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Timestep splitting in Lagrangian marine dispersion models

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TIMESTEP SPLITTING IN LAGRANGIAN MARINE DISPERSION MODELS

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Introduction

Lagrangian mathematical models, based on random walk methods, are well-established tools for the assessment of discharge dispersion in the aquatic environment. At HR Wallingford, the PLUME-RW suite of Lagrangian dispersion models is in regular use, and is applied with two-dimensional (2D) and three-dimensional (3D) finite element flow models. The range of applications is currently:

- Dissolved pollutant dispersion; for conservative or decaying pollutants.
- Particulate pollutant and suspended cohesive sediment dispersal, deposition and re-suspension.
- Non-cohesive sediment transport.
- Oil slick transport and fate.

Whilst Lagrangian models have long been acknowledged as practical and highly flexible tools for assessing pollutant dispersion in the marine environment, there remain limitations in their application, largely associated with timestep sensitivities. In particular, as discussed by Mead [1], sensitivities associated with the representation of vertical mixing processes have been identified. These sensitivities have been considered in recent years by various authors, and both pragmatic and rigorous mathematical solutions have been proposed. This paper presents an approach aimed at improving accuracy over the traditional approach, while avoiding excessively long model run times.

Recently, Ross and Sharples [2] have reviewed in detail the criteria for timestep selection in Lagrangian models with spatially-varying diffusivity, and have presented methods for minimising boundary effects and the effects of density discontinuities in such models. The work presented in this paper utilizes the Ross and Sharples [2] analysis, which is referred to hereafter as RS04. In both 2D and 3D models, techniques including the use of shorter timesteps for vertical processes than for horizontal processes are employed.

In the context of the present work, the term “2D model” refers to a Lagrangian model which takes the results of a 2D-in-plan, depth-averaged flow model as input data. A “3D model” uses the results of a fully 3D flow model, based on sigma-coordinates. The 2D modules of the PLUME-RW suite are actually quasi-3D, as they calculate model particle movements in all three dimensions, using analytic profiles to extrapolate depth-averaged quantities to vertical profiles.

Models based on random walk methods employ random number generators to calculate model particle movements associated with turbulent mixing. During the studies described in this paper, an unexpected dependence of model solutions on the sequencing of calls to the random number generator was identified. To the author's knowledge, this is not a well-known aspect of the use of random number generators in Lagrangian models, so details are given in the paper.

1. Equations: 1) Lagrangian model formulation

RS04 quote the full equation for vertical particle motions in Lagrangian models with vertical diffusivities, K_z (m^2/s), which vary in the vertical direction:

$$z_{n+1} = z_n + K_z'(z_n)\Delta t + r \left[\frac{2K_z(z_n + \frac{1}{2}K_z'(z_n)\Delta t)\Delta t}{R} \right]^{1/2} + w_p\Delta t \tag{1}$$

where z_n and z_{n+1} are the vertical particle locations (m) at consecutive timestep numbers n and $n+1$ respectively, K_z' (m/s) is the first derivative of K_z with respect to z , Δt is the model timestep (s), w_p is a vertical velocity (representing, for example, sediment settling) and r is a random number from a distribution having zero mean and variance, R . In this notation, $x(\dots)$ denotes the value of x at the position given within the brackets, whereas $y[\dots]$ denotes the multiplication of y by the contents of the brackets. In Lagrangian models used in marine dispersion applications, Equation (1) is usually applied with reflecting boundary conditions at the sea surface and seabed. If r is selected from a normal distribution, then $R=1$, but if the distribution is uniform in the range ± 1 , then $R=1/3$.

Equations: 2) Timestep sensitivities in Lagrangian models

The 2D modules of the PLUME-RW suite use a parabolic form for K_z , which defines a profile having minima at the seabed and the sea surface, and a maximum at mid-depth. In 3D applications, a mixing length model is employed to modify the profile for vertical density and velocity gradients. Mead [1] noted that, for relatively long timesteps, use of Equation (1) with a parabolic K_z profile can result in model

particle accumulations in the middle of the water column, with associated particle number depletions near the sea surface and seabed. Similar departures from expected particle distributions can occur near density interfaces in 3D models.

Mead [1] suggested a solution to the difficulty outlined above, based on the observation that models tend to exhibit the required properties at relatively short timesteps. Whilst it would be impractical to reduce all of the processes represented in Lagrangian models to timesteps at which the correct behavior occurs, it should be possible to implement a sub-timestep for the vertical processes. The work presented in this paper involves the implementation of such a procedure.

