Check if the udpated flow and state variables satisfy equation (11), failing which, compute a better guess for updated temperature and return to step d.

## DISCUSSION

A computer program developed to follow the solution procedures outlined above is currently being used to simulate the two-phase blowdown from a liquid propane pipeline. Various differencing schemes are being tested with the objective of obtaining one that would optimize the solution procedure in terms of computation speed as well as stability. With the schemes that have been used, the time step has been limited to only a fraction of a millisecond and the simulation of the blowdown process has been accomplished for about 400 milliseconds. The void fraction and pressure at the exit are found to oscillate with time from the results of this simulation. While there is some experimental evidence that such oscillations are indeed present (5), it is considered desirable to test the program further to ensure that the predicted oscillations are not caused by numerical instabilities.

s. Guess the updated temperat

Along the pipe axis, the liquid-vapor interface is observed to have waves. Further, pressure gradient is rather steep at the point where two-phase region ends and one-phase region begins. Due to these reasons, it appears to be necessary to use a rather fine spatial grid. The stability criterion, then, restricts the time step to very small values and the computation speed has, therefore, been very slow. To simulate the two-phase blowdown of multicomponent mixtures, such as NGL, another computer program has been developed assuming that Moody's model can be used to predict the boundary condition at exit. The computational speed for this program is even slower because phase equilibrium calculations (which are iterative in nature) have to be performed at each stage of the iteration. Further improvement of the existing program is, thus, necessary in order to make it practical to be used for the analysis of hazard resulting from breaks in liquified hydrocarbon pipelines.

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#### I. CHEM. E. SYMPOSIUM SERIES NO. 71

THE EVAPORATION OF HAZARDOUS MATERIALS FROM SOLUTION.

M.H. Hilder\*

Conventional procedures for estimating the rate of evaporation of hazardous materials are based on the evaporation of pure liquids. With materials in solution one must not only take account of the reduced vapour pressure but also of the liquid phase resistance to mass transfer; this can have a marked influence on the rate of release and on the surface concentration of the material and hence on its dispersion in the atmosphere. Experimental and theoretical evidence is presented which should help in estimating the magnitude of these effects.

INTRODUCTION

Conventional procedures for estimating the rate of evaporation of potentially hazardous material (3, 4) are based on the evaporation of pure liquids and obviously do not need to take account of any liquid phase resistance to mass transfer.

The evaporation of (soluble) flammable or toxic materials from solution, although normally less of a potential hazard, sometimes require evaluation as well. If the same conventional procedures are applied, without making any allowance for liquid phase resistance, the results could be wildly inaccurate and could therefore lead to the wrong conclusions being drawn.

The present paper stems from a practical example where the liquid phase resistance was neglected, although the consequences in this particular case were negligible.

The potential emission of acetone from an open tank of 2 x 8.8 m surface area containing aqueous effluent at 20°C assumed to be contaminated with 0.1 wt.<sup>§</sup> acetone was estimated by a conventional procedure (3) to be 5.4 mg/m<sup>2</sup>s at a wind speed of 2 m/s. The corresponding acetone-in-air concentration at the water-air surface was taken to be equal to the equilibrium concentration, which is 1270 mg/m<sup>3</sup>.

This estimate was considered dubious because it did not take account of any liquid phase resistance. Measurements and calculations of the plate efficiency for acetone-water distillations (8) have shown that the liquid phase resistance can be considerable at low acetone concentrations. Another indication was that a 0.1 wt.% solution of acetone in an open sample bottle did not produce a tell-tale smell of acetone, except shortly after being shaken, although the equilibrium concentration is above the smell threshold.

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It was therefore decided to study the problem in more detail.

#### EXPERIMENTS.

Experimental procedure.

PORTARY AD

Two experiments were carried out on laboratory scale with the object of confirming and, if possible, quantifying the effect of the liquid phase resistance.

A row of eleven petri-dishes, each containing a known weight of a 0.1 wt. solution of acetone-in-water was placed in the opening of a fume cupboard. Each petri-dish had a diameter of 88 mm and contained 45-65 gm of solution, resulting in a liquid depth of 7.5 - 10 mm.

