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CLOUD: A vapour–aerosol dispersion model accounting for plume 3D motion and heat and mass transfer between phases☆

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Abstract

The CLOUD (concentration levels of unconfined dispersion) code has been developed, the nucleus of which is an innovative two-phase fluid dispersion model characterized by conservation equations for mass, momentum, energy and species, averaged over a volume slice transverse to the direction of plume motion.

The initial and boundary conditions for the above equations are determined either by using auxiliary models or by direct input of the space distribution, and respectively of the time evolution, of the relevant variables. The initial conditions model for an instantaneous, puff release has been based on an experimental programme carried out at the Swiss Federal Institute of Technology. The boundary conditions for semi-continuous, jet releases have been based on literature models for critical two-phase flow at the rupture. The code has been validated with data from three large scale release test series: the Desert Tortoise series (ammonia), the Goldfish series (HF), and the Thorney Island series (heavy gas).

Keywords: Vapour–aerosol dispersion; 3D dispersion model

1. Introduction

Most of the currently available tools for predicting the dispersion of hazardous materials still use, for heavier than air releases, lumped parameter (box) models. On

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the other side there are three-dimensional models, like FEM3 [1], that need long computing times on large computers.

An intermediate approach [2, 3], due originally to Colenbrander, is an extension of the box model, where, instead of a symmetric cloud slumping under gravitational forces and convected with the wind, a true one-dimensional approach is considered.

Another one-dimensional approach, where conservation equations of mass, momentum and energy along the release path are solved, has been developed by Ooms [4] to predict the behavior of a stack plume, in steady-state conditions.

The aim of the CLOUD (concentration levels of unconfined dispersion) model was to generalize and unify the approaches of Colenbrander and Ooms in order to obtain a unified one-dimensional model able to describe all types of release to the atmosphere both in steady-state and in transient conditions as well as two-phase fluids.

2. Conservation equations and closure relationships

A diagram showing a typical plume is shown in Fig. 1. The plume contains a mixture of air, noxious substance and water in more than one phase and is surrounded by the external air. In order to derive a set of one-dimensional conservation equations, the plume is averaged across a cross-sectional slice perpendicular to the plume centerline and the rate of change of a scalar Ψ within this slice is considered. The space coordinate s lies along the plume centerline, which is not fixed in space and time.

The following general conservation equation can be derived for a plume of rectangular cross section of height H and half-width B:

$$\frac{\partial}{\partial t}(BH\langle\rho\Psi\rangle) + \frac{\partial}{\partial s}(BH\langle\rho\Psi(v_s - u_s)\rangle) - \rho_{\text{ext}}\Psi_{\text{ext}}(2B\hat{w} + H\hat{v}) - BH\langle\rho\hat{S}\rangle = 0, \quad (1)$$

where $\hat{v}$ and $\hat{w}$ are, respectively, the horizontal and vertical components of the entrainment velocity.

The following points should be made concerning the application of this equation:
- v_s is the fluid velocity, whose direction is coincident at any point with the centerline direction;
- u_s is the component of the velocity of the points belonging to the centerline along the centerline direction at a given time, and arises because of the moving slice boundaries.

Substituting 1 for Ψ and 0 for $\hat{S}$ the mass conservation equation can be obtained from (1). Similarly, by substituting for Ψ the three Cartesian components of the fluid velocity and including the appropriate source terms, the three momentum conservation equations can be obtained.

Substituting $\Psi = h$, $\Psi = h_\ell x_\ell$ and the appropriate source terms, the total energy and liquid energy conservation equations can be derived, while the species conservation equations can be obtained by substituting $\Psi = m_{ki}x_k$ and the source terms at the external boundary and at the phase interface.