RS04 present an extensive analysis of similar difficulties to those discussed by Mead [1]. They note that, for Equation (1) to be applied in Lagrangian models, it is necessary for the functional forms of both K_z and K_z' to be continuous and differentiable. This is never achievable at diffusivity discontinuities such as model boundaries and discrete pycnoclines (although RS04 present two mathematical procedures for minimising the difficulty), but is achieved elsewhere if a particular criterion is satisfied which relates Δt to K_z'' (s^{-1}), the second derivative of the vertical diffusivity with respect to z . In practice, RS04 found a more stringent criterion for Δt to be applicable:

$$\Delta t \ll f \text{ MIN} \left(\frac{1}{|K_z''|} \right) \tag{2}$$

where f is a constant, and $\text{MIN}(\dots)$ denotes the minimum value of the bracketed term over the water column. RS04 found

“artificial” particle accumulations to be indistinguishable from statistical variations for $f=1/200$, provided appropriate measures are taken to minimize boundary effects (see below), whilst for $f=1/100$, errors in expected particle distributions were no more than 1%.

The timestep sensitivities discussed by Mead [1] are fully consistent with the results presented by RS04; for Figures 2b and 2c of Mead [1], the timesteps used correspond to f values (see Equation (2) above) of $1/125$ and $1/4$ respectively, so uneven particle distributions were to be expected for the longer timestep. The somewhat uneven particle distributions in the vicinities of the boundaries with the shorter timestep (Figure 2b of Mead [1]) were due to boundary effects which, following RS04, require correction additional to the use of a timestep which satisfies Equation (2). Mead [1] reports only negative departures from expected particle numbers in the vicinities of model boundaries for long timesteps, whereas RS04 report negative departures as boundaries are approached, switching to large, positive departures immediately adjacent to boundaries (Figure 5 of RS04). The absence of such positive departures from the results presented by Mead [1] was entirely due to the limited vertical resolution of the grid chosen to present the results, and subsequent analysis using enhanced resolution has revealed the presence of positive departures consistent with RS04.

Equations: 3) Procedures for minimising the effects of K_z discontinuities

RS04 present two methods for minimising artificial particle distributions in the vicinities of diffusivity discontinuities, and these were tested in the PLUME-RW code during the course of the work described here; the creation of random mixed layers in the vicinities of the boundaries (hereafter referred to as the RML method) was tested in the 2D code, and forcing $K_z'=0$ at the discontinuities (hereafter referred to as the

KZ0 method) was tested in the 3D code. Both methods are applicable in both types of model. However, whereas the RML method only provides improved results at the sea surface and seabed, the KZ0 method also provides enhancements at density interfaces within the water column in stratified models, so is the preferred method in 3D. At the time of writing, the KZ0 method has not been tested in the 2D code, although this is desirable.

Equations: 3.1) The RML method

This method involves the creation of layers at the sea surface and seabed, so that particles entering those layers are mixed according to a uniform random number distribution. The thicknesses of the layers are required to be equal to, or to exceed, the maximum possible particle displacements at the layer edges away from the boundaries. It follows from Equation (1) that the heights (m) of the edges of the sea surface and seabed boundary layers above the seabed, z_t and z_b respectively, are given by:

$$h - z_t = K_z'(z_t)\Delta t + r_{\max} \left[\frac{2K_z(z_t + \frac{1}{2}K_z'(z_t)\Delta t)\Delta t}{R} \right]^{\frac{1}{2}} \quad (3a)$$

$$z_b = - \left\{ K_z'(z_b)\Delta t + r_{\min} \left[\frac{2K_z(z_b + \frac{1}{2}K_z'(z_b)\Delta t)\Delta t}{R} \right]^{\frac{1}{2}} \right\} \quad (3b)$$

where r_{\min} and r_{\max} are the minimum and maximum values of r respectively in Equation (1), and h is the total water depth (m).

Equations: 3.2) The KZ0 method

As discussed by RS04, the use of a reflecting boundary condition at the sea surface and seabed in Lagrangian marine dispersion models is equivalent to the application of diffusivity profiles on the out-of-water sides of these boundaries, with the out-of-water profiles being mirror-images of the profile within the water column. Consequently, K_z' is

discontinuous at the boundaries, and Equation (1) becomes inapplicable, causing unrealistic particle distributions in the vicinities of boundaries. The KZ0 method reduces this difficulty by smoothing the diffusivity profile, including the out-of-water, mirrored extensions using a cubic spline, which gives $K_z = 0$ at the boundaries.

Model enhancement and testing

Historically, when running PLUME-RW, timesteps were chosen to be less than the horizontal node spacing of the square output mesh divided by the maximum current speed in the study area. This approach yielded timesteps which were sufficiently short to prevent plume fragmentation, but generally long enough to achieve practical run times. The timestep criterion in Equation (2) requires much shorter timesteps than had traditionally been used in PLUME-RW, thus introducing the risk of impractical run times. This was addressed by introducing a sub-timestep loop into the code, so that use of the traditional criterion could continue for the main timestep, with the more stringent Equation (2) being used to select a sub-timestep used for the vertical particle movement computations. In this way, computational overheads associated with the use of Equation (2) were minimised.

Inevitably, the introduction of the sub-timestep loop increased model run times, but the increases in run length were considerably less than would have been expected had the shorter timestep been used for all the computations (estimated as the original run time multiplied by the number of sub-timesteps in each timestep).