The fume cupboard was fitted with a conventional extraction fan so that, by adjusting the position of the "sash-window", the air flow over the petri-dishes could be varied. The air velocity during the first experiment was 2 m/s and during the second 0.1 - 0.15 m/s.

The temperature of the solution was measured by placing a thermometer in one of the petri-dishes. The air temperature and humidity were also measured at regular intervals.

At hourly intervals after the beginning of each experiment, two dishes were removed and replaced by blanks. The final weight of each dish was recorded and the acetone concentration of the combined residual solution was determined by COD-analysis.

# Experimental results.

The two sets of figures relating total weight loss and acetone concentration as a function of time were used to calculate the rate of water evaporation and acetone emission.

Water evaporation. The weight loss of acetone was negligible in comparison to the total weight loss and therefore the rate of water evaporation per unit area was derived from a plot of total weight loss per unit area against time, as shown in Figure 1.

The relevant experimental conditions and the calculated mass transfer coefficients for water evaporation are summarised in Table 1.

TABLE 1 - Experimental water vapour mass transfer coefficients.

Expt. no.	nevnos a 1,6 5etamética	a asw emologies fortw F.O
Air velocity (m/s)	2	0.13
Air temperature ( <sup>O</sup> C)	17.5	17.7 Mind Trups
Air humidity (%RH)	51	51
Solution temperature ( <sup>o</sup> C)	14	for according to
Rate of evap. (kg/m <sup>2</sup> hr)	0.43	0.058
Mass transfer coeff. (m/s)	2.7 10-2	5.5 10-3

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The mass transfer coefficients were calculated using the conventional expression for mass transfer

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whereby the water vapour concentrations at the surface of the solution  $(C_{wi})$  and in the bulk air flow  $(C_w)$  were derived from the saturated vapour pressure at the corresponding solution and air temperatures.

In this case there is no liquid phase resistance and hence the experimental mass transfer coefficients are gas-side coefficients; they agree well with the calculated gas-side coefficients as shown in Figure 3.

Acetone emission. In the case of acetone emission both the gas-side and liquid-side resistance to mass transfer have to be taken into consideration.

$'' = k_1 (0)$	$C_1 - C_{1i}$	$= k_g$	(Cgi	$-C_g$ )					•	•	•	•	•	•	•	•	•	(2)	)
----------------	----------------	---------	------	----------	--	--	--	--	---	---	---	---	---	---	---	---	---	-----	---

The expression on the LHS represents the mass transfer in the liquid phase and the expression on the RHS the gas phase mass transfer. Assuming that the acetone concentrations at the interface are in equilibrium and obey Henry's law ( $C_{1i} = H \ C_{gi}$ ), Equation 2 can be expressed in terms of an overall liquid side mass transfer coefficient

ass transfer in Doth experiments.

	$\phi'' = K_1 (C_1 - HC_g)$			•	•	•	• •	•	•	•	•	• •	•	•	•		•	•	•	•	•	•	(3)	
here																								
	$\frac{1}{1} = \frac{1}{1} + \frac{H}{1}$	1000	fred	and	-63		diffe	de	i voi	here	510	ha				25			-			1.12	(4)	
	$K_1  k_1  k_g$	bid	aple	in		dan.	shot	\$2.58	al s	17 3	odd												10	

In the case of the two experiments, the main air stream was free of acetone and  $C_g = 0$ . However, in analysing the experimental data it was necessary to take account of the change in volume of the liquid in the petri-dishes due to the evaporation of water; the mathematical treatment of this correction is dealt with in Appendix 1. The results of the two experiments in terms of the fraction of acetone remaining after a given time are shown in Figure 2. The corresponding mass transfer coefficients and other relevant data are summarised in Table 2.

TABLE 2: Experimental acetone mass transfer coefficients.

Expt. no.	shiping a hispite	add the 2 and 1 and a ship
Air velocity (m/s)	2	0.13
Solution temp. ( <sup>O</sup> C)	offer 14 perando a	12 de la contentanse
Equilibrium coefficients H (-)	1090	1220
Mass transfer coefficients		
- overall K <sub>1</sub> (m/s)	2.0 10-6	4.5 10-7
- gas-side kg (m/s)	1.8 10-2	3.7 10-3
- liquid side k <sub>1</sub> (m/s)	2.3 10 <sup>-6</sup>	5.3 10 <sup>-7</sup>

tespectively.

