

EVALUATION OF CFD MODELLING OF GAS DISPERSION NEAR BUILDINGS AND COMPLEX TERRAIN

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Uncertainties in Computational Fluid Dynamics (CFD) modelling of gas dispersion in the vicinity of buildings and complex terrain have been investigated in two recent studies reported here. The EMU project (*Evaluation of Modelling Uncertainty*) evaluated the variability of results due to the way in which a CFD code is applied and the accuracy of predictions for realistic scenarios. The second study focused on the applicability of CFD for modelling dense gas dispersion over much larger distances around an industrial site located in complex terrain. These studies have provided useful insights on the modelling strategies which can be used to tackle such applications and the likely accuracy of the predictions.

Keywords: CFD, dispersion, buildings, complex terrain, uncertainty

INTRODUCTION

Currently, a range of 'simple' tools are used to predict the dispersion of gases over flat terrain; however, actual industrial sites are usually much less straightforward and involve complex topography and buildings. CFD techniques offer the capability to simulate realistic industrial problems in greater detail and its use, with the widespread availability of sophisticated commercial software packages and powerful workstations, for safety-related applications is increasing.

EVALUATION OF MODELLING UNCERTAINTY

The validity of CFD predictions is generally uncertain for two important reasons. Firstly, the way in which a CFD code is applied to a specific problem depends on the constraints on staff costs, timescales and computer resources, and can have a critical impact on the final results. Secondly, there is a disparity between the generally simple scope of model validation studies and the complexity of the actual industrial scenarios. To investigate these problems, the European Commission funded the EMU project (*Evaluation of Modelling Uncertainty*). The specific objectives were:

- to evaluate the spread in results due to the way in which a CFD code is applied;
- to evaluate the accuracy of CFD predictions in large, complex gas dispersion situations.

The EMU project involved a group of four organisations undertaking CFD simulations for a series of realistic near-field dispersion test cases. The organisations were: WS Atkins Consultants Ltd (UK); EnFlo Research Centre, University of Surrey (UK); ARIA

Technologies (France); and NCSR “Demokritos” (Greece). The project was coordinated by WS Atkins. All four partners undertook CFD modelling and EnFlo undertook wind tunnel modelling of certain cases. An overview is presented here of the methodology adopted and the results obtained. Full details are reported by Hall (1).

Methodology

CFD Codes. A key aspect of the project was the use of the same CFD code by all four partners for each particular test case. Actually, two CFD codes were used during the course of the project. Most of the cases were tackled using a commercial CFD code, STAR-CD (Computational Dynamics Ltd (2)). The second code, ADREA-HF (Andronopoulos *et al.* (3)), has been developed specifically for atmospheric dispersion modelling by NCSR “Demokritos” (Greece) and the Joint Research Centre, Ispra (Italy).

Test Cases. The test cases were chosen to provide information on a number of specific factors which have an important influence of the variability and accuracy of CFD results. These factors included: the resources available to the modeller, the problem geometry, gas release conditions (source terms), meteorological conditions, and mesh architecture. The test cases were conceived during the course of the project, rather than being drawn from existing datasets, in order to ensure that each new test case geometry had not been previously encountered by any of the four partners. Furthermore, the test cases were all tackled ‘blind’, that is without reference to any wind tunnel data.

The test cases are summarised in Table 1. They were specified in three stages of increasing complexity, as noted below.

Table 1 Summary of Test Cases

	Stage A			Stage B							Stage C	
	A1	A2	A3	B1	B2	B3	B4	B5	B6	B7	C1	C2
continuous	✓			✓		✓		✓	✓	✓	✓	
transient		✓	✓		✓		✓					✓
area source	✓											
simple jet		✓				✓		✓	✓	✓		
simple cloud			✓									
‘realistic’ jet				✓							✓	
‘realistic’ cloud							✓					✓
buoyant		✓						✓				
neutrally buoyant	✓								✓	✓		
dense			✓	✓	✓	✓	✓				✓	✓
L-shaped building	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
additional building						✓	✓		✓	✓		
cliff									✓	✓		
trench										✓		
industrial site											✓	✓
atmospheric conditions	D5	D5	D5	F2	F2	D5	D5	F2	F2	F2	D5	D5
wind direction	0	45	45	45	45	255	45	45	345	345	N	NW
wind tunnel case	✓	✓				✓		✓	✓		✓	
CFD code: STAR-CD	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
ADREA-HF								✓		✓		

