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# A dense vapour dispersion code package for applications in the chemical and process industry

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**Abstract**

A computer code package for dispersion of dense vapour clouds in obstructed terrains is presented. The package consists of three models: a detailed fully three-dimensional model and two models (a 1-D and a 2-D) based on the shallow layer concept. The models are validated by the application of three field tests with different degrees of geometrical complexity. The first test was performed on flat terrain under isothermal conditions. The second was a cold jet release with a straight fence perpendicular to the flow. In the last test a semicircular fence obstructed the flow. The validation exercise indicated that the dimension of the model applied should preferably be of the same order as the geometry to be described.

*Keywords:* Dense gas; Dispersion; Shallow layer models; Complex terrain

## 1. Introduction

A joint development work on computer models for simulation of denser-than-air vapour clouds has during the last years been going on at the Joint Research Centre, Ispra, Italy, and the Research Centre 'Demokritos' in Athens.

The accident scenarios studied include instantaneous releases resulting from complete failures of containment as well as continuous releases from leakages in tubes or vessels. The main application areas are assessment of consequences in terms of damage to the public and installations, and optimization of safety engineering features for accident mitigation.

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Due to the diversity in the model application areas, it is desirable to have access to models with different levels of detail in the description of the dispersion phenomena. A code package has therefore been developed comprising three models of different complexity. These models will be presented in the following, and their capabilities will be demonstrated by application of data from three full-scale field experiments.

## 2. The one-dimensional shallow layer model

The simplest of the three models in the package is the one-dimensional (1-D) shallow layer model [1]. As basis of this model are the conservation equations for mass, mass of dense gas, enthalpy, and momentum in the downwind and crosswind direction. They are all formulated as one-dimensional partial differential equations with time and downwind coordinate as independent parameters. These equations are integrated over the cloud height and the cloud width. An additional equation couples the velocity in the crosswind direction with the cloud width. Thus the system of equations to be solved consists of six coupled non-linear differential equations.

The turbulent mixing between the dense gas cloud and the surrounding air is described by means of an entrainment velocity. This parameter is the velocity by which the surrounding air enters (entrains) the top and edge of the cloud, and thereby dilutes the dense gas. The concentration and temperature calculated by the model are (like the velocities) averaged over the cloud height and width. Experimental data however show that the concentration and the relative temperature deficit (defined as the difference between the cloud and the ambient temperature divided by the latter) vary in the vertical and crosswind direction. A Gaussian profile in the crosswind direction and a power profile in the vertical direction are therefore assumed for the concentration and the relative temperature deficit.

The model is capable of taking into account the presence of simple obstacles as permeable or solid walls. The influence of an obstacle on the cloud momentum is modelled by means of a friction factor, which is a function of the ratio between the cloud height and the obstacle height. If this ratio is less than unity and the wall is impermeable the friction factor is set to infinity.

The equations are discretized in space by means of a first (or an optionally second)-order upwind scheme for the convective terms. The integration in time is fully implicit, permitting large time steps. The implicit discretization results in six sets of linear equations which, due to the banded structure of the matrices, are solved by a direct method. The coefficients in the linear equations are however highly non-linear, so the overall solution is found by an iterative procedure.

## 3. The three-dimensional model ADREA-HF

ADREA-HF [2] is the most detailed model in the package. It is able to handle cases where the terrain is characterized by a high degree of complexity including non-rectangular obstacles and anomalous surfaces. Also cases where the ambient conditions are complex (e.g. stable, unstable or stagnant meteorological conditions) or cases where the source is a two-phase mixture can be handled properly by this model.

Here the conservation equations are fully three-dimensional, and they include three equations for the momentum. Besides the six conservation equations a one-dimensional equation for the ground heat transfer (with the vertical direction and time as independent variables) can be included in the solution.

The working fluid is treated as a mixture of two fluids in thermodynamic equilibrium. Both fluids may contain several components. The fluid kinetics is described by assuming a slip velocity between the liquid phase and the ambient gas.

The interaction between the ambient air and the cloud is described by means of turbulent viscosity terms. The vertical turbulent viscosity is assumed to be a function of the turbulent kinetic energy and a turbulent length scale. The horizontal turbulent viscosities are assumed to be simple multiples of the vertical. The turbulent kinetic energy is found by solving a conservation equation where one of the most important terms is the turbulent energy dissipation. The dissipation is assumed to be a function of the turbulent kinetic energy and the length scale. Thus the turbulence model is a one-equation ($k - l$) closure model. Further details can be found in Ref. [2].