The acetone vapour-liquid equilibrium coefficients H were calculated using the correlation quoted by Stockar and Wilke (1), which was based on the experimental data of Othmer et al (2). These data also confirm that Henry's law holds and that the equilibrium coefficient is constant over the experimental range of concentrations.

The gas-side mass transfer coefficients for acetone were derived from the corresponding experimental mass transfer coefficients for water evaporation. The details of this derivation are given in Appendix 2.

## Discussion of experimental results.

Both the form of the acetone concentration versus time plot (Figure 2) and the relative magnitudes of the corresponding mass transfer coefficients (Table 2) indicate that the acetone emission was primarily determined by the liquid phase resistance.

The fact that the (extrapolated) concentration versus time plot intercepts the t = o axis at  $CV/C_0V_0 = 0.8 \pm 0.06$  is in itself an indication of the dominance of the liquid phase resistance. The theoretical value for a stagnant layer with zero gas phase resistance is about 0.8. The experimental mass transfer coefficients confirm this and show that the liquid phase resistance accounted for about 85% of the total resistance to mass transfer in both experiments.

It is more difficult to give a water-proof explanation of the absolute value of the liquid mass transfer coefficients. In spite of the considerable uncertainty (+ 25%) of each individual COD-based concentration measurement, the mutual consistency of the data and the probable physical limitations suggest that the mass transfer coefficients are accurate to within + 10-20%.

The lower limit of the liquid phase mass transfer coefficient is given by

 $Sh = \frac{k_1 \delta}{D} = 2.5 \dots (5)$ 

This represents the mass transfer in a stagnant layer by pure molecular diffusion, in the absence of any natural of forced convection. In the present case, with an acetone-in-water diffusivity of  $D = 1.2 \ 10^{-9} \ m^2/s$  and a layer thickness of  $\delta \sim 8.5 \ 10^{-3}$  m, the limiting value is  $k_1 \sim 3.5 \ 10^{-7} \ m/s$ .

Any liquid motion however slight will inevitably enhance the liquid side mass transfer. The higher experimental values are possibly due to the effect of the air flowing over the liquid surface. Assuming this air flow causes the liquid to circulate across the surface, down and along the bottom of the petri-dish, one can postulate that mass transfer occurs according to the penetration theory with a characteristic surface exposure or contact time  $t_e$ , in which case

Based on the experimental mass transfer coefficients this would mean a contact time of 300 s with an air velocity of 2 m/s and a contact time of 5500 s at 0.13 m/s; assuming an average effective surface flow path of about 5 cm this would in turn suggest liquid surface velocities of 1 cm/min. and 0.05 cm/min. respectively.

. . . (6)

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Although this is no more than a hypothesis, the figures suggest that it is plausible. Surface velocities of this magnitude are too low to have been observed with the naked eye under normal circumstances. The ratio of air velocity to surface velocity is approximately the same for both experiments. Extrapolation of the figures to zero surface velocity give a physically feasible result.

Another possibility of course is that similar circulation currents are caused by natural convection due to small temperature differences created by the water evaporating.

#### PREDICTION IN PRACTICE

In practice, assuming that the atmospheric dispersion characteristics are known, two parameters are required to estimate the potential hazard caused by the evaporation of a flammable or toxic material:

- the rate of evaporation or emission of the material, and - the concentration of this material above the evaporation surface. These two parameters provide the starting point for any dispersion calculation.

For pure liquids the estimation of these two parameters is relatively simple and well documented. For flammable and toxic materials in solution the situation is more complex and no standard methods are available.

### Rate of emission.

When estimating the rate of emission from a solution one must take account, not only of the reduced equilibrium vapour pressure, but also of the relative magnitudes of the gas and liquid phase mass transfer coefficients.

Gas phase mass transfer. The conventional equations for estimating gas phase mass transfer coefficients (3, 4) are based on the well known fundamental expression for turbulent flow over a flat surface. Both this expression and the corresponding one for laminar flow are given in Appendix 2.