In preliminary model tests with the sub-timestep loop, simulations were carried out in 2D, with vertical particle distributions which should have remained approximately uniform during the runs. It proved impossible to achieve the expected, uniform vertical particle distributions in these tests, whatever the value of the sub-timestep. This problem was traced to the revised sequencing of calls to the random number generator introduced with the sub-timestep loop. Before the introduction of the loop, the code had carried out calculations for all the model particles sequentially, before moving on to the next timestep. When the sub-timestep loop was introduced initially, vertical calculations were carried out for each model particle for all sub-timesteps within each timestep, before moving on to the next particle. The effects of this on the sequencing of calls to the random number generator are illustrated in the table below:

	Before introduction of sub-timestep loop	With initial implementation of sub-timestep loop
Sequence of calls to random number generator	Particle 1, Timestep 1 Particle 2, Timestep 1 Particle 1, Sub-timestep 1, Timestep 1 Particle 1, Sub-timestep 2, Timestep 1 etc	Particle 1, Sub-timestep 1, Timestep 1 Particle 1, Sub-timestep 2, Timestep 1 Particle 2, Sub-timestep 1, Timestep 1 Particle 2, Sub-timestep 2, Timestep 1 Particle 1, Sub-timestep 1, Timestep 2 Particle 1, Sub-timestep 2, Timestep 2 Particle 2, Sub-timestep 1, Timestep 2 Particle 2, Sub-timestep 2, Timestep 2 etc

To address this difficulty, the coding of the sub-timestep loop was revised so as restore the original sequencing of time- and particle-stepping used in calls to the random number generator. This was achieved through generating and storing whole random number sequences within the code, rather than generating random numbers only at points within the code where they are used. Once the code revision had been made, it became possible to achieve approximately uniform particle distributions with appropriate choices of model timesteps and sub-timesteps. The requirement for this correction was unexpected. It is, however, consistent with the findings of Hunter et al [3], who found that the output of standard random number generators used in Lagrangian models had different statistical properties, depending on whether loops over particles were nested within loops over time, or *vice versa*. To the present author's knowledge, this is not a well-known aspect of the use of random number generators in Lagrangian models.

The following were implemented in the Lagrangian model code:

- The sub-timestep loop for vertical particle movements (as discussed above).
- Random mixed layers at the sea surface and seabed, using the method of RS04, discussed above (in the 2D model).
- Curve fitting, using a cubic spline, to the profiles of vertical diffusivities calculated from the flow model current and density fields (in the 3D model).
- Forcing of $K_z=0$ at the sea surface and seabed (in the 3D model).

Model enhancement and testing: 1) 2D model testing

The enhanced 2D code was tested using a convenient time-varying flow field for the coastal waters around Bahrain. An area

with a reasonably level seabed was chosen initially, so that the results would not be complicated by the effects of varying bathymetry, but the findings were confirmed subsequently for a more complex area, with higher current speeds. At the chosen release point, the mean water depth was some 20m, and the maximum depth-averaged current speed was about 0.2m/s. The results illustrated in this paper were those of 50-hour simulations, with 200,000 particles distributed evenly over the water column at the start of the simulations. The particles were tracked in the time-varying flow and should, if the model algorithms reproduce the correct physical behavior, have remained evenly distributed through the water column. For results presentation, the average numbers of particles over the simulations were calculated for 200 layers, each of approximately 0.1m thickness. In the figures, the results are presented as percentage departures from the expected number of particles per layer (1,000).

Model enhancement and testing: 1.1) Effects of the introduction of the sub-timestep

Figure 1 shows the results of three tests undertaken after all of the model enhancements listed above applicable to the 2D model had been implemented, except the introduction of boundary random layers. The three tests all had a main timestep of 300s, with sub-timesteps of 300s (Test 28; timestep and sub-timestep equal, so effectively no sub-timestep), 5s (Test 29) and 1s (Test 30). These sub-timesteps correspond to f values (Equation (2)) of 1/8, 1/500 and 1/2,500 respectively.