The conservation equations are formulated in terms of the finite volume method in space and are fully implicit in time. They are solved by means of a method, based on the SIMPLER algorithm [3]. This method involves a transformation of the total mixture mass equation into a full pressure equation. The resulting linear equations are solved iteratively by a Gauss–Seidel point iteration method.

## 4. The two-dimensional shallow layer model

The 2-D shallow layer model is based partly on the 1-D model and partly on the 3-D ADREA-HF model. The geometrical description of the solution domain as well as the numerical solution method is derived from the 3-D code. For the turbulence description use is made of the entrainment velocity concept adopted in the 1-D model. The two-dimensional conservation equations are integrated in the vertical direction over the cloud height. A vertical power profile is applied for the concentration and temperature deficit. This model, which is in the development phase, offers the same possibilities as the 3-D model for describing a complex terrain, but it requires less computer time and storage.

## 5. The Thorney Island trial No. 8

The capabilities of the three models will now be demonstrated by simulations of different field experiments.

The first experiment is one regarding instantaneous releases in an unobstructed terrain performed at Thorney Island in 1982–1983 [4]. This experimental programme was organized by the Health and Safety Executive and sponsored by the Commission

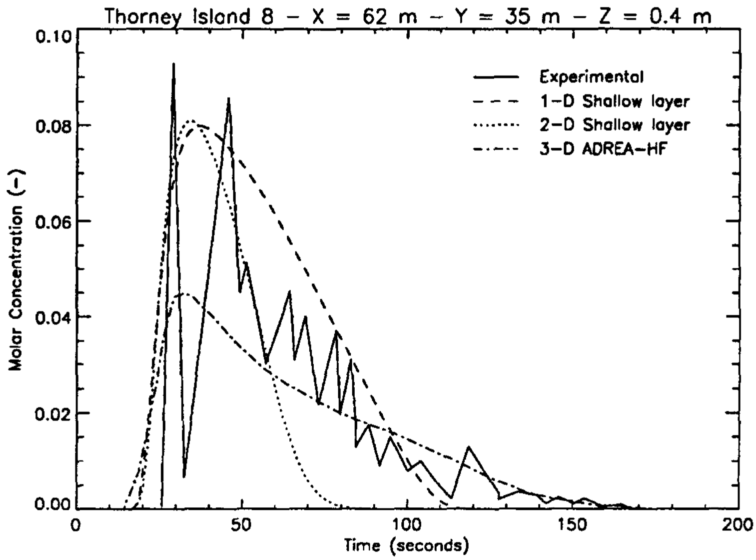


Fig. 1. Thorney Island 8. Comparison between experimental and calculated concentration histories. The sensor position is $X = 62$ m downwind, $Y = 35$ m crosswind the source at an elevation from the ground of $Z = 0.4$ m.

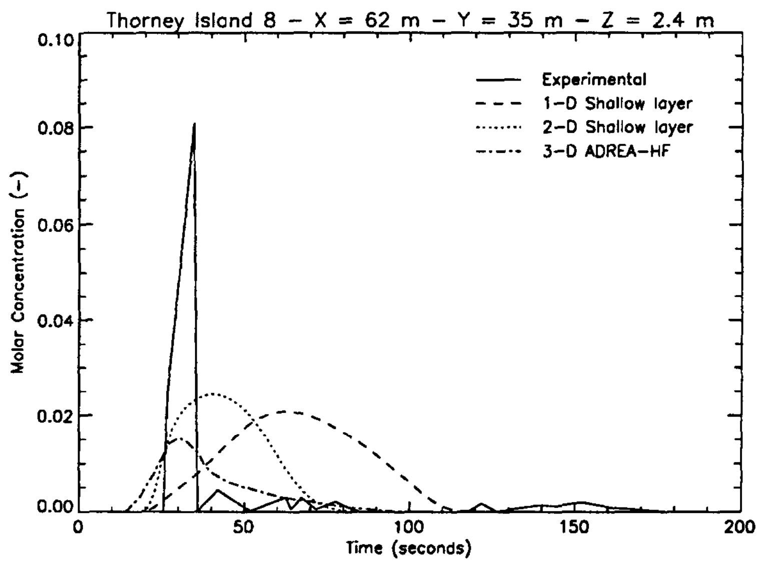


Fig. 2. Thorney Island 8. Same horizontal position of the sensor as in Fig. 1 but at an elevation of 2.4 m from the ground. The sensor is close to the upper boundary of the cloud.