- Stage A comprised three cases, A1 to A3, involving a simple building on flat ground. The cases were modelled using STAR-CD. Simplicity was an important consideration because three of the four partners had no prior experience of this code. For this reason, also, only neutral atmosphere and isothermal conditions were considered.
- Stage B incorporated increases in complexity of the geometry (*i.e.* terrain, obstacles and number of buildings), release conditions (*i.e.* two-phase and non-isothermal releases) and meteorology (*i.e.* stability and wind speed). There were a total of 7 test cases. Phase I comprised four cases, B1 to B4, all of which were tackled using STAR-CD. Phase II comprised cases B5 to B7 and involved the ADREA-HF code for the first time.
- Stage C concerned an actual industrial site, featuring numerous buildings and complex local topography. Two scenarios involving chlorine releases were studied.

In addition to the factors described above, it was possible during the course of the project to observe the importance of the user's familiarity with the CFD code. At the start of the project only WS Atkins was familiar with the STAR-CD code and only NCSR "Demokritos" was familiar with the ADREA-HF code. Short training courses were held for the purpose of learning how to run the software packages. Much more time is needed, however, for users to become familiar with such complicated tools. The series of test cases provided the opportunity to assess how much time was really needed for experienced dispersion modellers to switch codes.

Wind Tunnel Modelling. Experiments were performed in EnFlo's large stratified wind tunnel (working section measuring 20m long x 3.5m wide x 1.5m high) at a model scales between 1/133 and 1/250. Measurements were made of mean concentrations using an 18-channel FID gas sampling system. Continuous jet releases of dense, buoyant and neutrally-buoyant gases have been simulated in neutral or stably stratified atmospheres.

Example Results. Figures 1 and 2 show typical meshes used for the simplest and most complex cases respectively. Results were presented in the form of iso concentration surfaces (examples in Figures 3 and 4), cross stream concentration profiles (Figure 5) and vertical concentration profiles (Figure 6). Figures 5 and 6 also show the way in which results were plotted to demonstrate the differences between each partner's results (P1...P4) and the experimental (wind tunnel) data. For transient releases, presentation and comparison of results is less straightforward; Figure 7 shows a typical comparison between cloud shapes predicted by CFD with those predicted by a 'simple' dispersion model, HGSYSTEM (Post (4)).

Analysis of Results. The CFD results were analysed in a number of ways:

- a qualitative assessment of the four partner's results for each release;
- a comparison of overall cloud quantities of practical relevance, such as peak concentration-downwind distance and concentration-width plots;
- a statistical analysis for point-based results, for the cases for which wind tunnel results were available. Two measures were used, namely the geometric mean bias and the geometric variance, as defined by Hanna *et al.* (5);
- a comparison with the results of HGSYSTEM.

Comparison between Different CFD Modellers' Results

CFD requires a very large number of inputs from the user, particularly when designing the mesh, and this inevitably gives scope for variability. During this project, the variability was indeed found to be large. It is difficult to summarise this simply in quantitative terms, but the following gives some indications:

- Considering a concentration level of 1% of the source concentration, for illustrative purposes, the maximum of the hazard ranges predicted by the four partners varied by a factor of 1.5 to 5 greater than the minimum of the predicted hazard ranges. The variation of overall cloud width was of a similar magnitude.
- At higher concentrations, the magnitude of the differences was generally smaller, e.g. for a case involving a continuous dense jet release at a real industrial site, the maximum of the hazard ranges was a factor of 2.4 greater than the minimum at the 10% concentration level and a factor of 3.1 greater at the 1% level.

The particular aspects which contributed most to variability were found to be:

Human factors. Familiarity with the CFD software was an important issue, since the initial learning phase took about 4-6 man-months. User errors were not uncommon, such as the wrong sign for the ground heat flux in a stable atmosphere case (in which case, scatter relative to experiments increased to a factor of 10^4). Interpretation of specifications, conversion of concentrations from mass fractions, used in the CFD models, to other units, and extracting cloud size information caused a surprising number of mistakes.

