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A Comparison between the uses of Passive Scalar Diffusion and Trajectory Following Techniques for Short Range Dispersion

by

J R Kemp

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Met O (APR)
(Atmospheric Processes Research)
Meteorological Office
London Road
Bracknell
Berks, RG12 2SZ

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1 Introduction

In this brief study, a comparison is made between two methods of calculating dispersion using numerical models of the fluid flow. The two methods are (i) following individual particle trajectories and (ii) using the advection of a passive scalar. These experiments were carried out within the confines of an atmospheric turbulence simulation, utilising the turbulent flow fields generated to perform the dispersion. Trajectory routines can involve a considerable increase in the computational intensity of a model and require a completely separate module to be written, whereas the use of a passive scalar tracer can be included as an extension to the already present active scalars in the model (e.g. potential temperature). Using particle trajectories, however, does away with the complicated and subtle problems inherent in tracer advection schemes, such as the generation of negative concentrations and implicit diffusion.

A comparison between the two methods was attempted using the techniques of Large Eddy Simulation (LES) under neutral conditions. Three types of advection scheme were used, namely the schemes of Piacsek-Williams, Van Leer and Leonard. These schemes are described below along with a description of the trajectory model used. Only dispersion out to reasonably short times (1000 seconds) has been examined so far.

2 Advection Schemes

Whether we are using a passive scalar or particle following, the underlying requirement is the same, i.e. a solution to the diffusion equation:

$$\frac{\partial c}{\partial t} + \underline{u}.\nabla c = \nabla.(K\nabla c). \tag{1}$$

where c is the concentration field, $\underline{u}$ is the velocity field and K is the diffusivity.

In the passive scalar approach, equation (1) is approximated using finite difference methods. The advective and diffusive terms are calculated separately, the same time-lagged scheme being used for the diffusive term with all three advection schemes.

The Piacsek-Williams (1970) scheme is centred in both space and time and is solved explicitly in time. The advective scheme for a scalar variable ϕ in one dimension is,

$$\phi_i^{t+1} = \phi_i^{t-1} - \frac{\Delta t}{\Delta x}(u_i^t \phi_{i+1}^t - u_{i-1}^t \phi_{i-1}^t)$$

where δt is the time-step used and δx is the grid spacing. u and ϕ are stored on a staggered mesh with u_i lying between ϕ_i and ϕ_{i+1}. It conserves both mass and mean square scalar and is the cheapest of the three to run. In regions of high gradient or strong advection, however, it will produce spurious oscillations leading to negative concentrations in the scalar field.

The other two schemes used are both TVD (Total Variance Diminishing) schemes, with the property that an initially positive field will remain positive for all time (positivity preserving), which is essential for the advection of our scalar concentration field. Unfortunately, to achieve this desirable result, a rather less desirable introduction of artificial diffusion is required. Furthermore the schemes are non-variance conserving and more computationally expensive to run.

The Leonard (1991) scheme (called ULTIMATE), is the most expensive to run, but has the advantage of being slightly less diffusive than the van Leer (1974) scheme. It uses a third order upwind scheme to calculate the scalar flux through a grid-cube face, which is then limited depending on the updated value falling within a certain range. The van Leer scheme is based upon a second-order upwind Lax-Wendroff scheme. It is faster than the Leonard scheme because the positivity preserving property is inherent in its base scheme and thus explicit limiting is not required.

3 The Trajectory Model

The method used for following particle trajectories is as follows. At each time-step, the velocity of each particle was estimated using a simple linear interpolation from the surrounding 8 gridpoints and the particle displaced by a distance $V_{int}\delta t$ in each coordinate direction, where V_{int} is the interpolated velocity in that direction and δt is the time-step. This method was found to produce accurately reversible trajectories and hence no higher order interpolation schemes were considered necessary. The test for reversibility in this case involved running a number of particles forward in time for 1000 timesteps through a turbulent velocity field held stationary in time, and then running them backwards form the end points for another 1000 steps. All the particles were found to return to their start-points to within a few percent of the distance travelled. Since LES has a finite resolution, only turbulent eddies on scales ranging between the domain size and mesh spacing, can be explicitly represented. There will be a significant proportion of turbulent energy at sub-grid scales (around 25% in the interior), and these motions must be parametrized in some way. This trajectory model uses a random walk type model involving the diffusivity obtained from the LES to account for sub-grid components. Random displacements in each of the three coordinate directions were given to the particles, where the random numbers had a Gaussian distribution of standard deviation σ_d given by

$$\sigma_d = (2K_{int}\delta t)^{\frac{1}{2}} \tag{2}$$

where K_{int} is the interpolated eddy diffusivity used within the LES. The results of this process are equivalent to those obtained from solving equation (1) if the diffusivity is constant. Since diffusivity is not constant in this simulation, however, it is found necessary to add an additional drift velocity of ∇K to account for this, without which particles tend to accumulate in regions where K is small e.g. at the ground. Reflective boundary conditions were imposed at both upper and lower boundaries, which are equivalent to the zero flux boundary conditions imposed for the schemes in section 2. This method, then, ignoring finite-differencing errors due to the time-step, is equivalent to solving (1). Tests showed that an initially well mixed distribution remained well mixed even after 10,000 seconds of simulation.

4 Runs

Initially, a reasonably steady, neutral boundary layer was setup by the following method. A 1-d run with a $10ms^{-1}$ imposed geostrophic wind was used to initialize the 3-d simulation, whose domain consisted of a 32 cubed set of gridpoints evenly spaced in the x and y directions and stretched in the z direction, covering $3200m$ horizontally and $1000m$ vertically. Turbulence was generated by disturbing the system from equilibrium with random velocity additions in the lower half of the domain. The value of the surface roughness, Z_0, used was $0.1m$. The boundary layer was then allowed 25,000 seconds to settle down to a reasonably steady state.

Two types of release were attempted, namely instantaneous point releases and instantaneous area releases. In both cases the release was made from halfway up the domain i.e. at 500m. The point source was simulated by setting the value for the passive scalar concentration, Q, to zero everywhere except on one gridpoint, or alternatively, (for the trajectory model), a number of particles (around 15,000) were released from the same point. The method for an area source was identical except that the particles or Q values, were released over an entire horizontal slice, spanning the domain.

At various times out to 1000 seconds after the release, dispersion data was stored. This included vertical concentration profiles, vertical spread (σ_z), mean height of the puff and vertical and horizontal slices through the domain.