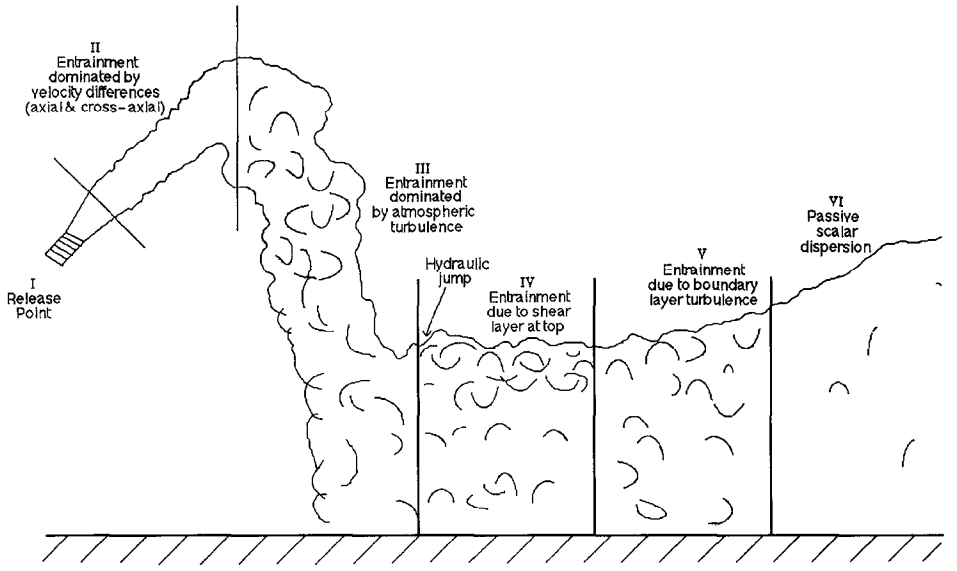

Fig. 1. Sketch of typical plume.

A further differential equation is needed to calculate the side spreading of the ground bounded plume. This is a simple kinematic equation for the total Lagrangian derivative of the half-width B:

$$\frac{\mathrm{d}B}{\mathrm{d}t} = \left[\frac{\partial}{\partial t} + (v_s - u_s)\frac{\partial}{\partial s}\right]B = \hat{v} + v_g, \tag{2}$$

where $\hat{v}$ is the side entrainment velocity and v_g the gravitational spreading velocity (or frontal velocity).

Additional relationships are required in order to allow the solution of the set of differential conservation equations. These are the equation of state, the heat of mixing expression, and the saturated vapor pressure expressions at the gas–liquid interface for each species for a non-ideal liquid mixture. The remaining closure relationships concern the source terms for the mass, momentum, energy and conservation equations and for the kinematic differential equation for transverse spreading.

The entrainment velocity is surely the most important among the source terms, in view of the high sensitivity of the results to air entrainment into the released cloud/plume. A sketch of the different phenomena affecting the entrainment of air into the plume is shown in Fig. 1.

In region I, where depressurization and acceleration of the jet occurs, no entrainment is considered but only momentum conservation is assumed. In regions II and III the entrainment of air into the free plume is modelled according to Ooms' [4] methodology. The entrainment model to be used for the ground bounded plume in

regions V and VI is based on Colenbrander's methodology [2, 3]. In region IV, a transition between the free plume situation and the ground bounded situation is assumed to occur. Downstream of this region a limitation to the maximum fluid velocity is given based on a characteristic propagation velocity:

$$c = \sqrt{\frac{g(\rho - \rho_a)H}{\rho}} + v_a. \tag{3}$$

Transverse profile functions have been adopted consistent with the entrainment models, i.e. a Gaussian profile as suggested by Ooms [4] for the free plume region and a Gaussian profile in the horizontal direction with an exponentially decreasing profile in the vertical direction as suggested by Colenbrander [2] for the ground bounded cloud/plume.

3. Numerical solution and code implementation

The conservation equations have been discretized using a staggered nodalization, with velocities defined at the cell edges and other quantities at the cell centers. An explicit donor-cell finite difference scheme has been adopted, which by convecting the cell center quantities consistently with the fluid direction, allows a stable numerical solution. The solution scheme is fast since no matrix inversion is needed. The explicit nature of the scheme has the drawback that the time step must comply with the Courant condition:

$$\Delta t_j/\Delta s_j < 1/(v_s - u_s)_j. \tag{4}$$

To speed up the computation, for jet type releases, a multiple time step scheme has been adopted with automatic time step increase where cells become larger and/or velocities decrease. Initial conditions for an instantaneous, puff type, release are computed by a specific model based on the experimental results obtained at the Swiss Federal Institute of Technology [5]. Boundary conditions for semi-continuous jet releases are computed by a critical flow model based on stagnation conditions inside the tank [6]. The code in its present version includes species conservation equations for three substances: air, water and the noxious substance. The properties of these substances are read from an external file. Properties input files for ammonia and hydrofluoric acid have been implemented, as well as for a mixture of R-12 and N_2, for code validation purposes.