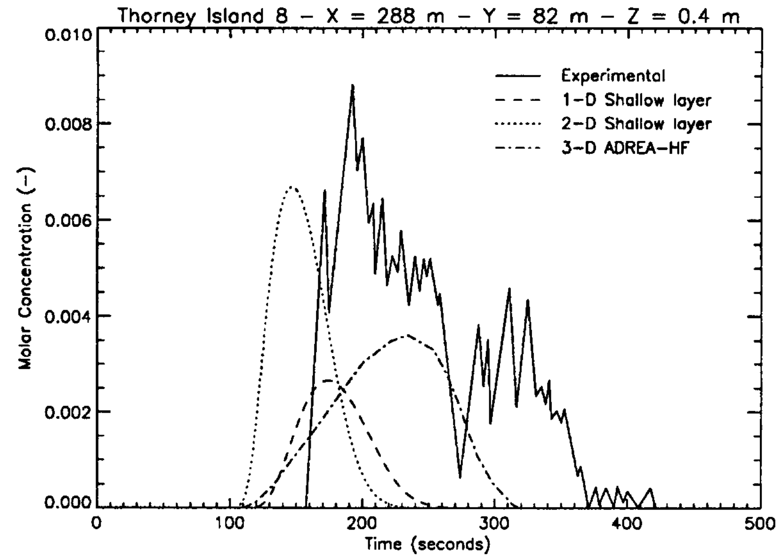


Fig. 3. Thorney Island 8. The sensor position is far downwind (288 m) the source.

of the European Communities. The source consisted of a ca. 2000 $m^3$ mixture of freon-12 and nitrogen. The relative density (to air) of the fluid was 1.63. The initial shape of the cloud was cylindrical with a diameter of 14 m and a height of 13 m. The wind velocity was 2.4 $m s^{-1}$ at 10 m height. The gas was detected by a total of 72 sensors located on 19 masts placed at distances ranging from 35 m to ca. 500 m in the downwind direction of the source.

Figs. 1 and 2 compare the experimental concentration history for sensors close to the source with results calculated by the three models. The calculations performed with ADREA-HF are described in more detail in Ref. [5]. Fig. 1 shows that all three models give reasonably good results, but that the best prediction is obtained with the 3-D model. Especially the residence time of the cloud is best evaluated by the ADREA-HF code.

In Fig. 2, where the elevation of the sensors is 2.4 m above the ground, the situation is quite different. It is seen that the cloud height is close to the sensor height since the experimental curve shows intermittency. This statistical behaviour cannot be described by the models but the 2-D and 3-D models are able to predict an initial concentration peak. The 1-D model predicts here the peak concentration to occur much later than measured.

In Fig. 3 data are shown for a position much further downwind. It is seen that here the concentration level is an order of magnitude lower. The general tendency is the same as before. The 3-D model provides a better value of the cloud residence time, but the concentration level is predicted well by all three models.

Thus, from this field test it can be concluded that when an isothermal release on a flat terrain has to be modelled, a 2-D or a 3-D model is necessary only in case a detailed knowledge of the concentration distribution is required.