In practical situations flow is nearly always turbulent but in some cases, in particular in small scale tests, the flow will be laminar and the relation between air velocity, flow path length and mass transfer coefficient will be different. It is therefore important to know the limits of the laminar and turbulent flow regimes and to be able to compare the corresponding mass transfer coefficients.

Liquid phase mass transfer. The liquid phase mass transfer coefficient is more difficult to predict since it is strongly dependent on the degree and extent of any liquid motion which is not usually very easy to define.

For stagnant, rigid layers of liquid the initial rate of mass transfer is determined by the exposure time  $t_e$  and the instantaneous mass transfer coefficient is given by

$$k_1 = \sqrt{\frac{\mathbb{D}}{\pi t_e}}$$
 for  $\delta > \sqrt{\pi \mathbb{D} t_e}$  .....(7a)

or, averaged over the total exposure time, by

These expressions are derived from the so-called penetration theory.

Eventually the mass transfer coefficient reaches a constant, minimum value given by

$$Sh = \frac{k_1 \mathcal{S}}{\mathbb{D}} = 2.5$$

transfer from or to the sea surface.

the liquid surface can be derived from Equation 2.

be correspondingly lower.

confirmed in practice.

of about 1 s.

be of great benefit.

Laboratory tests.

Surface concentration.

concentration will be.

for

$$r \quad \delta < \sqrt{\pi \, \mathbb{D} \, t_e} \, \dots \, \dots \, \dots \, (8)$$

Since in most cases the diffusivity is of the order of D  $\sim$  10<sup>-9</sup> m<sup>2</sup>/s it is unlikely that this lower limit will have any practical relevence for layers

more than a few millimeters thick. For layers thicker than a few millimeters

it is unreasonable to expect the layer to remain stagnant so long in practice.

Hence the practical lower limit of the liquid phase mass transfer coefficient for materials with a diffusivity  $D = 1 - 2 \ 10^{-9} \ m^2/s$  will be  $k_1 \sim 1 \ 10^{-6} \ m/s$ ;

for high molecular weight materials with a lower diffusivity the limit will

An upper limit can also be given based on experience with mobile or moving

liquids. For mobile drops, jets and films of liquid Beek (5) quotes values

These values were predicted by the penetration theory for various aeration

equipment (with characteristic exposure times of 0.2 - 1 s) and have been

A value of  $k_1 = 0.5 \ 10^{-4}$  m/s was also given (5) for mass transfer from the

surface of a moderately agitated liquid. A similar value of  $k_1 = 0.55 \ 10^{-4}$ m/s is given by Liss and Slater (6) as the result of measurements of oxygen

The upper limit for the liquid mass transfer coefficient for materials with a diffusivity of  $D = 1 - 2 \ 10^{-9} \ m^2/s$  can therefore be taken as

 $k_1 = 5 \ 10^{-5}$  m/s; for materials with different diffusivities the upper limit can be estimated from the penetration theory assuming a surface exposure time

It is clear that the factor 20 between the upper and lower limits is too

information on practical values for stagnant pools, flowing rivers etc. would

An expression for the gas phase concentration of the evaporating material at

This expression provides a means of estimating the surface concentration and shows that the greater the liquid side resistance, the lower the surface

Laboratory tests can be useful to determine or confirm the order of magnitude

of emission rates and the relative importance of gas and liquid phase

with the sort of equipment and facilities available in any laboratory.

resistance. Our own results illustrate that such tests can be carried out

 $C_{gi} = \frac{C_1 k_1 + k_g C_g}{k_1 H + k_g}.$  (9)

great to allow reliable estimates to be made in many cases. Additional

of  $k_1 = 0.5 - 1 \ 10^{-4}$  m/s for materials with a diffusivity  $\mathbb{D} = 1 - 2 \ 10^{-9} \ \text{m}^2/\text{s}$ .

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The design and analysis of any experiments are obviously important if the correct conclusions are to be drawn from the results. One method has been described in this paper but other methods could also be used. Dilling (7) has described measurements of the emission rates of 27 chlorohydrocarbons from aqueous solution in a stirred beaker. Unfortunately, he simply assumed the previously derived (6) mass transfer coefficients for sea surface conditions and did not determine the coefficients applicable to his own apparatus.