5 Results

Figures 1 to 3 show vertical concentration profiles using trajectories and two advection schemes, Piacsek-Williams and Ultimate, respectively, for an area source situated at $500m$. Profiles are displayed for 10 times out to a maximum of 1000 seconds. Concentrations are plotted on an arbitrary scale. The profiles are encouragingly similar, (that produced from the van Leer scheme was indistinguishable from the Leonard scheme and is not shown here), and appear to suggest that there is little to choose between the four methods. It should be noted, however, that for the Piacsek-Williams scheme negative concentrations at individual points were produced, although the horizontal mean shown in the figure does not give an indication of this. Figure 11 displays a contour plot of concentration in a vertical (x-z) slice through the LES domain. Large areas of negative concentrations, shown by dashed lines, are clearly visible in the slice. Figures 4 and 5 show plots of σ_z and mean height against time for the four cases. The results are very similar out to around 500 seconds, but as time progresses further the simplistic Piacsek-Williams scheme tends to diverge away from the other schemes. The Ultimate scheme appears to give the results most similar to those from using trajectories.

The results from a point release, however, show up differences between the various methods much more clearly. Figures 6, 7 and 8 show concentration profiles produced from a point release at $500m$ using trajectory following, Piacsek-Williams advection and Ultimate advection respectively. The differences are much more clearly shown up. The release was made into a region of negative vertical velocity as is obvious from the downward progression of the concentration maximum as time progresses. The Piacsek-Williams profiles with large negative spikes contrast sharply with the smooth profiles produced using trajectory following methods. Ultimate advection produces profiles very similar to those in figure 6, but with increased spread in the vertical due to the implicit diffusion involved in such an advection scheme. The plots of σ_z and mean height (Figs 9 and 10), show a much greater variation between the different methods than in the area source case. Further point source runs have shown additionally that the individual performances of the various schemes compared to that of the trajectory following scheme, vary considerably with changes in initial conditions i.e. where the release was made from. No absolute correlation was found between the effects of releasing into updraughts or downdraughts and the performance of the various schemes.

6 Conclusion

This study has shown up some of the differences between methods of dispersion modelling. Trajectory following methods are clearly superior to scalar diffusion methods. They are more flexible and more statistical information (e.g. Lagrangian statistics following individual particles), can be retrieved from them. On the down side, however, they do introduce a significant increase in computational cost compared to the scalar advection methods. A simple advection scheme has a great deal of problems coping with point releases and the generation of negative concentrations is clearly unacceptable. There is little to choose between the two TVD (Total Variance Diminishing) schemes although the

Leonard Ultimate scheme performed slightly better in general. For a point source, however, the differences between these methods and trajectory following are still significant. Additionally use of these schemes does introduce a notable increase in cost, but not nearly so high as a suitable trajectory scheme.

References

Piacsek, S.A. and Williams, G.P. (1970): Conservation properties of convection difference schemes. *J. Comp. Phys.* **6**, 392-405.

Leonard, B.P. (1991): The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection. *Comput. Methods Appl. Mech. Engrg.* **88**,17-74.

Van Leer, B. (1974): Towards the ultimate conservative difference scheme. II. Monotonicity and conservation combined in a second-order scheme. *J. Comp. Phys.* **14**, 361-370.

Figure Captions

Figure 1 – Vertical concentration profile using trajectory method from an area source.

Figure 2 – Vertical concentration profile using Piacsek-Williams scheme from an area source.

Figure 3 – Vertical concentration profile using ULTIMATE scheme from an area source.

Figure 4 – Growth of σ_z with time using all four methods from an area source.

Figure 5 – Variation of mean height of plume with time using all four methods from an area source.

Figure 6 – Horizontally integrated concentration profiles using trajectory method from a point source.

Figure 7 – Horizontally integrated concentration profiles using Piacsek-Williams scheme from a point source.

Figure 8 – Horizontally integrated concentration profiles using ULTIMATE scheme from a point source.

Figure 9 – Growth of σ_z with time using all four methods from a point source.

Figure 10 – Variation of mean height of plume with time using all four methods from a point source.

Figure 11 – Vertical slice through concentration field generated from an area source using the Piacsek-Williams scheme. Solid and dashed lines indicate positive and negative concentrations respectively.