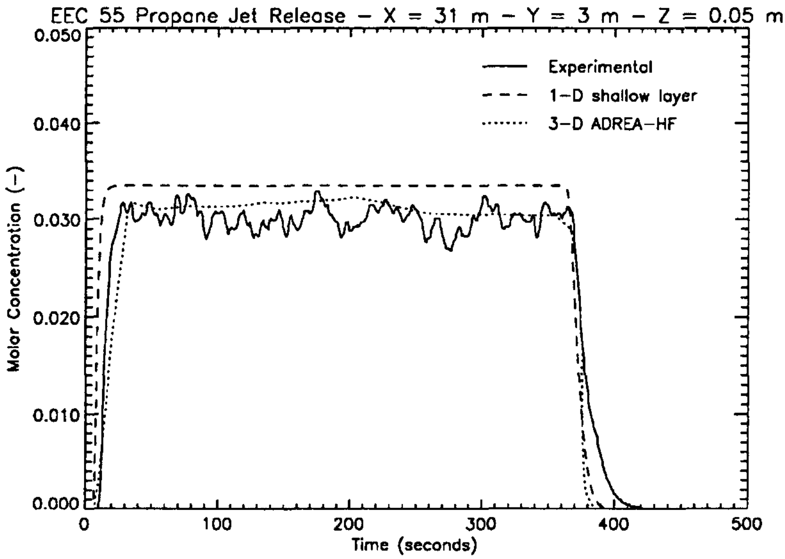


Fig. 4. EEC 55 propane jet release. Comparison between experimental and calculated concentration histories. The sensor position is 31 m downwind and 3 m crosswind the jet source. The elevation of the sensor from the ground was 0.05 m.

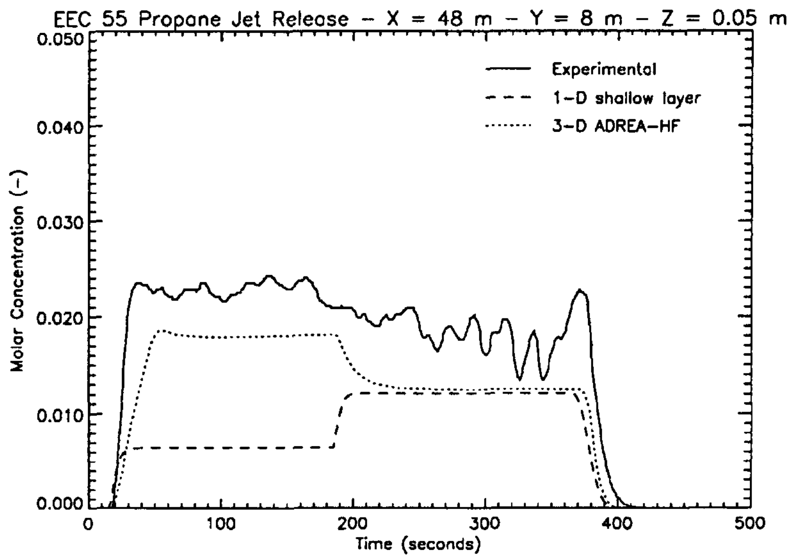


Fig. 5. EEC 55 propane jet release. The sensor position is close to the upwind side of the fence, which is removed at 185 s.

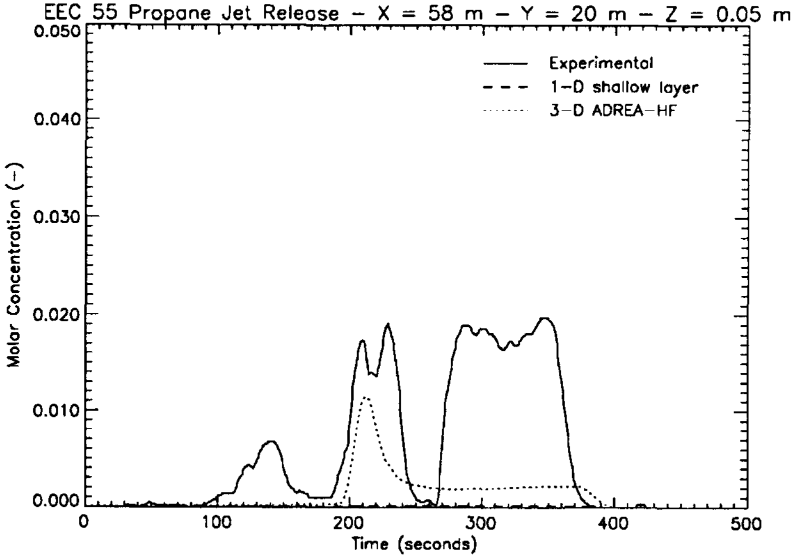


Fig. 6. EEC 55 propane jet release. The sensor position is close to the edge of the cloud 10 m behind the fence. The 1-D model predicts a too small cloud width, so the calculated concentration becomes negligible.