Ideally one should try to simulate the practical situation, in particular as regards the gas and liquid phase mass transfer coefficients. A method of estimating the laboratory conditions (usually laminar flow) required to ensure equal gas phase coefficients is described in Appendix 2. The experiment at an air velocity of 0.13 m/s gave the same gas phase coefficient as that calculated for the practical example given in the introduction. Our experimental results also illustrate the advantage of being able to determine the actual gas phase coefficient during the same experiment by measuring the rate of evaporation of the solvent at the same time.

Simulation of the liquid phase coefficient is obviously more difficult until further information on both practical and laboratory coefficients are available.

## Example.

The data presented above allow a more realistic estimate to be made of the example quoted in the introduction.

Assuming  $k_1 = 1 \ 10^{-6}$  m/s (lower limit) the rate of emission would be 0.8 mg/m<sup>2</sup>s and the surface concentration 200 mg/m<sup>3</sup>, each being a factor 6 lower than the original estimate.

Taking the upper limit of  $k_1 = 5 \ 10^{-5}$  m/s the rate of emission would be 4.8  $mg/m^2s$  and the surface concentration 1150  $mg/m^3$  which is a negligible decrease.

This illustrates once again the importance of a reliable estimate of the liquid phase mass transfer coefficient.

A more realistic estimate in this case is  $k_1 = 2.5 \ 10^{-6}$  m/s which corresponds to the experimental value for an air velocity of 2 m/s and is equivalent to a surface exposure time of 4 min. The corresponding rate of emission would be 1.7 mg/m<sup>2</sup>s and the surface concentration 400 mg/m<sup>3</sup>, which are each a factor 3 lower than the original estimate.

Acetone is in fact a poor example since it has a large equilibrium coefficient. There are however, many substances with a much lower equilibrium coefficient (7) which will be totally dependent on the liquid phase resistance over a wide range of conditions.

# CONCLUSIONS.

The potential hazard from (soluble) flammable or toxic materials evaporating from solution will in most cases be less than that created by the evaporation of the pure liquid. Nevertheless, it is important that reliable and physically consistent methods are available to estimate the effect of evaporation from solution.

The experimental results reported in this paper show that the liquid phase resistance can play a dominating role in the evaporation of hazardous materials from solution. This is confirmed by the results of other investigators (6, 7). This liquid phase resistance affects not only the rate of evaporation but also the concentration of the material at the liquid surface and hence has a double effect on the subsequent dispersion calculations.

The prediction of evaporation rates from solution is difficult due to the lack of reliable data on liquid phase mass transfer coefficients in practice. The large difference between the estimated upper and lower limits of this coefficient illustrate this point.

The experimental results also illustrate that useful information can be gleaned from simple laboratory scale tests as long as they are carefully designed and analysed.

In conclusion, I trust that you will accept this paper for what is is: a contribution from a factory-based engineer, who

- has been confronted in practice with this sort of hazard evaluation;
- does not have the time to follow developments in this specialised field (and therefore regrets omitting any references to other relevant sources);
- but who is concerned that reliable and practical methods should be developed for the assessment of hazards.

Acknowledgements. I would like to thank Ir. W.J. Smeenk for his meticulous experimental work and Ing. C.J. van Leeuwen and Ir. H.J. van den Berg for their own contributions to the final result.

#### SYMBOLS USED

A = liquid surface area in petri-dish  $(m^2)$ 

- $C = concentration (kg/m^3)$
- $\mathbb{D}$  = diffusion coefficient (m<sup>2</sup>/s)
- H = Henry's equilibrium coefficient ( )
- k = mass transfer coefficient (m/s)
- K = overall mass transfer coefficient (m/s)
- L = flow path length (m)
- t = time(s)
- t<sub>e</sub> = surface exposure time (s)
  u = gas velocity (m/s)
- V =liquid volume in petri-dish (m<sup>3</sup>)
- Re = Revnolds number (-)
- Sc = Schmidt number (-)

Sh = Sherwood number ( - )

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- = evaporation rate (kg/m<sup>2</sup>s)
- = layer thickness (m)
- = solution density  $(kg/m^3)$ P
- = kinematic viscosity (m<sup>2</sup>/s) 2

# Subscripts.

- = in the gas phase
- = at the interface
- = in the liquid phase
  - = initial
- = total
- = of water vapour

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# APPENDICES

APPENDIX 1 - Analysis of the experimental acetone emission data.