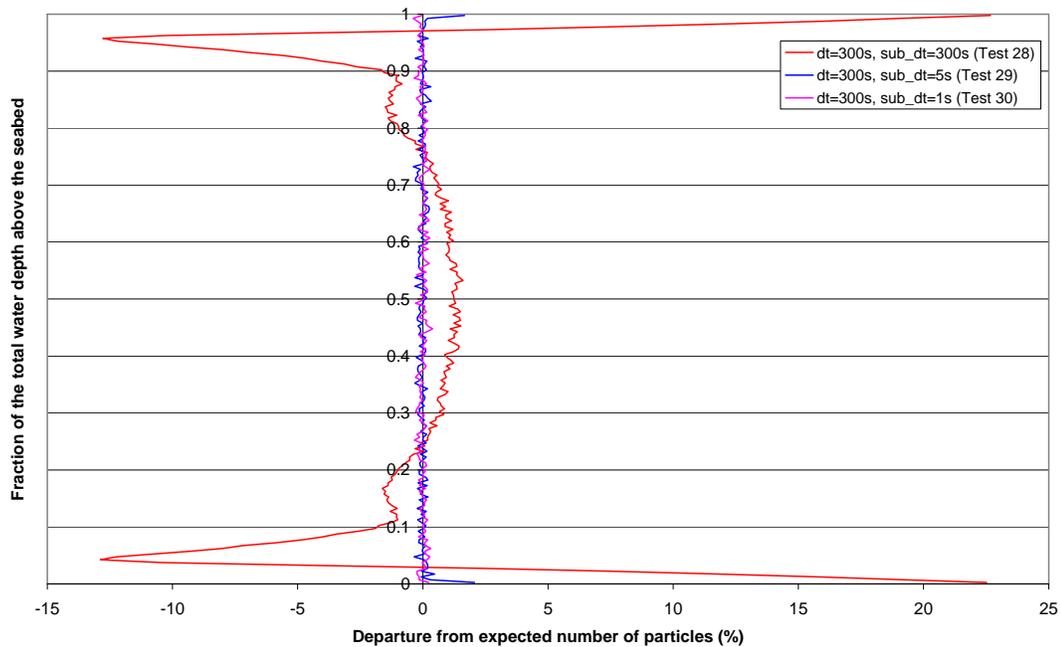


Figure 1 Sub-timestep sensitivity of the vertical particle distributions in the enhanced model without boundary random mixed layers; Bahrain tests

Clearly, Figure 1 shows that there were significant departures from an even particle distribution for $\Delta t_s=300s$, where Δt_s is used to denote the value of the sub-timestep (s). Positive departures from expected particle numbers in the immediate vicinities of the boundaries were up to 23%, whilst adjacent negative departures were up to 13%. Near the centre of the water column, positive particle number departures were around 1%. The form of the particle number distribution for Test 29 is similar to that reported by Mead [1] (Figure 2c) and RS04 for relatively long timesteps. The exceptions to this are the positive particle number departures from expectation in the immediate vicinities of the boundaries, which were not resolved by water column layering applied by Mead [1].

For $\Delta t_s=5s$ ($f=1/500$), the particle distribution was approximately even over the water column (given that some small, statistical fluctuations are inevitable in Lagrangian solutions), except in the immediate vicinities of the boundaries, where positive departures from expected

particle numbers were some 2%. With $\Delta t_s=1s$ ($f=1/2,500$), particle number departures from expectation adjacent to the model boundaries were essentially indistinguishable from the statistical fluctuations through the water column.

It is evident from the results discussed in this section that use of a sub-timestep for vertical particle motions has the potential to reduce unrealistic features of model particle distributions, without the need to use very short timesteps for all of the model computations. This finding applies even without further measures to deal with boundary effects, provided sufficiently small sub-timesteps are used. Whilst the form of the particle distribution for Test 28 ($f=1/8$) would probably be judged unacceptable for most model applications, those of the distributions for Tests 29 ($f=1/500$) and 30 ($f=1,2500$) would be satisfactory for most purposes. The particle accumulations at the boundaries in Test 29 are very small in practical terms.

Table 1 Computation time increases with sub-timestep implementation in the 2D model

Test	Sub-timestep (s)	Timestep/sub-timestep	Slow-down factor from equal timestep and sub-timestep
30	1	300	43
29	5	60	9
28	300	1	-

In any model application, sensitivity tests are required to ensure that a sufficiently short sub-timestep is used; as is shown below, the use of boundary mixed layers allows relatively long sub-timesteps to be applied.

Based on Tests 28-30, Table 1 summarizes the run time increases associated with the implementation of the sub-timestep in the 2D model. The increases in run time for smaller sub-timesteps are 6-7 times less than those which might be expected if short timesteps were applied for all the model processes, rather than through the use of separate timesteps for the horizontal and vertical processes. This clearly demonstrates the benefit of the use of the sub-timestep in terms of run time.

Model enhancement and testing: 1.2) Effects of the introduction of the boundary mixed layers (the RML method)

Figure 2 shows the results of three tests undertaken after all of the model enhancements listed above applicable to the 2D model had been implemented, including the introduction of boundary random layers with thicknesses calculated using Equation (3). The three tests all had a main timestep of 300s, with sub-timesteps of 5s (Test 32, mixed layer thicknesses of 0.2m), 10s (Test 33, mixed layer thicknesses of 0.4m) and 20s (Test 34, mixed layer thicknesses of 0.8m). These sub-timesteps correspond to f values (Equation (2)) of 1/500, 1/250 and 1/125 respectively.