## 6. The EEC propane experiment No. 55

The EEC propane experiments [6–8] were performed under non-isothermal conditions on flat terrain with an obstacle. They were carried out in Lathen in Germany in 1989 by TüV and Risø and sponsored by the Commission of the European Communities.

Experiment no. 55 was performed as a jet release with a nozzle diameter of 15.5 mm. The release material was liquified propane which became superheated at the outlet, where the pressure dropped to atmospheric causing a very fast evaporation (flashing). The release rate was 3 kg $s^{-1}$ and the momentum of the jet was estimated to be 208 N, giving an exit velocity of 69.3 m $s^{-1}$ .

The release time was 480 s and the wind velocity at 10 m elevation was 2.6 m $s^{-1}$. A 2 m high and 51.2 m long impermeable fence was placed 48 m from the source perpendicular to the ideal wind direction. The wind in this experiment was 12° off this ideal direction. 185 s after the start of the experiment, the fence was removed instantaneously allowing a comparison with the unobstructed case under the same meteorological conditions. The relative density (with respect to air at ambient temperature) of propane vapour at saturation temperature (231 K) was assumed to be 1.89.

The concentration at ground level was measured by ca. 20 sensors placed 5 cm above the ground. Vertical concentration and temperature profiles were measured at two masts located 38 and 63 m from the source.

The comparison between experimental and calculated results is shown in Figs. 4–7. Fig. 4 shows the concentration time history for a position at ground level, close to the

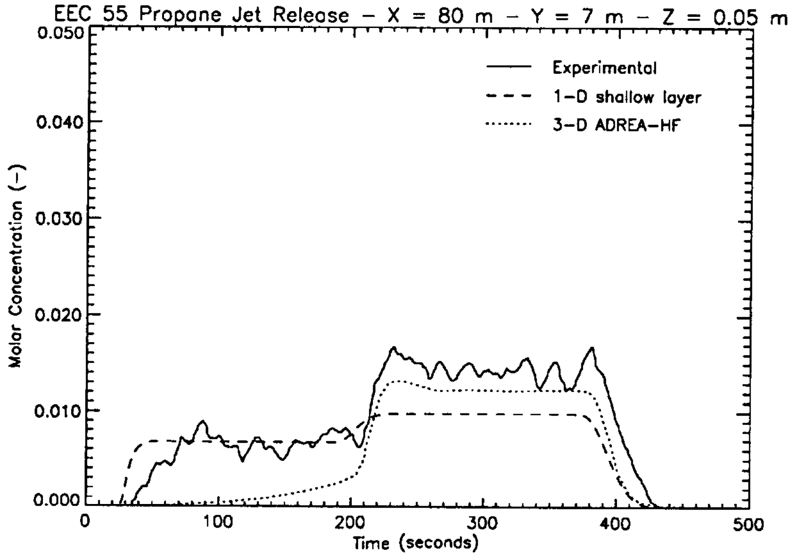


Fig. 7. EEC 55 propane jet release. The sensor position is 32 m downwind the fence.

midplane of the jet. The experimental (nearly) steady-state conditions are reproduced very well by both the 1-D and the 3-D models. In Fig. 5 the situation is shown close to the upwind side of the fence. In this case it is seen that the decrease in the concentration, when the fence is removed, is correctly predicted by the 3-D model, whereas the 1-D calculation indicates a slight increase in the concentration. The concentration level is however predicted satisfactorily by both models.

Fig. 6 shows the situation close to the edge of the cloud behind the fence. The concentration history exhibits here an intermittent behaviour arising from the meandering of the cloud. The 1-D model predicts here a too small cloud width, so the calculated concentration becomes negligible. Also the 3-D model predicts a too small cloud width when the fence is present, so here also the calculated concentration becomes zero. The 3-D model is however able to predict an increase in the concentration when the fence is removed.

In Fig. 7 the situation further downwind is illustrated. As before it is seen that when the sensor is placed inside the cloud, also the 1-D model gives reasonably good results. Here the influence of the fence is underestimated by the 1-D model, but overestimated by the 3-D model.

From these figures it can be concluded that the 3-D model gives the best description of the influence of the obstacle, but that the 1-D calculations are in acceptable agreement with the experimental values. Only in the vicinity of the cloud boundary the models fail to give a reasonable estimate of the concentration level.