Applying Equation 3 to batch evaporation of acetone from a volume V of solution in a petri-dish with a liquid surface area A.

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Since in this case 
$$- dV \rho = \emptyset_t^{"} A dt$$
 it follows that

$$\frac{d(C V)}{C V} = \int_{\mathscr{O}_{t}}^{\mathscr{O}_{t}} \frac{K_{1}}{V} \frac{dV}{V} \quad .$$

which on integration yields

This expression can be used as it stands but an expression in terms of time is often preferred and is easier to handle.

Multiplying top and bottom of the RHS by

one obtains

The experimental data can then be plotted and analysed in terms of a corrected time (t\*) and initial volume ( $V_0^*$ ), such that

where

The average initial volume of 55 ml was used for  $V_{\rm o}^{\ \star}$  in the analysis of the experimental data.

APPENDIX 2 - Gas phase mass transfer in laminar and turbulent flow.

The basic expressions for mass transfer for fluid flowing over a flat surface are:

Laminar flow ( $Re < 3 \ 10^5$ )

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These equations can be used to relate and/or compare mass transfer coefficients in different situations.

Example 1. The mass transfer coefficients of different materials under otherwise identical "evaporation" conditions are simply related by their respective diffusion coefficients. For both laminar and turbulent flow

This expression was used to calculate the mass transfer coefficient for acetone ( $\mathbb{D} = 1.1 \ 10^{-5} \ m^2/s$ ) from the experimentally determined mass transfer coefficient for water vapour ( $\mathbb{D} = 2.0 \ 10^{-5} \ m^2/s$ ).

Example 2. The same gas phase mass transfer coefficient can be achieved in either laminar or turbulent flow if the following criterion is satisfied:

1	$\left(\frac{\text{u L}}{\mathcal{V}}\right)$	0.5	lam.	= 0.056	$\frac{1}{L}$	$\left(\frac{u L}{v}\right)$	0.8	turb
			Tan.		100 100 100	1 1 1	1000	turp.

This expression can be used to relate small scale test to full scale, practical conditions.

A graph relating the gas phase mass transfer coefficient for laminar and turbulent flow is shown in Figure 3 for the acetone-in-air system.



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FIGURE 2: Experimental acetone evaporation results.





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SPREADING AND DISPERSION OF DENSE VAPOURS AND GASES

D. J. Gunn\*

The emission of dense vapour at ground level from a vessel or pipe failure spreads by gravity and forms a cloud of dense gas in the neighbourhood. Spreading is controlled by fluid velocities and lateral pressure gradients set up by density difference. Momentum and continuity relations for the cloud are derived from basic equations. The rate of dispersion into the atmosphere and the rate of emission into the cloud are boundary conditions. The description is compared with other models presented in the literature.

#### INTRODUCTION

The consequences of a major leak of volatile and flammable liquid, or the emission of a flammable vapour in a major hazard plant may be simulated if models of the emission, vapour dispersion and blast propagation are available. The failure of a pipe or vessel is invoked, and the period and rate of leakage are estimated from details of the nature of the failure and the inventory of the vessel or connecting vessels. The intention of the simulation is to examine the consequences of a major loss of containment in which the whole contents of a vessel are expelled, for example.

The concentration of vapour is followed by a dispersion calculation with the object of estimating the extent of the flammable environment as a function of time. If there is a significant possibility of ignition, the consequences of the subsequent explosion and blast may be examined to estimate the extent of plant and neighbourhood damage.

The object of this paper is to consider the importance of velocity, turbulence and other transport processes in the dispersion of vapour into the atmosphere and to examine the effect of density upon dispersion particularly when the density of the emitted vapour is greater than the density of air.

Methods that are available at present for dispersing gas clouds are related to this background. The development of an alternative method is suggested. The discussion is related to the spreading and dispersion of non-buoyant gases.

### Transport Processes in the Atmosphere

When an efflux of dense gas takes place at a rate that is large enough to affect the local atmospheric distribution of velocity, a shallow cloud of gas

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