Mesh design and numerics. This depends on the available computing hardware and project timescales, which force the modeller to consider smaller and coarser resolution meshes than desirable. Each modeller followed their own or published 'design rules' for domain sizes, but there was no consensus between the details of such rules. Crosswind transport was not always adequately accounted for. Preliminary scoping calculations were helpful to determine appropriate domain sizes. Solutions obtained using finer meshes and higher-order differencing schemes showed much more flow structure in the vicinity of buildings, and tended to exhibit reduced scatter, relative to the experimental data, in comparison with the solutions obtained with coarse meshes and upwind differencing. General mesh architecture and the extent of local mesh refinement varied substantially.

Source conditions. These are fundamental inputs to any dispersion model and tuning of other model parameters will not make up for errors here. Variability was greatest for large-scale instantaneous releases for which the initial cloud shape and flow conditions inside the cloud are uncertain for realistic scenarios.

Turbulence model. For STAR-CD, changes to the k- ϵ model by one partner produced minimal differences in dispersion results relative to the standard model. For ADREA-HF, the differences were more substantial (e.g. hazard range doubling) when the k- ϵ model was used instead of its default k-l model.

Atmospheric conditions. Inlet velocity profiles were similar, but inlet turbulence conditions varied considerably. Rather unrealistic profiles were used by some modellers; others used empirically-based profiles and checked them for self-consistency. For stably stratified cases, temperature profiles and ground treatment added to the variability.

Representation of geometry. Simplification is often necessary or desirable and depends upon the required and available precision of the geometry data. For the real site, the process involved the building shapes and locations being modified and small details and certain buildings being omitted.

Comparison of CFD and Wind Tunnel Results

The most important point demonstrated by the results was:

- The 'best' CFD solution (that free from any numerical errors) will not necessarily be the same as that from the experiments because of turbulence modelling inadequacies. A coarse mesh model can sometimes give better agreement than a fine mesh model, due to some cancelling out of mesh and turbulence modelling errors. This complicates the definition of accuracy.

Some overall conclusions relating to accuracy for continuous releases are given below:

- For hazard ranges, STAR-CD solutions (using the standard or modified k- ϵ turbulence model) tended to exceed experimental values by significant amounts, e.g. a factor of 2 to 3 greater at the 1% concentration level. In a few solutions, however, the hazard ranges were under-predicted.
- For STAR-CD, the agreement between predicted and measured concentrations, in neutral conditions, varied between about a factor of 5 and 100, with best performance at high concentrations and worst at low concentrations.
- There was little evidence that solutions based on a large number of cells (typically, 120k to 180k) are much better than those based on more modest numbers (typically, 60k to 80k). With finer meshes and higher-order differencing schemes, the results exhibit less scatter relative to experimental measurements, but the overall bias depends on the capabilities and limitations of the turbulence model.
- For ADREA-HF, there was a slight bias towards over-prediction in one case, but no significant bias in a complex, industrial case. For this case, the agreement between predicted and measured concentrations was within a factor of 10, even though numbers of mesh cells varied from about 35k to 130k.
- The limited evidence available suggests that the k-l turbulence model in ADREA-HF performs better than the k- ϵ model for atmospheric dispersion applications.
- Agreement for one stable atmosphere case (B5) was generally poor. The results obtained with STAR-CD showed huge spread, biased to under-prediction. One of the ADREA-HF solutions appeared to be much better, although the degree of uncertainty arising from the experiments themselves was significant.

EVALUATION OF A PRACTICAL APPLICATION

This second study considered CFD modelling of continuous releases (44 kg/s) and instantaneous releases (80 tonnes) of chlorine, in neutral (D5) and stable (F2) atmospheric conditions, around an industrial site located in complex terrain. Two wind directions were studied. The problem was much more difficult in modelling terms than those encountered in the EMU project, due to the more complex terrain effects (significant topography) and the

greatly increased downwind distances of interest. The EMU-C2 model shown in Figure 2 measured about 1 km long x 660 m wide and the ground height varied by less than ± 25 m relative to the release point. In this study, the main challenge was to balance the need to maintain reasonable near-source detail with a domain measuring some kilometres in length. In view of this, aspects of the CFD modelling strategies which needed close attention included:

- the size of domain needed to establish toxic dose contours around the industrial site;
- the design of the computational mesh and the accuracy with which buildings and structures are represented in a large-scale problem;
- simulation of the wind field over complex terrain, including the specification of realistic atmospheric conditions at the boundaries of the model domains.