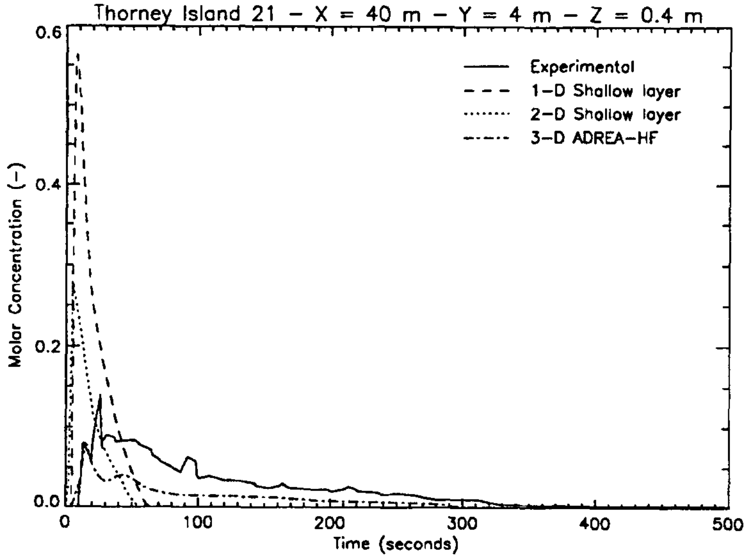


Fig. 8. Thorney Island 21 trial with a semicircular fence. The sensor position is 40 m downwind and 4 m crosswind the source. Due to the 3-D fence the 1-D model fails to give a reasonable prediction.

## 7. The Thorney Island trial No. 21

This Thorney Island trial [4] concerned, like the previously described No. 8, an instantaneous release of ca. 2000 $m^3$ freon-12/nitrogen mixture (here with a relative density of 2.02). However, in this field test a 5 m high impermeable semicircular fence was erected in the downwind direction. The radius of the semicircle was 50 m, and the centre coincided with the centre of the cylindrical source. The wind direction was ca. 6° off the ideal direction, and the wind velocity was 3.8 $m\,s^{-1}$ in 10 m height.

In Figs. 8–10 the results calculated with the three models are compared with the experimental data. The 3-D calculations are described in more detail in Ref. [9]. In contrast to the previous two cases, it is seen that the 1-D model here fails to give reasonable results. This is due to the three-dimensional nature of the obstacle. Fig. 8 shows a comparison of the data for the case when the sensor is positioned 40 m downwind the source. It is seen that the 1-D model, due to the inherent assumption of a straight fence (perpendicular to the wind direction), predicts a too low cloud residence time and a far too high peak concentration. The 3-D calculation, where the geometry of the fence is properly modelled, agrees well with the experimental curve.

The situation on to the downwind side of the fence is illustrated in Figs. 9 and 10. In Fig. 9 the downwind distance from the fence is 25 m, and in Fig. 10 this distance is ca. 250 m. The tendency shown in Fig. 8 is also seen in these two figures, but the

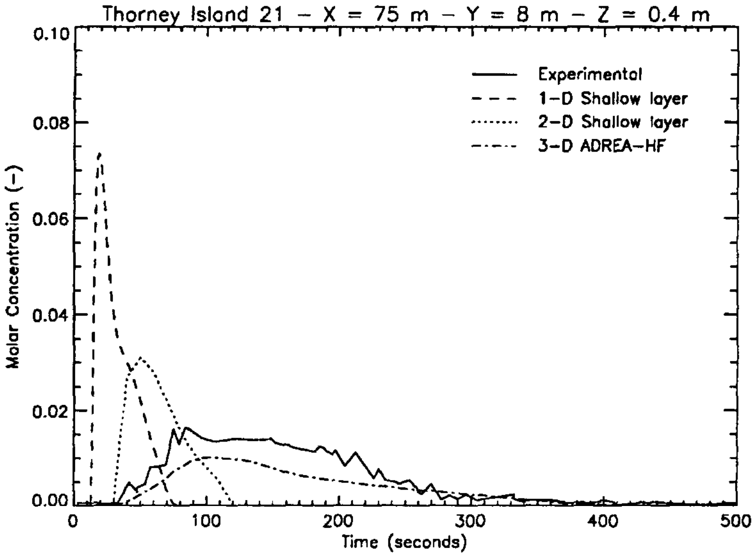


Fig. 9. Thorney Island 21. The sensor position is 25 m downwind the fence. Like in Fig. 8 the 1-D model fails to predict the concentration level.