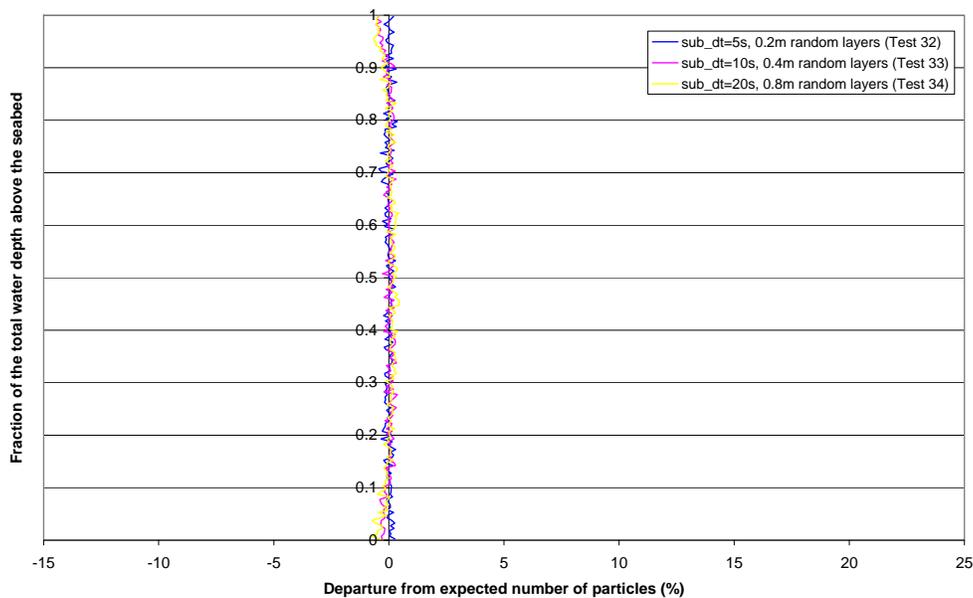


Figure 2 Sub-timestep sensitivity of the vertical particle distributions in the enhanced model with boundary random mixed layers; Bahrain tests

The results of Tests 29 (Figure 1) and 32 (Figure 2) are directly comparable to illustrate the effects of the introduction of random mixed layers in Test 32, because the two tests were identical in all other respects. The particle distribution in Test 32 did not exhibit the small, near-boundary departures of particle numbers from expectation. It is, therefore, evident that unrealistic particle accumulations can be prevented through the use of longer sub-timesteps in combination with boundary random mixed layers than is possible without such layers. The use of somewhat longer sub-timesteps with mixed layers (Tests 33 and 34) introduced slight curvature to the particle distributions but, at less than 1% departures of particle numbers from expectation, these results would be suitable for almost all practical model applications.

Model enhancement and testing: 2)

3D model testing

The enhanced 3D code was tested using an approximately steady flow field for a flat-bedded area of coastal waters. The water depth was approximately 15m, and the current speed was about 0.17m/s. Initially, the model was run without any density variation through the water column, whilst in subsequent tests a two-layer density structure with a step discontinuity was imposed. The results illustrated in this paper were those of 23-hour simulations, with 200,000 particles distributed either evenly over the water column (Tests 12-16 and Test 21) or at the sea surface (Tests 17 and 18) at the start of the simulations. The particles were tracked in the flow. For the initially-uniform particle distributions, the particles should, as for the 2D model, have remained evenly distributed through the water column. To present the results of the tests with initially-uniform particle distributions, the average numbers of particles over the simulations were calculated for 200 layers, each of approximately 0.075m thickness. In the

figures, the results are presented as percentage departures from the expected number of particles per layer (1,000). To present the results of the tests with particle release at the sea surface, the numbers of particles in each of the 0.075m layers are shown at various times through the simulations.

For practical reasons, the sub-timestep loop was introduced in the 3D code at the same time as the implementation of the KZ0 method for dealing with model particles in the vicinities of the sea surface and seabed. Consequently, unlike the 2D tests, it is not possible to demonstrate the separate effects of the sub-timestep and the KZ0 method on model particle distributions.

Figure 3 shows the results of four tests undertaken, without any density variation through the water column, after all of the model enhancements listed above applicable to the 3D model had been implemented. The four tests all had a main timestep of 25s, with sub-timesteps of 25s (Test 12; note that the timestep and sub-timestep were equal), 5s (Test 14), 1s (Test 15) and 0.5s (Test 13). These sub-timesteps correspond to f values (Equation (2)) of 1/4, 1/20, 1/100 and 1/200 respectively.

The results shown in Figure 3 demonstrate the same tendency towards expected, uniform particle distributions for shorter sub-timesteps (smaller f values) noted for the 2D model. For $f=1/4$ (Test 12), 16% of the released particles actually left the water column. In the previous version of the code, such behavior would have been prevented by the reflecting boundary condition, but this would have worsened the non-uniformity of the Test 12 results shown in Figure 3, rather than improving it.