Modelling Strategies

The general methodology comprised the following stages:

- a) Scoping calculations using HGSYSTEM to predict the dispersion of chlorine releases over unobstructed, flat terrain;
- b) CFD simulations of wind flow and chlorine dispersion over unobstructed, flat terrain;
- c) CFD simulations of wind flow and chlorine dispersion in a 4 km x 4 km region, using 100 m x 100 m planwise mesh resolution and including topography but excluding buildings and structures (the 'far-field model'). This was intended primarily to provide realistic atmospheric boundary conditions at the boundaries of the more detailed near-field model domain (see below).
- d) CFD simulations of wind flow and chlorine dispersion in a smaller region, measuring 2.5 km long x 1.6 km wide, using cells of planwise dimensions up to 32 m x 32 m to resolve the complex terrain, and including the site buildings (the 'near-field model').

To model the continuous two-phase jet release, HGSYSTEM was used to predict the complex initial jet behaviour and these results were then used to define a pure vapour source in the CFD model. This source was defined at the point where the aerosol fraction had dropped to about 1%. Numerical 'sinks' were defined to take account of the entrainment of air by the jet. The presence of tanks and pipework near the gas source were neglected, both in this case and also for the instantaneous release.

Lessons Learnt

For modelling of wind and dispersion behaviour in complex terrain, some key points arising were as follows:

- With a domain extending 2 km downwind of the source, each transient case had to be run for a modelled duration of about 20 minutes (compared to only 5 minutes in the EMU-C2 case). With over 100,000 cells in the near-field model, the computing time required was in excess of 5 days, which was felt to be at the upper limit of acceptability.
- The near-field domains were clearly not large enough to avoid the clouds impacting on the upwind and side boundaries in some cases. Some transient solutions had to be cut short for this reason and, in these cases, it was not possible to determine the relevant dose contours.

- The far-field modelling showed that the predicted wind fields varied rather significantly when 50 m x 50 m cells were used instead of 100 m x 100 m cells. Smaller cells (32 m x 32 m) were used in the near-field model to try to resolve the terrain effects more accurately.
- Using the far-field model results to define the atmospheric conditions at the near-field model boundaries proved to be difficult, mainly because the two meshes were not quite compatible for this operation. The approach eventually adopted was much simpler and only took account of the upwind fetch but not of wind variations across the width of the domain.

Regarding mesh resolution, it was judged that the details of the site buildings and structures would probably not affect the concentration distributions significantly after several hundred metres. Coarse representations were therefore implemented. It was judged that the extra effort involved in defining a more realistic geometry would probably not have yielded a major improvement in accuracy. For example, it was decided not to define storage tanks as being circular, since such details would have been purely cosmetic in view of the coarse mesh resolution. Clearly, it was not possible to model all the important features in accordance with the 'best practice' principles identified in previous studies.

Dispersion Results

For the flat terrain cases, the CFD results were compared with those obtained using HGSYSTEM. The main points arising from this were:

- For continuous releases in neutral (D5) conditions, the peak ground level downwind concentrations predicted by the CFD models generally exceeded the HGSYSTEM values by a factor of 1.5-2. In stable (F2) conditions, the CFD solutions under-predicted concentrations by a factor of 2-3.
- For the instantaneous release, the CFD solutions showed both under- and over-predictions of peak ground level downwind concentrations by a factor of up to 2.
- The results suggest that the performance of the k-ε turbulence model is worse for stable atmospheres than for neutral atmospheres.

For the near-field dispersion cases, the following trends were observed for the effects of the complex site and local terrain, in comparison with the flat terrain cases:

- For the continuous jet release in neutral (D5) conditions, the peak concentrations between 500 and 2000 m downwind of the site were 3-5 times less for the two wind directions considered. In stable (F2) conditions, the peak downwind concentrations were roughly 2-4 times less for both wind directions.
- For the instantaneous release, the peak concentrations at 500 m downwind of the release point were a factor of 1.3-2.4 higher than for flat terrain. Further downwind, however, the peak concentrations were lower than for flat terrain, eg. at 2000 m the peak concentrations were 30-60% less for both wind directions.