Figure 1

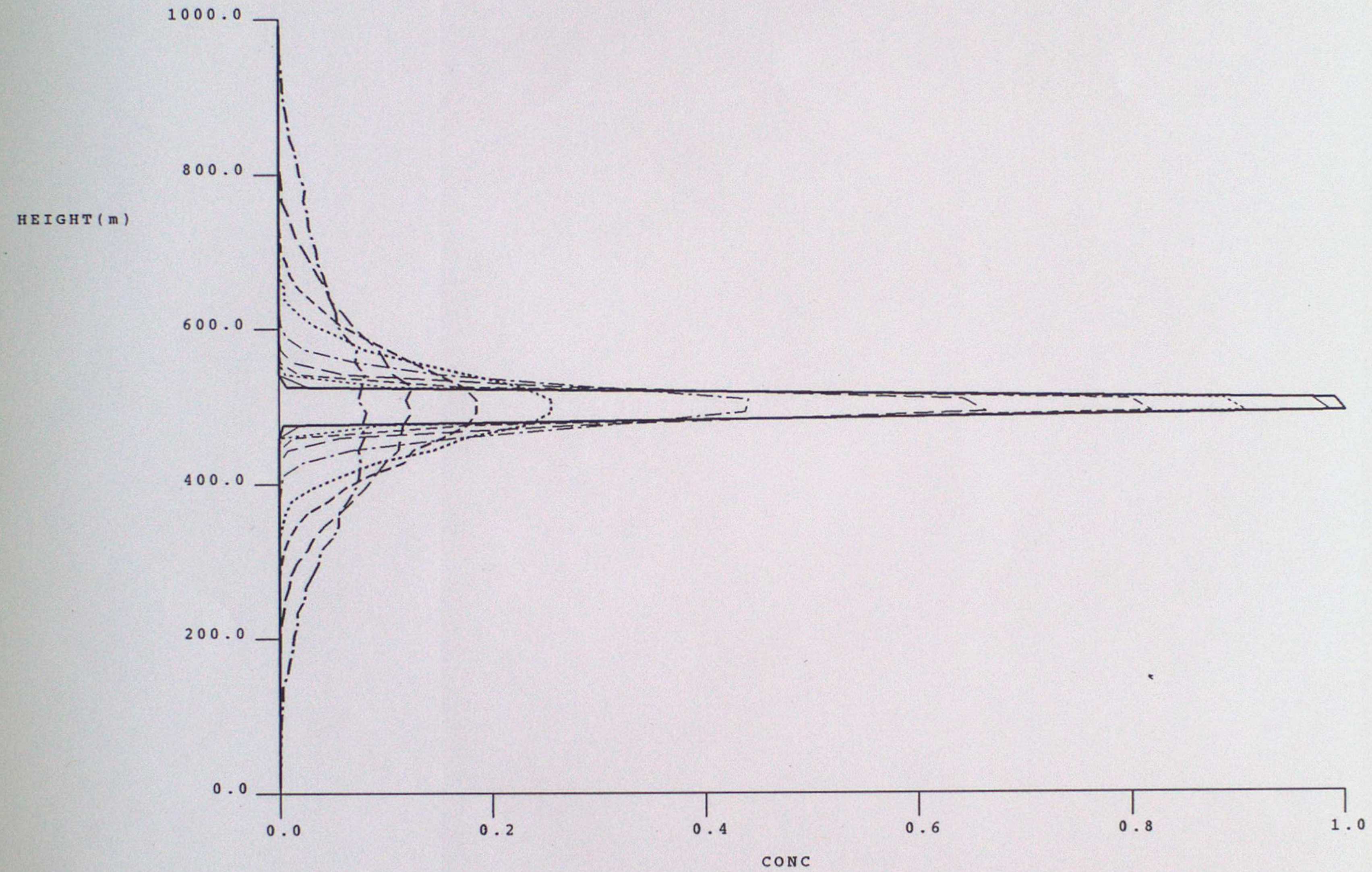
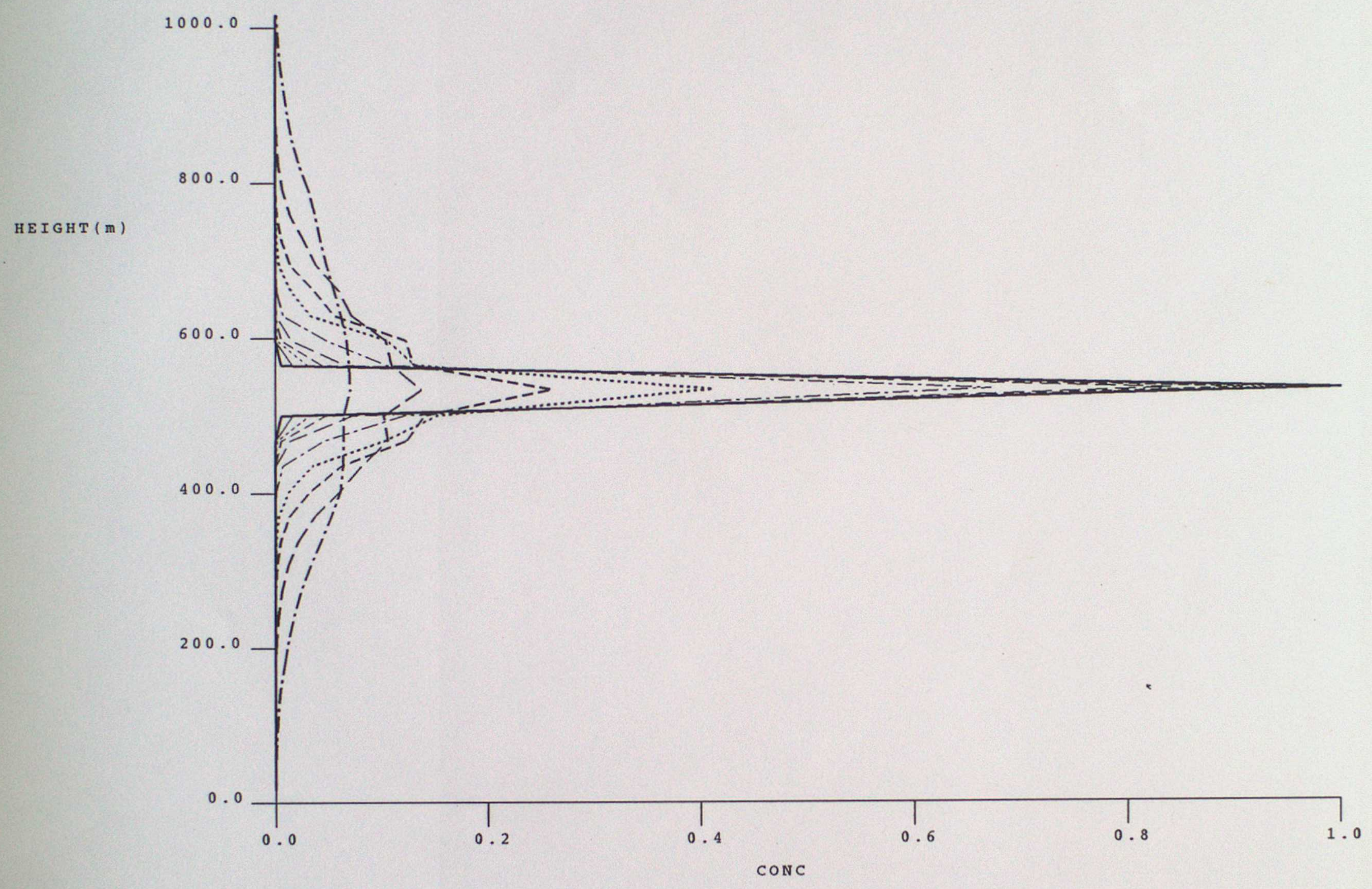