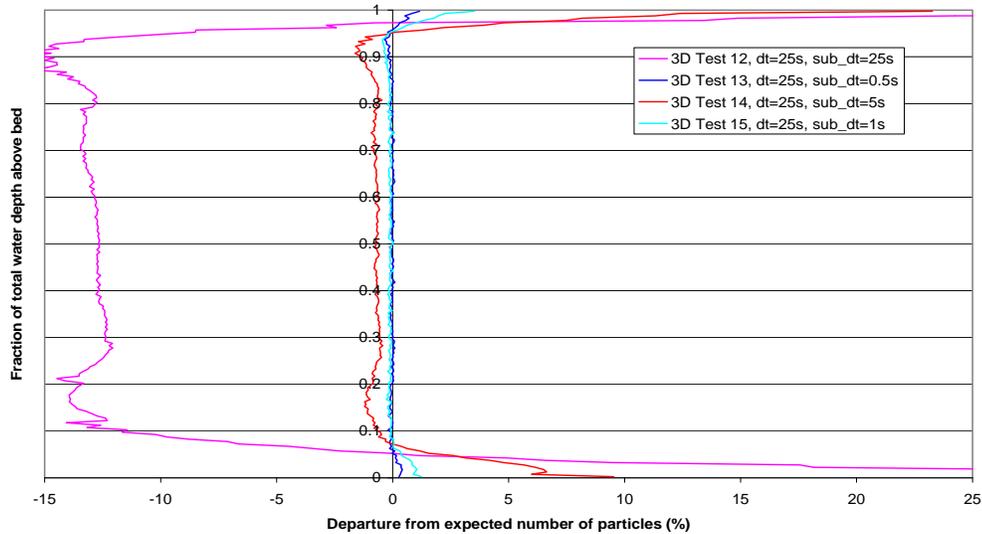


Figure 3 Sub-timestep sensitivity of the vertical particle distributions in the enhanced model with $K_z=0$ at the boundaries; flat-bedded model tests, zero density variation

The results for Test 12 would be judged unacceptable for most model applications, as they show major departures from uniformity at the sea surface and seabed (202% and 73% respectively), with compensating departures of order 10-15% over the remainder of the water column. At the other extreme of the range of sub-timesteps, the results for Tests 13 and 15 ($f=1/200$ and $f=1/100$ respectively) would be acceptable for most applications, with departures from expected particle numbers of 1% and 4% respectively at the sea surface, and <1% and 1% respectively at the seabed.

To test the effects in the enhanced 3D model of density variations through the water column, a two-layer density structure was imposed on the flow model results used for Tests 12-15, with uniform densities of $1,010\text{kg/m}^3$ and $1,020\text{kg/m}^3$ above and below mid-depth respectively. The resulting density discontinuity is sharper than is likely to occur in nature, and so represents a stringent test of the enhanced code. Figure 4 shows the results of Tests 16 and 21, which are equivalent to Tests 15 (sub-timestep 1s) and 13 (sub-timestep 0.5s) respectively, with the density discontinuity included. The particle

distributions for Tests 16 and 21 show positive departures from expected particle numbers at the density interface, with the departure being smaller for the smaller sub-timestep. However, at 6% and 3% for the sub-timesteps of 1s and 0.5s respectively, these particle accumulations are only slightly larger than those at the sea surface and seabed in the same runs, and are much smaller than those noted in previous studies. The response to the halving of the sub-timestep between Tests 16 and 21 indicates that further reductions in the particle accumulations at the density interface could be achieved by using still smaller sub-timesteps. In view of the extreme nature of the density discontinuity in these tests, however, further attempts to reduce the particle accumulations at the interface have not been undertaken.

Tests were undertaken to assess the effects of the density discontinuity on the rate of spreading of model particles through the water depth. For these tests, 200,000 particles were released instantaneously at the sea surface, and were tracked for 23 hours. Both tests had a timestep of 25s and a sub-timestep of 1s. Test 17 was based on the discontinuous density structure described above, whilst Test 18 had no

vertical density variations. The distributions of model particles in these tests are shown in Figure 5 at 1 hour, 5 hours and 23 hours. At 1 hour (Figure 5a), particles have spread through the water depth in both cases; there are gradients in particle numbers between the sea surface and seabed, with a significant discontinuity at the density interface in the stratified case. There is much more uniformity through the depth at 5 hours (Figure 5b), with a noticeable two-layer structure in the stratified case, whilst at 23 hours (Figure 5c) both particle distributions are approximately uniform. This behavior is qualitatively reasonable, but is difficult to validate quantitatively. The rate of spreading above the density interface (that is, in a region of uniform density) was checked against an analytic solution, and found to be satisfactory. This gives confidence that this particular random walk model is well-formulated, in that results consistent with Fickian diffusion are achieved for a particular diffusivity profile. Given that the diffusivity profile is based on well-established algorithms, it is to be expected that the model will reproduce rates of spreading of dissolved substances in varying density fields in nature.

However, a quantitative calibration exercise is required to give full confidence in the model.