CONCLUSIONS

For near-field atmospheric dispersion modelling, the geometric scales of interest range from less than 1m up to 1-2km, forcing the user to compromise between accuracy and computational cost

when designing the mesh. It is worth stressing that, for practical 3D simulations of dispersion in the wake of one or more buildings, one cannot hope to attain mesh independent solutions with current work-station based CFD technology. Choice of numerical model and mesh design are thus highly important, and this is a major cause of variation between different modellers' results.

It could be argued that the accuracy required of CFD simulations for near-field dispersion need only be equivalent to the accuracy currently achieved by analytical flat terrain models, (*ie.* to within a factor of 2) or that they should be much lower. However, from the above arguments, a major problem with such an approach is that the potential variability of CFD results between different modellers (and, therefore, organisations) would be great if coarse resolution models were used.

The use of a single CFD model to provide information both for on-site considerations and for evaluating far-field off-site effects is rather over-ambitious for the current generation of 'standard' workstations. However, if targeted more specifically at near source or on-site or far-field effects, then CFD can provide useful information on the combined effects of complex releases, realistic atmospheric conditions and the effects of buildings and complex terrain.

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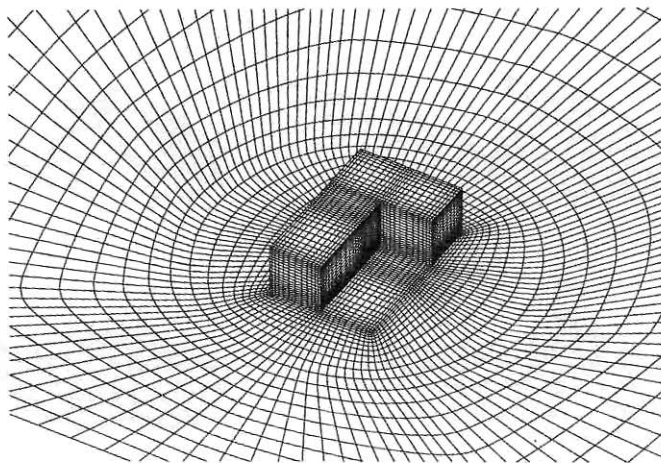