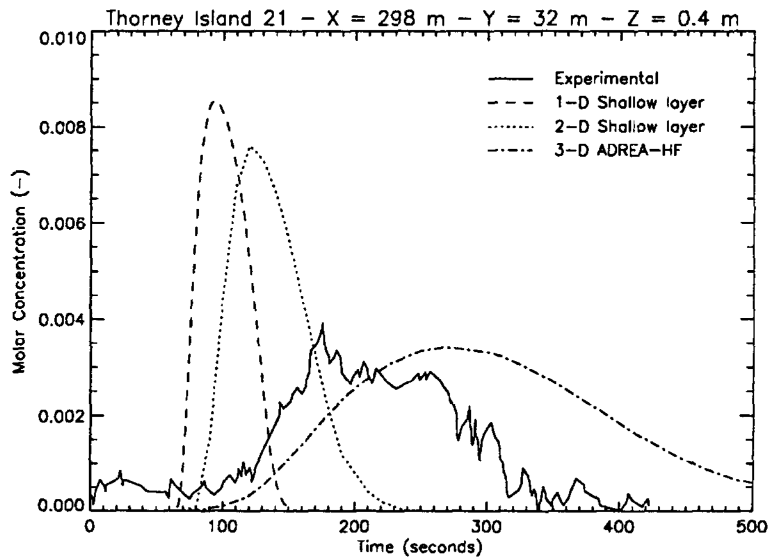


Fig. 10. Thorney Island 21. The sensor position is here 250 m downwind the fence. The disagreement between the 1-D calculation and the measured curve is now reduced, due to the smaller influence of the fence.

discrepancy between the 1-D calculation and the experimental curve diminishes when the distance from the fence increases. This is caused by the reduced influence of the obstacle. The agreement between the 3-D calculation and the experiment is very satisfactory in both cases.

From this exercise it can be concluded that if the influence of three-dimensional obstacles has to be modelled properly, a fully 3-D (or at least a 2-D shallow layer) model calculation is required.

## 8. Summary and conclusions

A computer code package for dense vapour cloud dispersion has been presented. The package consists of three models: a detailed fully three-dimensional model and two models (a 1-D and a 2-D) based on the shallow layer concept.

The package has been validated against three different field experiments: the Thorney Island trial Nos. 8 and 21 and the EEC propane release No. 55.

The first field test was an instantaneous, isothermal release over a flat terrain. The comparison between the experimental and the calculated results showed that all three models were applicable under these conditions.

The EEC test was carried out with a cold jet source and a fence (perpendicular to the flow), which was removed during the experiment. Here the 1-D model predicted well the undisturbed jet, but was not able to simulate in detail the influence of the fence. However the predicted concentration level was in acceptable agreement with the measured data. The agreement between the experiments and the 3-D calculations was good except very close to the boundary of the cloud, where the concentration history shows an intermittent structure.

Finally the second Thorney Island trial (with a semicircular fence) showed that in the case of a three-dimensional obstacle, a 3-D calculation is necessary in order to obtain a satisfactory prediction. In this case the 1-D calculation failed, due to the inherent two-dimensional description of the three-dimensional obstacle.

Based on the above validation exercise, one can conclude that the model to be selected for a given case should have the same dimension as the geometry to be described. Thus, for the case of dispersion in flat terrain, where the main concern is the concentration distribution on ground level in the downwind direction, the application of the 1-D model will probably give satisfactory results. If 3-D obstacles (e.g. buildings) are present and detailed information of the distribution is needed, the 3-D model is required. However, if the computer requirements are prohibitive (e.g. in the case of a parametric study with the 3-D model), it seems possible to obtain a reasonable simulation by choosing a model with one dimension lower than the geometry (e.g. a 3-D fence simulated by a 2-D model). The required CPU-time and memory size will in that case be significantly reduced.

Before definite conclusions can be drawn, more validation exercises have to be performed with the dispersion code package presented here.

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