The input required by the code is very limited in size and reflects the four possible cases dealt with by the code: jet release or puff release with boundary/initial conditions intrinsically computed or externally assigned as input values.

The output of the code, beyond a standard printout file, features specific files for interfacing with plotting devices and 3D graphics packages, allowing to track the space–time evolution of the hazardous susbtance concentration.

4. Droplet behavior

An assumption commonly made in the modelling of droplet evaporation is that the droplet is well mixed and is at a uniform temperature throughout. Using Fourier methods, estimates of the timescales for mixing and thermal diffusion have been made by Seinfeld [7]. This evaluation suggests that, while perfect thermal mixing inside the droplets can be assumed with negligible errors, for what concerns the mass diffusion account should be taken of the concentration difference between the center and surface of the droplet. The heat transfer coefficient on the gas side to be used for computing heat transfer at the interface is expressed as

$$\alpha = F_{vh} k_g / 2 r_d \tag{5}$$

where F_{vh} is a ventilation factor accounting for droplet vertical motion due to gravity, k_g the gas conductivity and r_d the droplet radius. The molar flux of the species i at the surface of the droplet on the gas side is expressed, according to Newbold and Amundson [8], assuming positive flux to the droplet, as

$$J_i = -F_{vm} C_2 \frac{C_T D_{lm}}{r_d} \ln(C) \frac{Y_{id} \exp\left(\frac{D_{lm}}{D_{im}} \ln C\right) - Y_{i,\infty}}{\exp\left(\frac{D_{lm}}{D_{im}} \ln C\right) - 1} \tag{6}$$

where F_{vm} is a ventilation factor, C_2 a factor accounting for temperature dependence of diffusion coefficient, C_T is the total molar concentration, and:

$$C = Y_{I,\infty} / Y_{I,d}. \tag{7}$$

The subscripts d and ∞ denote values of the molar fractions Y, respectively, at the droplet surface and in the bulk gas stream, while subscript I denotes the noncondensible phase (air). The diffusion coefficients D_{im} are mixture values weighted by species fluxes. The equation for diffusive transport inside the droplet of component i in a binary solution is:

$$N_i = -D_{1,2} C_T \nabla X_i + X_i (N_1 + N_2) \tag{8}$$

where X_i is the molar fraction of component i and N_i is the net molar flux relative to stationary coordinates. Eqs. (6–8) are used to determine the source terms for mass in the species conservation equations.

5. Code validation

The large scale experimental data employed for the validation of the CLOUD code concern the release of three different substances: ammonia, hydrogen-fluoride and a heavier than air mixture of R-12 and nitrogen. The ammonia large scale release tests

were performed in 1983 at Frenchman Flat, Nevada, by the Lawrence Livermore National Laboratory (LLNL). These tests, called the Desert Tortoise series, concerned the release of pressure liquefied ammonia from high capacity tanker trucks, through an horizontal spill line having an orifice plate at the discharge point [9]. The

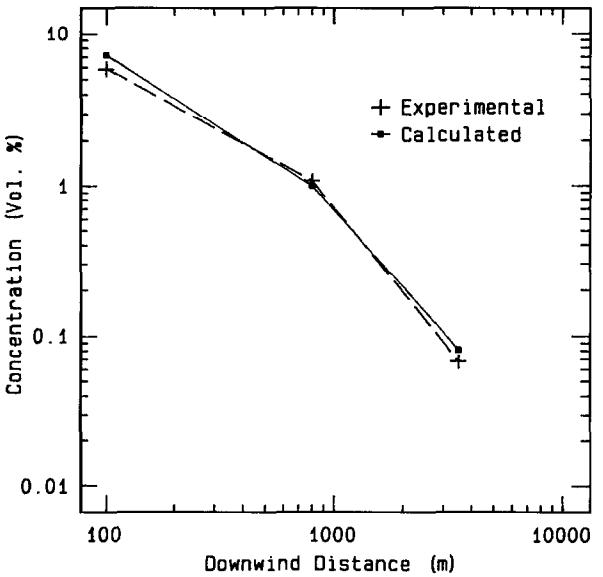

Fig. 2. Desert Tortoise test 1: comparison between experimental and calculated peak concentrations.