Figure 1 Sample mesh used for case A1

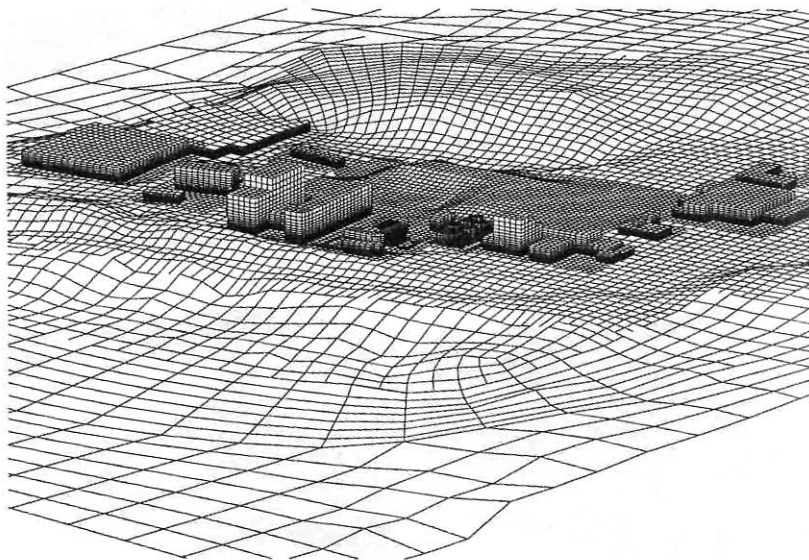


Figure 2 Sample mesh used for case C2

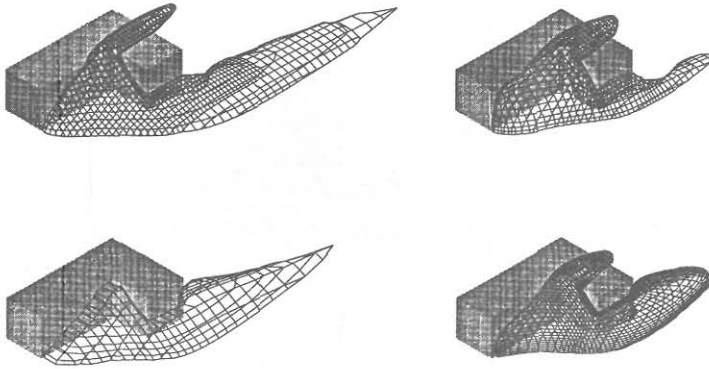


Figure 3 Comparison of partners' 5% iso-concentration surfaces for case A1

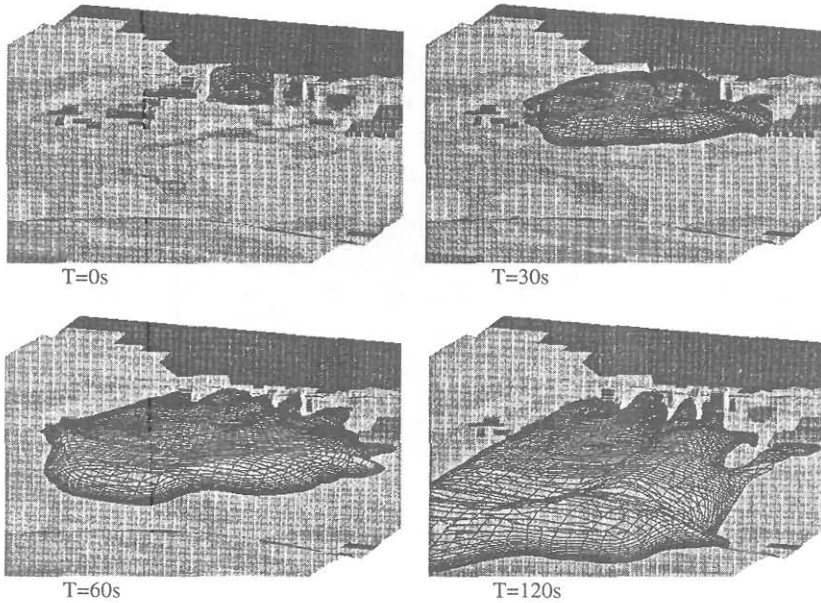


Figure 4 Sample sequence of 0.1% iso-concentration surface 'snapshots' for case C2

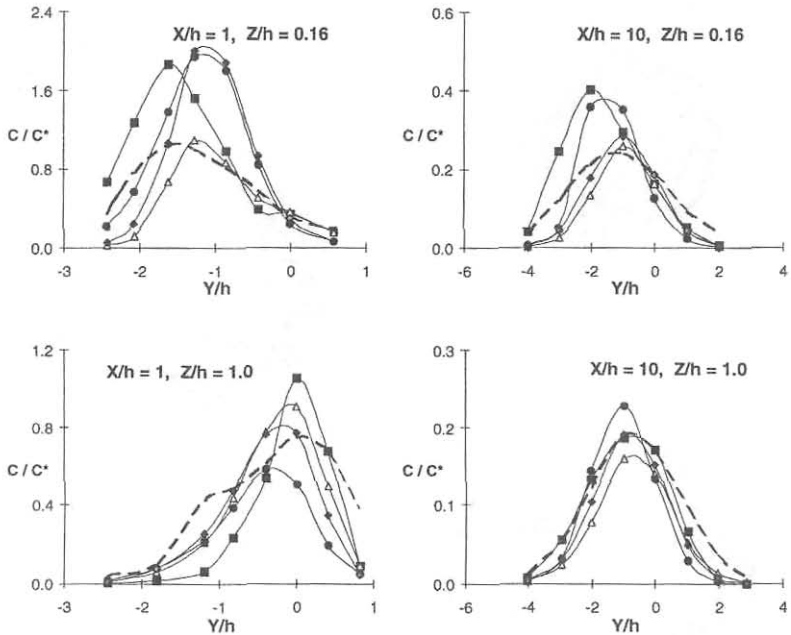


Figure 5 Cross-stream profiles of normalised concentration, $C/C^* = C.U_h.H^2/C_s.Q_s$ from CFD (partners P1-P4) and measurements, for case A1

