $\boldsymbol{u}_*$ and the atmospheric convective velocity $\boldsymbol{w}_*$, and was defined as

$$v^2 = (\alpha_2 \boldsymbol{w}_*)^2 + (\alpha_3 \boldsymbol{u}_*)^2 \tag{27}$$

where α_2 and α_3 are constants. Note that w_* is a property of the atmosphere; TWODEE considers only isothermal releases. Eidsvik was able, because he was working with an integral model, to use a cloud averaged value for v. Here, because of the shallow layer approach, a local value of v must be used. It is logical and convenient to use a weighted quadratic sum for v. It is clear that v, being a representative fluid speed, will have contributions from three distinct sources: (1) internally generated turbulence arising from the shear caused by the cloud having a different velocity from the ambient flow; (2) externally generated turbulence arising from the dense layer moving over the ground; and (3) externally generated turbulence present in the atmospheric boundary layer.

Although these three sources of turbulent kinetic energy contribute to v, the relative importance of each term is not clear and the model follows Eidsvik and others in the use of empirically determined constants. Thus

$$v^2 = k_1^2 u_*^2 + k_2^2 w_*^2 + k_3^2 |\mathbf{u}|^2 + k_4^2 |\mathbf{u} - \mathbf{u}_a|^2,$$

where u is the velocity of the cloud and u_a the ambient flow speed at the height of the cloud; the k_i are dimensionless constants.

Both to maintain consistency with Eidsvik, and to reflect the source of the turbulent energy, the k_i will be rewritten: $k_1 = 1$, $k_2 = \alpha_2$, $k_3 = \alpha_3 \sqrt{1/2(C_D)}$, and $k_4 = \alpha_7$. Combining the above arguments gives

$$v^2 = u_*^2 + (\alpha_2 w_*)^2 + \frac{1}{2} C_D \alpha_3^2 \mathbf{u}^2 + \alpha_7^2 |\mathbf{u} - \mathbf{u}_a|^2. \quad (28)$$

This is used in TWODEE. Both the friction velocity u_* and the ambient air velocity u_a may be obtained either by use of analytical results (such as using a standard logarithmic velocity profile), or by some numerical atmospheric flow field predictor. The latter approach could theoretically account for the complex flow seen near variable terrain such as recirculation zones.

4.3. Values for the free parameters

A brief discussion of the values taken by the free parameters follows. Full details are given by Hankin [4].

Britter [34] states that where Eq. (26) is used, $a = 0.4$ (von Karman's constant) and $b = 0.125$ are used, but note that the Richardson number used here differs from Britter's.

Here, u_* is the friction velocity and $\mathrm{Ri} = g'h/u_*^2$ is the Richardson number. Using von Karman's constant for a is consistent with experiment [34]; this value also has theoretical support [28], as Eq. (26) reduces to $w_t = av$ if $\mathrm{Ri} = 0$. Note that a's dependence on α should be weak [4] if the vertical distribution is exponential.

The exact value of von Karman's constant is uncertain. A range of 0.33 to 0.41 for k is offered by Pasquill and Smith [35]. This work will follow Britter and use $a = 0.4$.

Britter's value of b, 0.125, is discussed in relation to experimental results, in Part 3 of this paper; Britter used a different definition for h and $\bar{\rho}$ than here, but as will be shown, TWODEE is very insensitive to the exact value for this parameter.

The relative importance of a convective atmosphere is given by α_2. This work will follow Eidsvik and use a value of $\alpha_2 = 0.7$.

Ground roughness is measured by α_3 and C_D; this is classed as a peripheral variable by Britter and McQuaid [36]. In calm conditions (such as in the experiments of Schatzmann et al. [37]), the turbulence generated at ground level is comparable to that generated by the upper shear layer of the cloud. A reasonable value for α_3 is 1.3 (following Eidsvik) and this will be used here. The value of C_D may be estimated either from a knowledge of u and u_*, or of local ground characteristics.

The relative importance of shear is given by α_7. Values of $\mathscr{O}(1)$ are indicated and this study will follow Eidsvik and use $\alpha_7 = 1$.

The other free parameters in the model, which are not directly relevant to the top entrainment modelling, are the following.

- α_E, the edge entrainment coefficient. As discussed above, theoretical reasons suggest a value of zero for α_E in TWODEE.
- Fr, the front Froude number. It is convenient and conventional [3,12,18] to take Fr = 1 and this is used here; Britter and Linden [38] show that the front Froude number of a gravity current on a slope is only weakly dependent on slope angle. Although these workers use a different Froude number from that used here, the two definitions are identical on the assumption that buoyancy flux is constant along the current.
- S_1, the hydrostatic dimensionless shape parameter. Following Ellison and Turner [20], $S_1 = 0.5$ will be used.

5. Summary

The shallow water equations have been developed and generalized to include the effects of entrainment and nonuniform vertical profiles. Empirical correlations are required to determine the entrainment rate and a suitable method is presented. A set of standard values has been given.

The mathematical model has now been fully detailed. Part 2 of this paper will describe and use the computational model that implements the mathematical model; and part 3 will present validation against field data from McQuaid and Roebuck [2].

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