Figure 2



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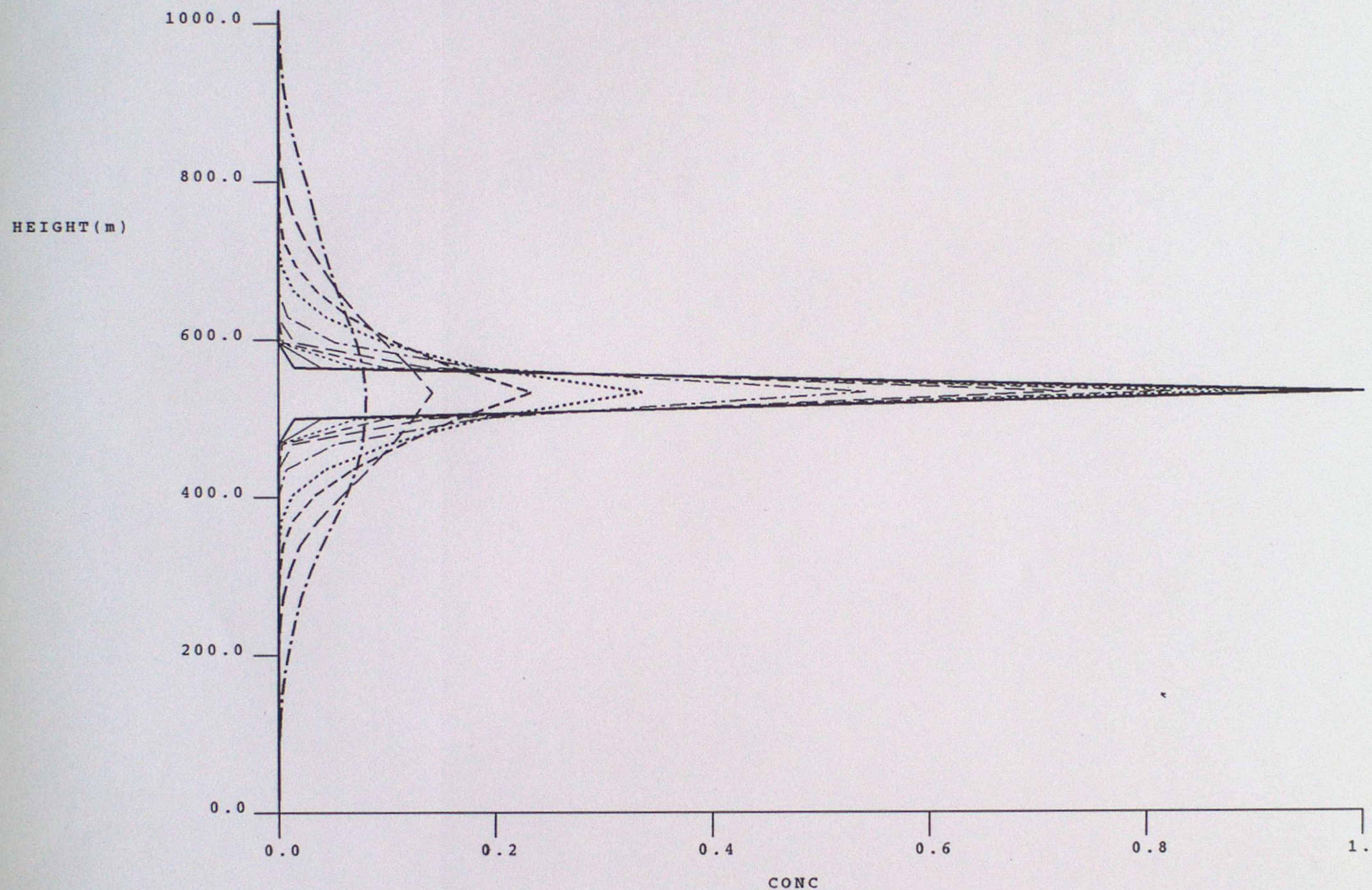


Figure 4

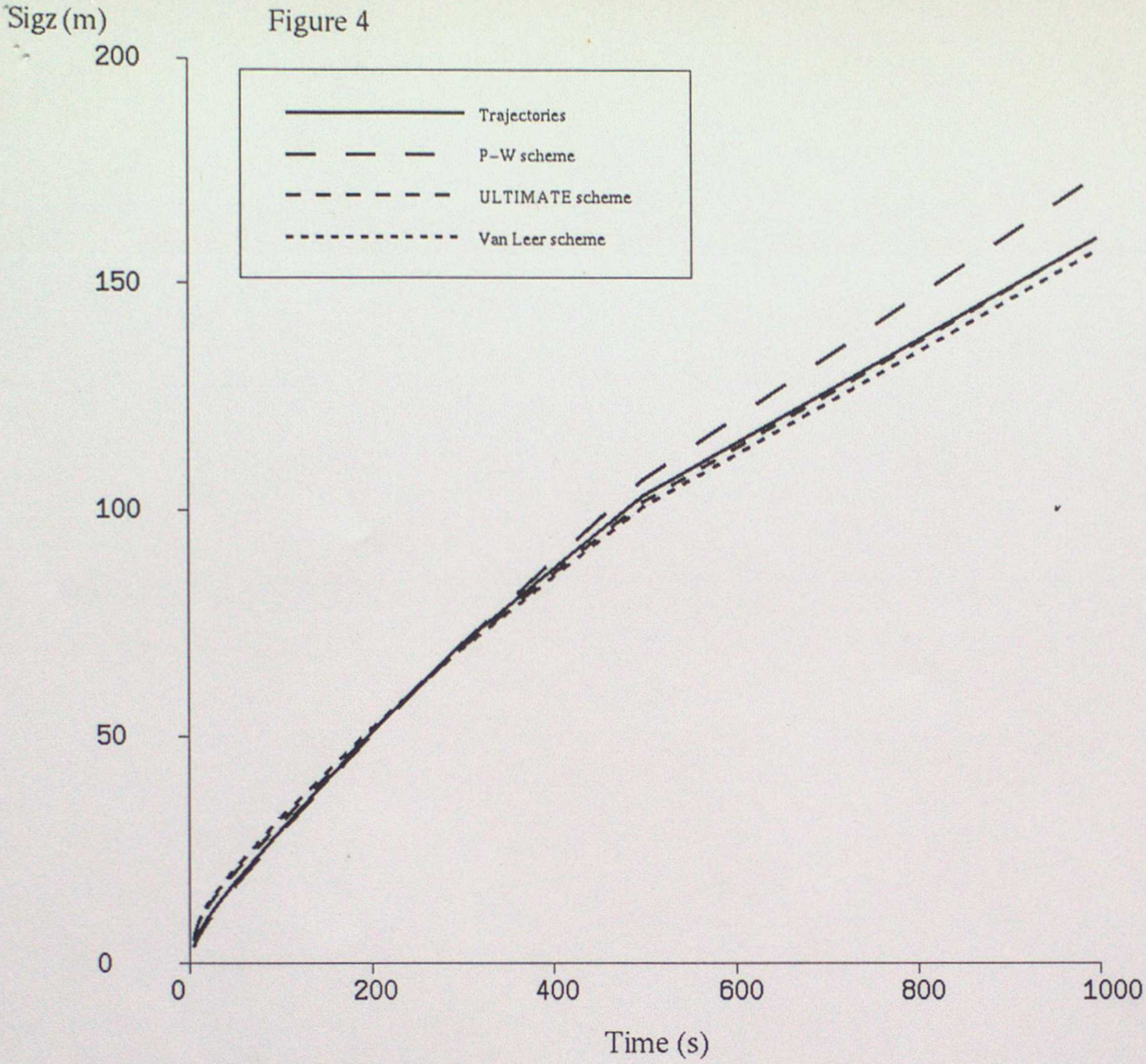

Sigz (m)
200
150
100
50
0
0
200
400
600
800
1000
Time (s)
Trajectories
P–W scheme
ULTIMATE scheme
Van Leer scheme