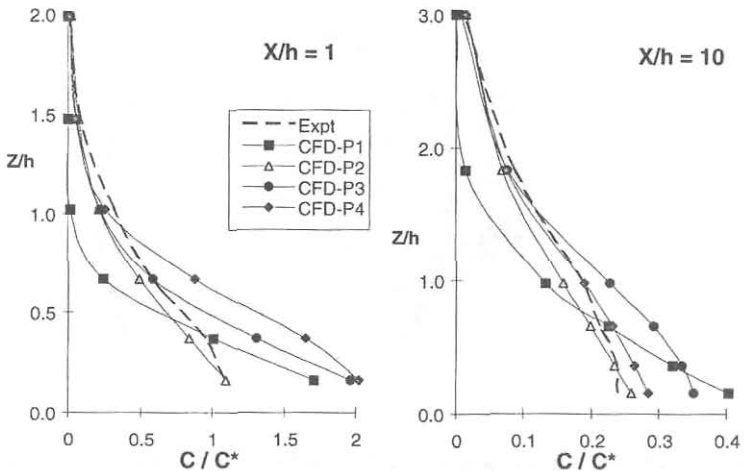


Figure 6 Vertical profiles of normalised concentration, $C/C^* = C.U_h.H^2/C_s.Q_s$ from CFD (partners P1-P4) and measurements, for case A1

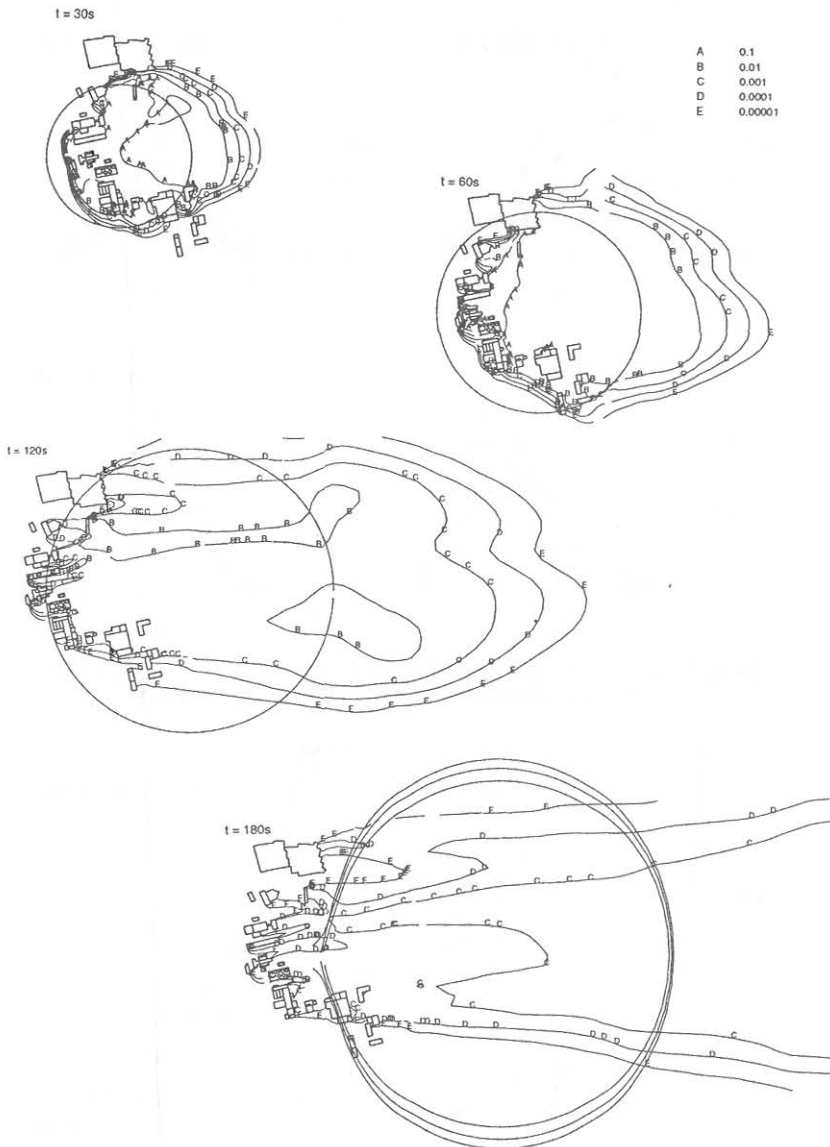


Figure 7 Comparison of ground level concentration contours predicted by a CFD model and HGSYSTEM for case C2

(HGSYSTEM concentrations: 10^{-2} @ $t=30, 60, 120s$; $10^{-3}, 10^{-4}, 10^{-5}$ @ $t=180s$)