Based on Tests 12-15, Table 2 summarizes the run time increases associated with the implementation of the sub-timestep in the 3D model. The increases in run time for smaller sub-timesteps are around half those which might be expected if short timesteps were applied for all the model processes, rather than through the use of separate timesteps for the horizontal and vertical processes. Whilst such run time savings are significant, they are much less than the savings achievable in the 2D model described above, and quite long run times may be required in some circumstances to achieve required improvements in model accuracy. The relatively small run time savings associated with the use of a sub-timestep in the 3D model relative to the 2D model are probably associated with the spline operations on the diffusivity profile in 3D. At the time of writing, it is considered that it may be possible to make further adjustments to the 3D model code to achieve lower slow-down factors.

Table 2 Computation time increases with sub-timestep implementation in the 3D model

Test	Sub-timestep (s)	Timestep/sub-timestep	Slow-down factor from equal timestep and sub-timestep
13	0.5	50	27
15	1	25	14
14	5	5	3
12	25	1	-

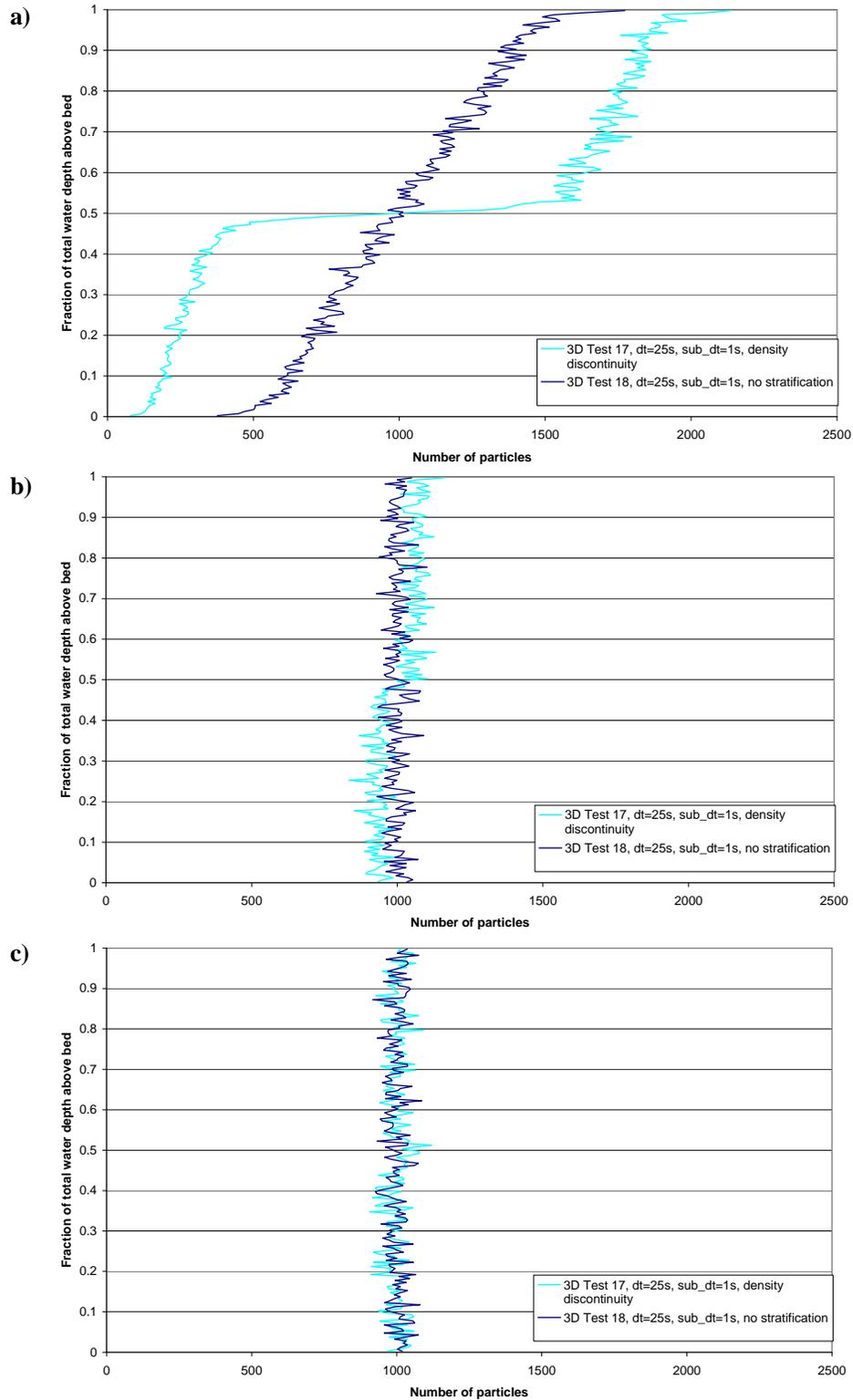


Figure 5 Vertical particle distributions at a) 1 hour, b) 5 hours and c) 23 hours in the enhanced model with $K_z'=0$ at the boundaries; flat-bedded model tests

Conclusions

A Lagrangian marine dispersion model has been enhanced to use different timestep values for horizontal and vertical particle movements. This has enabled unrealistic particle accumulations within the water column to be reduced, through the use of very short timesteps for the vertical movement calculations, without excessive increases in run time. It has been shown that particle accumulations can be reduced, or virtually eliminated, through the use of criteria presented by RS04 to select sub-timestep values. The criteria can be relaxed somewhat without particle accumulations becoming unacceptable for practical purposes. In the 2D case, longer sub-timesteps are practical if random mixed layers are introduced near the sea surface and seabed, as suggested by RS04, than is the case if such layers are not used.