Figure 5

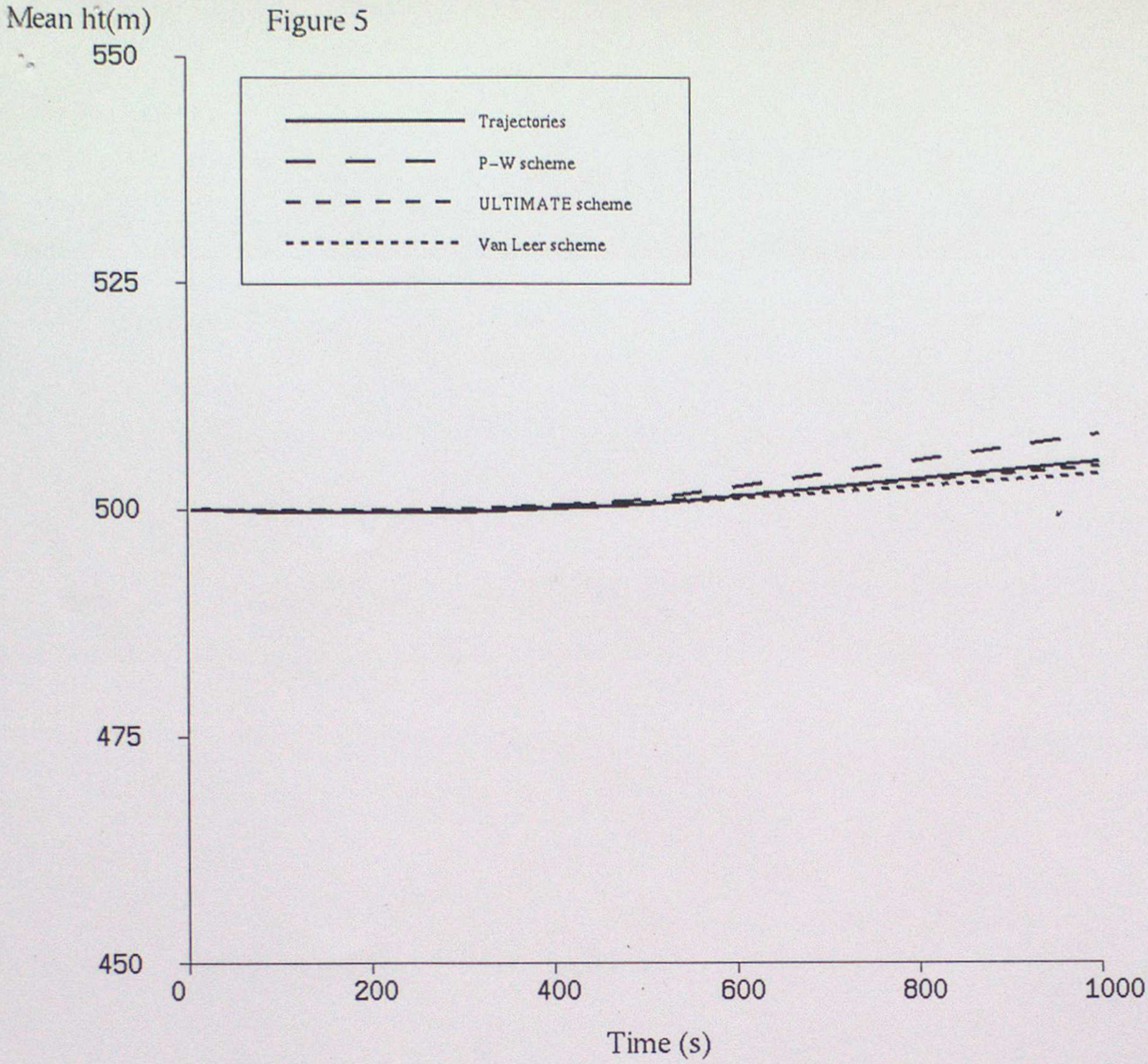

Mean ht(m)
550
525
500
475
450
0
200
400
600
800
1000
Time (s)
Trajectories
P-W scheme
ULTIMATE scheme
Van Leer scheme