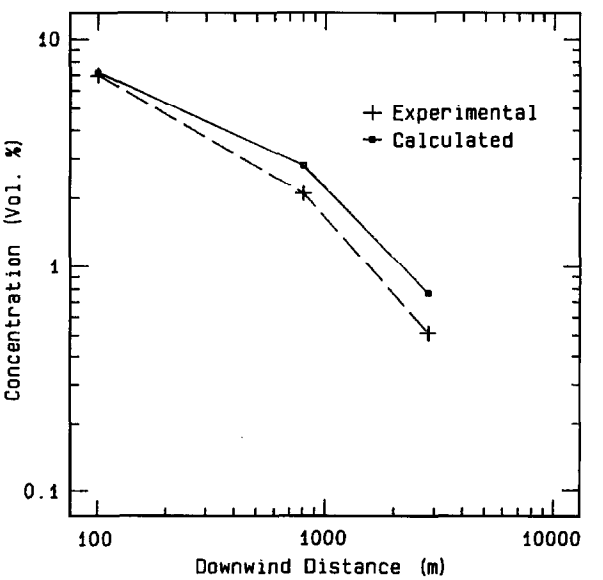

Fig. 3. Desert Tortoise test 4: comparison between experimental and calculated peak concentrations.

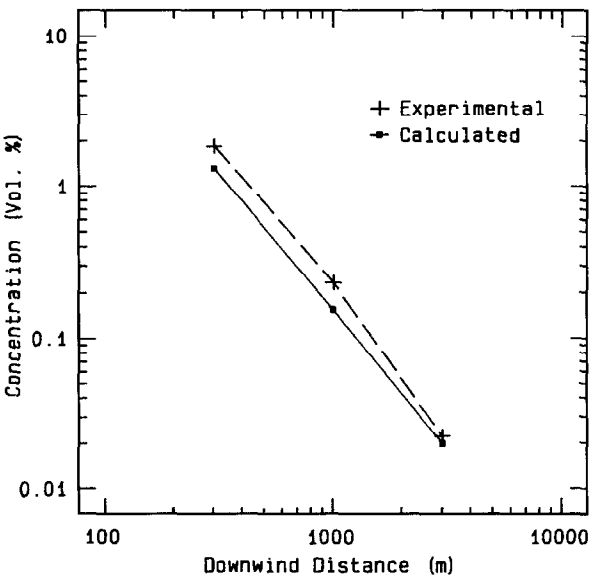

Fig. 4. Goldfish series test 3: comparison between experimental and calculated peak concentrations.

hydrogen-fluoride large scale release tests were performed by Amoco Corp. and LLNL in 1986 at the same test site Frenchman Flat, Nevada. This test series, called the Goldfish series, was also conducted using a pressurized tank, filled with liquid HF, and connected to an horizontal pipe, ending up at an orifice plate where flashing of the fluid occurred [10]. The heavy gas instantaneous release tests were performed at Thorney Island, West Sussex, UK, between 1982 and 1984 [11]. The gas was released from a nearly cylindrical container of about 2000 m^3, 13 m high, with a 14 m cross section diameter. The container walls collapsed and fell to the ground at the start of each trial, allowing free motion of the gas cloud.

Two different tests from the Desert Tortoise series have been chosen for comparison with the code predictions: test 1 and test 4. The comparisons between experimental and calculated peak concentrations are shown versus downwind distance from the spill point in Fig. 2 for test 1 and in Fig. 3 for test 4. The comparison with Goldfish Series release test 3 is shown in Fig. 4, in terms of peak concentrations. The comparisons with Thorney Island heavy gas release test 015 are shown in Figs. 5 and 6.