At the time of writing, separate methods have been established for dealing with boundary effects in the 2D and 3D codes. An obvious extension of the work would be the implementation in the 2D code of the procedure for forcing $K_z=0$ at the sea surface and seabed, which has only been implemented in 3D to date. The advantage of this over the random mixed layers method is that a model user would only be required to specify the sub-timestep at run initiation, whereas the use of mixed layers

requires the specification of both the sub-timestep and the layer thicknesses.

In the 3D code, the increases in run time for smaller sub-timesteps are around half those which might be expected if short timesteps were applied for all the model processes, rather than through the use of separate timesteps for the horizontal and vertical processes. In contrast, in the 2D code, run times are 6-7 times less than might be expected without timestep-splitting. At the time of writing, it is considered that it may be possible to make further adjustments to the 3D model code to achieve lower slow-down factors.

A quantitative calibration of the 3D model is required at the earliest opportunity. Models based on random walk methods employ random number generators to calculate model particle movements associated with turbulent mixing. During the model development described in this paper, an unexpected dependence of model solutions on the sequencing of calls to the random number generator was identified and corrected. To the author's knowledge, this is not a well-known aspect of the use of random number generators in Lagrangian models.

Dr Christopher Mead is a Principal Scientist, and team leader within the Hydrodynamics & Metocean Group of HR Wallingford Ltd. The team is responsible for all aspects of studies relating to marine discharge dispersion and water quality. Dr Mead has a PhD in physical oceanography, and some 25 years' experience in marine mathematical model application and development, including more than 20 years' specializing in marine dispersion studies at HR Wallingford. He developed the Company's PLUME-RW suite of Lagrangian dispersion models from first principles, and is now responsible for undertaking, supervising and managing a range of projects for water organisations and industrial clients.



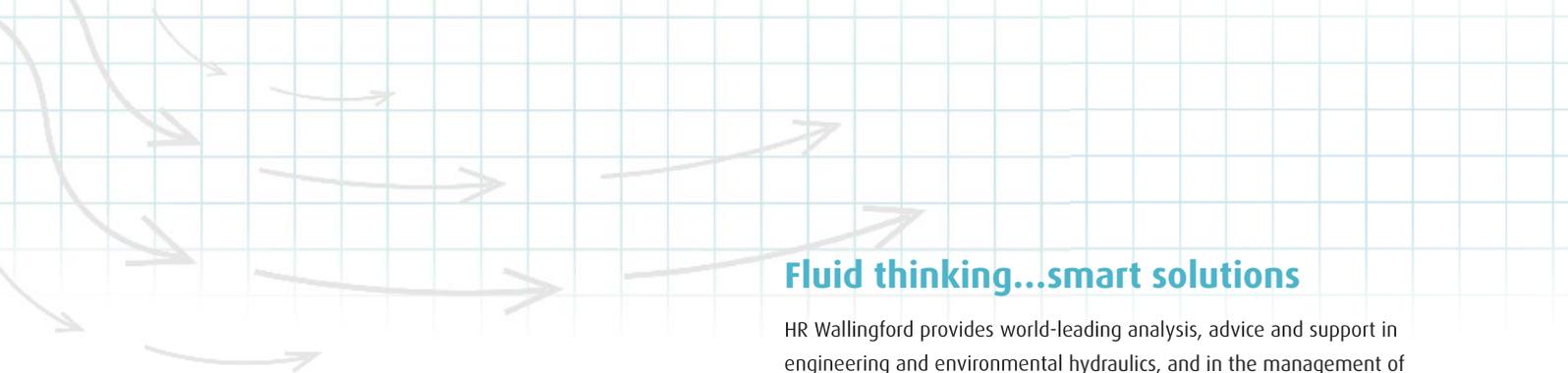


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Today, HR Wallingford has a 50 year track record of achievement in applied research and consultancy, and a unique mix of know-how, assets and facilities, including state of the art physical modelling laboratories, a full range of computational modelling tools, and above all, expert staff with world-renowned skills and experience.

The Company has a pedigree of excellence and a tradition of innovation, which it sustains by re-investing profits from operations into programmes of strategic research and development designed to keep it – and its clients and partners – at the leading edge.

Headquartered in the UK, HR Wallingford reaches clients and partners globally through a network of offices, agents and alliances around the world.



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