Figure 6

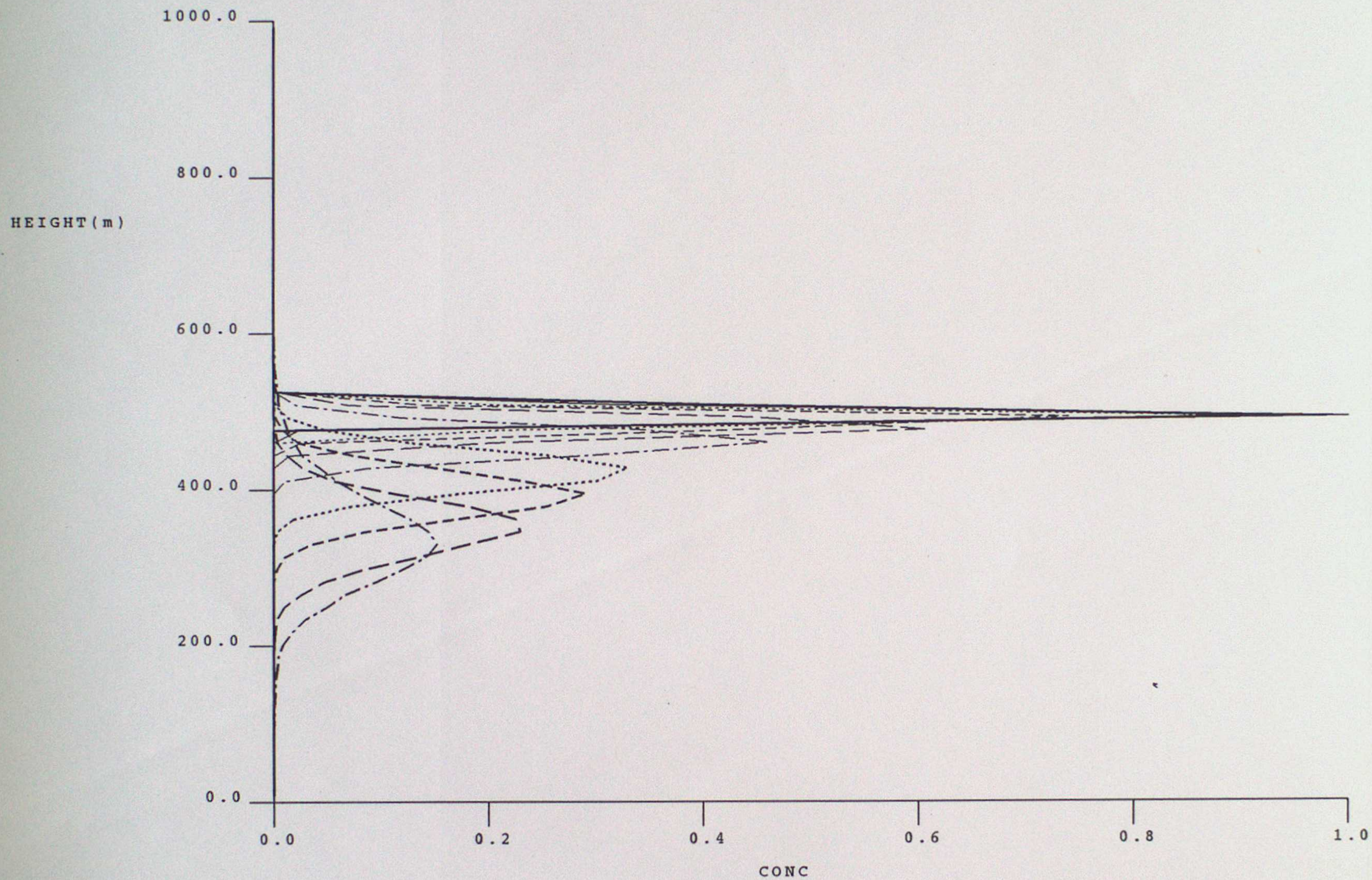


Figure 7

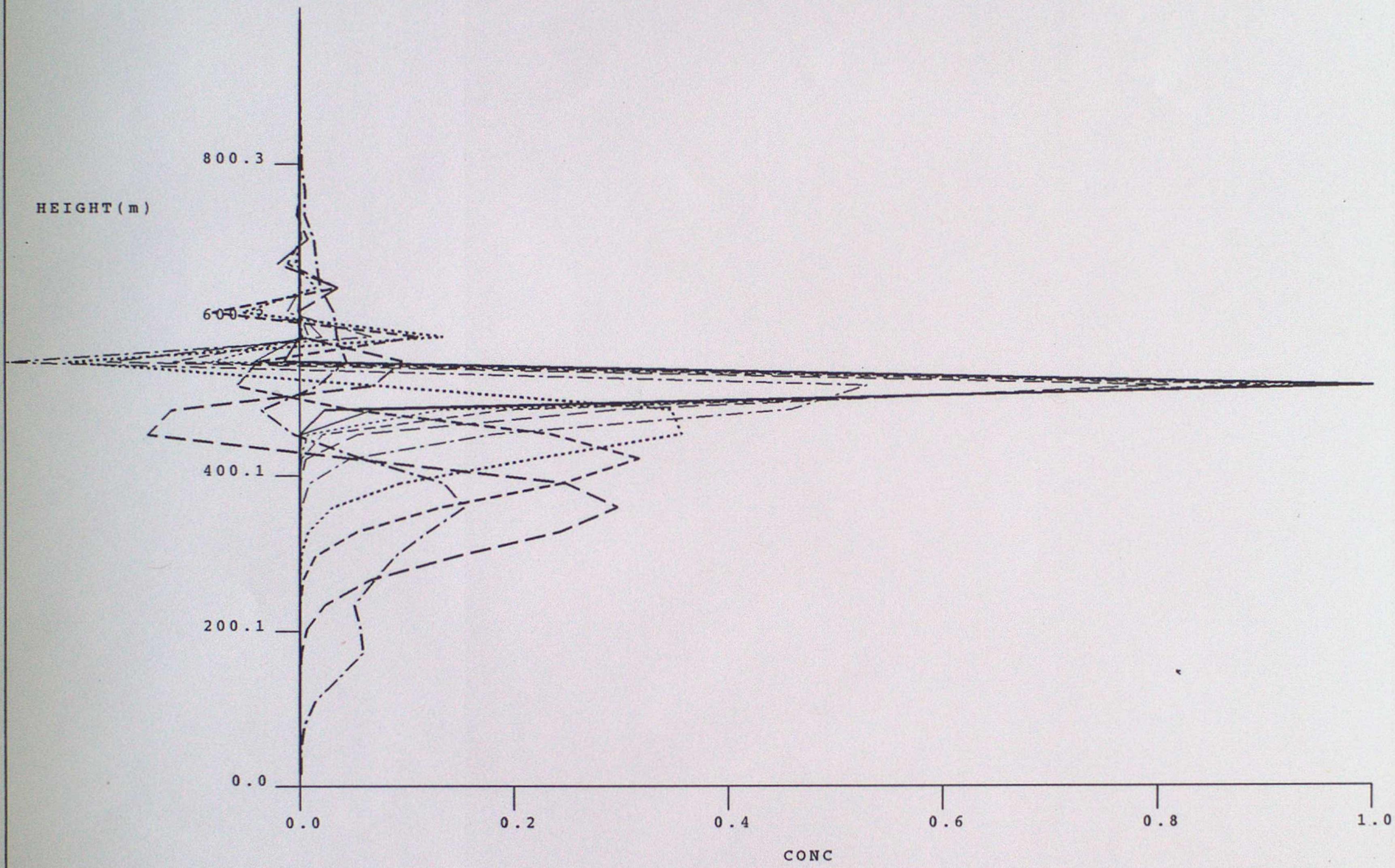


Figure 8

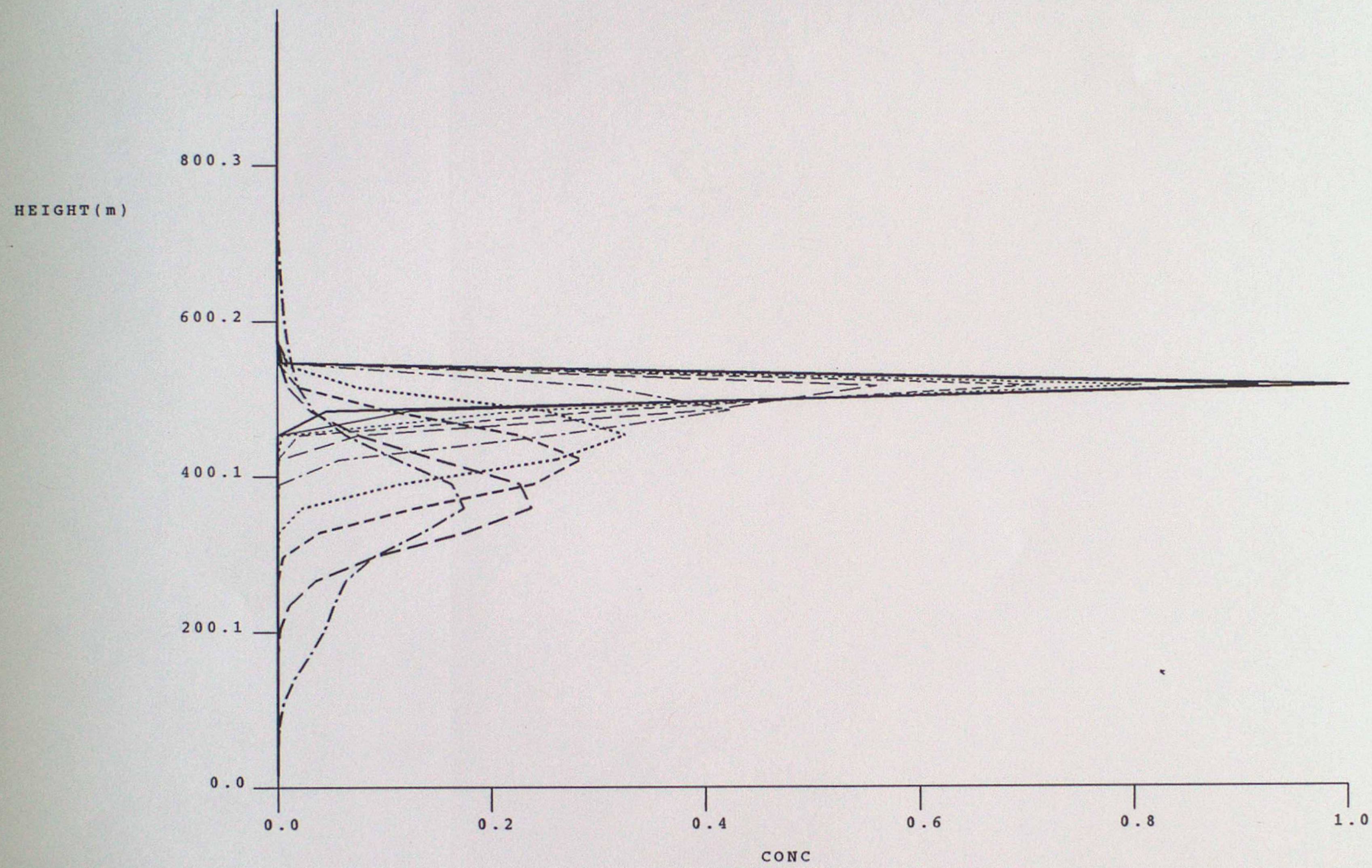


Figure 9

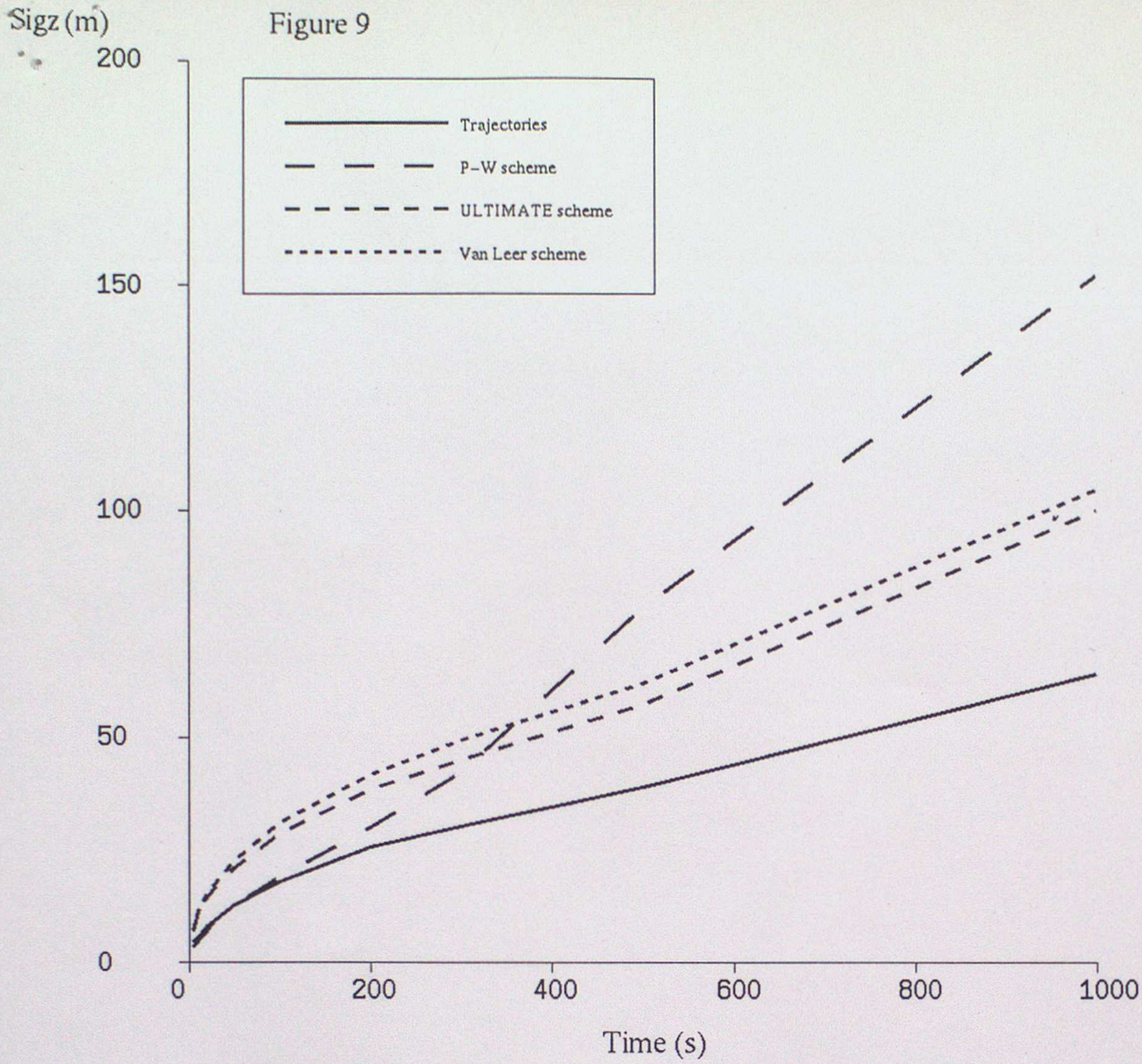
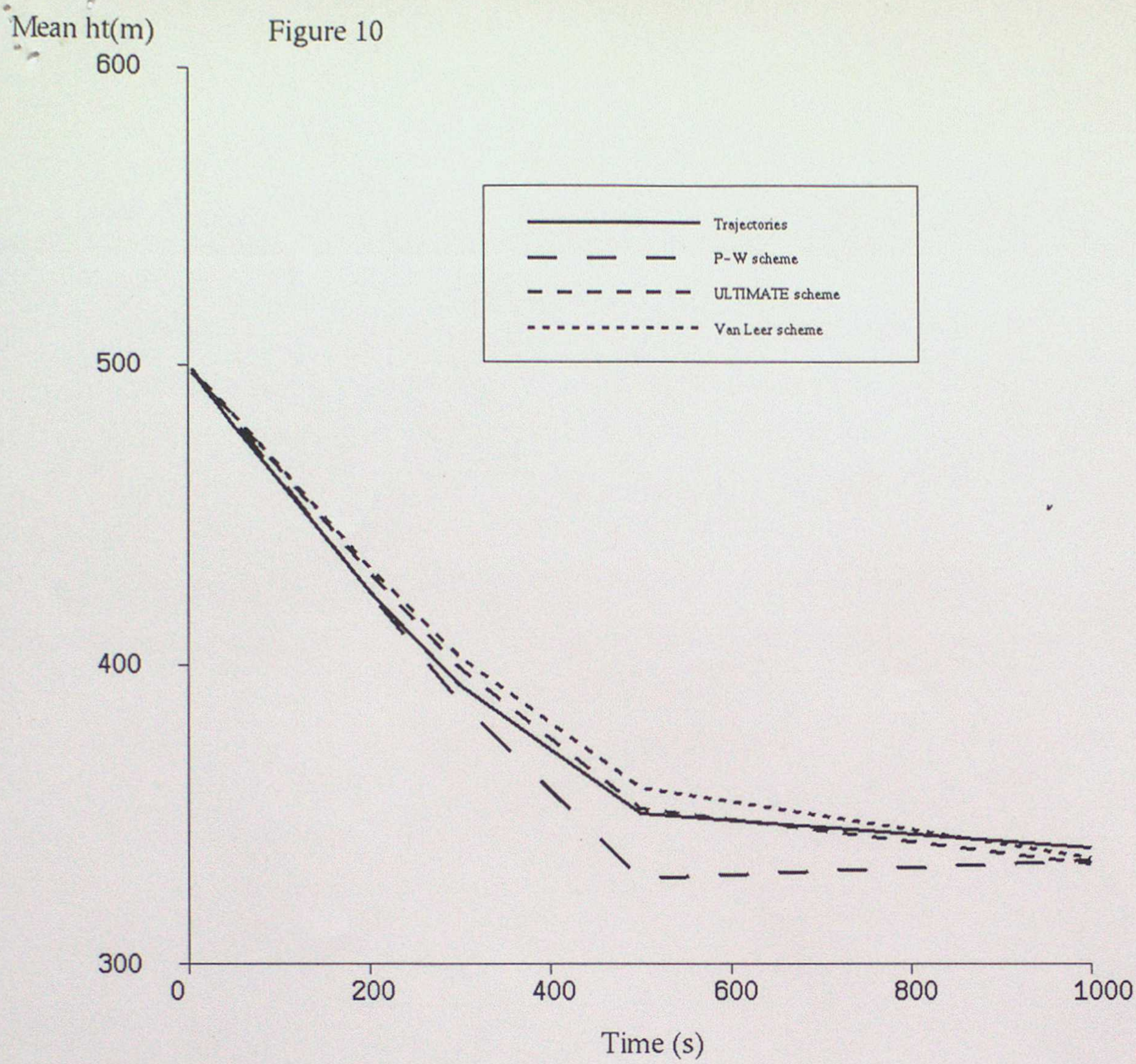