6. Conclusions

The CLOUD code is an efficient tool for predicting the dispersion of heavier than air releases implementing a complete set of one-dimensional conservation equations for mass, momentum, energy and species, together with proper closure relationships.

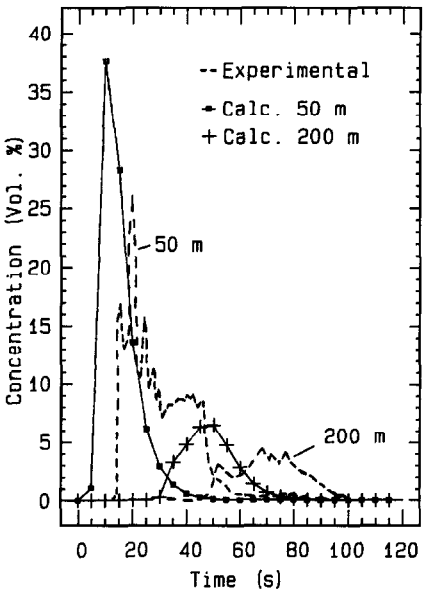

Fig. 5. Thorney Island trial 15: comparison between experimental and calculated concentrations at 50 and 200 m downwind.

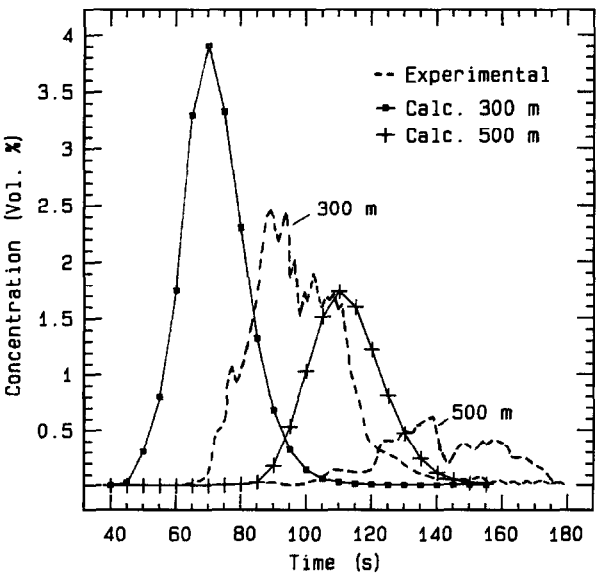

Fig. 6. Thorney Island trial 15: comparison between experimental and calculated concentrations at 300 and 500 m downwind.

These equations account also for two-phase fluid conditions and for a curvilinear trajectory of the cloud in space, under the action of inertia and gravity. The code can be used both for continuous or semi-continuous releases originating from a jet, and for instantaneous releases originating from sudden ruptures of vessels or tanks. The comparisons with the large scale release tests of pressure liquified NH_3 (Desert Tortoise) and HF (Goldfish Series) have shown the ability of the code to describe with good approximation very complex situations: the release source behavior at the jet efflux; the inertial dispersion phase characterized by intense mixing with air and velocity reduction, as well as by interfacial heat and mass transfer phenomena; and the mixed gravitational/diffusion driven growth of the gas plume far away from the release (up to 4000 m downwind). The comparisons with the heavy gas instantaneous release tests of Thorney Island have shown a tendency to overpredict the hazardous substance concentrations, particularly in the far field; but this results in a conservative behavior of the code.

Nomenclature

B	half-width of plume
C_T	total molar concentration
D	diffusion coefficient
F_v	ventilation factor
g	gravitational acceleration
H	height of plume
h	enthalpy
J	molar mass flux
m_{ki}	mass fraction of component i in phase k
N	net molar flux inside the droplet
r_d	droplet radius
$\hat{S}$	source term
s	curvilinear coordinate along plume/cloud centerline
t	time
v	fluid velocity
v_g	frontal velocity
X	molar fraction in liquid phase
x	gas mass fraction
Y	molar fraction in gas phase

Greek symbols

α	heat transfer coefficient
ρ	density

Subscripts and superscripts

a	air
ext	external
g	gas phase
h	heat transfer
i	component index
j	node index
k	phase index
ℓ	liquid phase
m	mass transfer
s	*s*-axis component

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