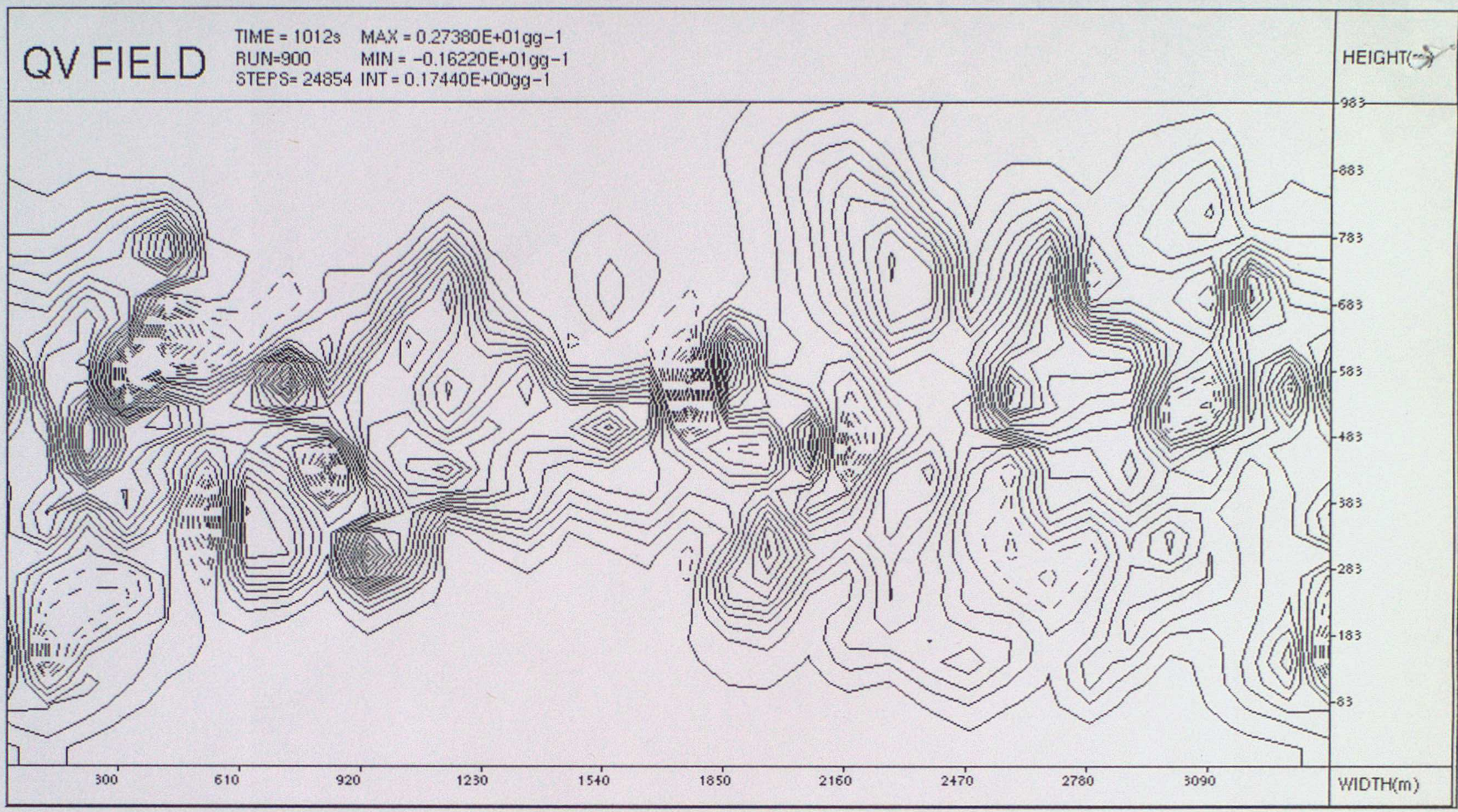

Sigz (m)
200
150
100
50
0
0
200
400
600
800
1000
Time (s)
Trajectories
P-W scheme
ULTIMATE scheme
Van Leer scheme

Figure 10



Mean ht(m)
600
500
400
300
0
200
400
600
800
1000
Time (s)
Trajectories
P-W scheme
ULTIMATE scheme
Van Leer scheme

FIGURE 11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STEPS= 24854 INT = 0.17440E+00gg-1
HEIGHT
983
883
783
683
583
483
383
283
183
83
300
610
920
1230
1540
1850
2160
2470
2780
3090
WIDTH(m)