

Memorandum

To: Ministry for the Environment Date: 24 March 2014

From: Graham Rickard Our Ref: MFE13305

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Subject: Review of the report "Dispersal of Pollutants: Numerical modelling of the dispersal of pollutants discharged to the sea from the wreck of the Rena"

Executive summary

A report on the dispersal of pollutants associated with the wreck of the Rena at Astrolabe Reef prepared by MetOcean Solutions Limited (MSL) has been reviewed by NIWA.

The report describes the dispersal of potential contaminants from the Rena wreck at Astrolabe Reef using a Lagrangian particle model. The particles are advected by hindcast flow fields derived from a MSL ROMS model (described in a companion MSL report), with added diffusion at each Lagrangian integration step in the form of a random walk term. A so-called "kernel bandwidth" method is then used to generate concentrations from the particle distributions in time and space. The time and space concentration distributions of each contaminant represent the main results of interest.

Our review finds that the numerical methods used are generally appropriate. Some aspects of variability are considered, e.g. differences implied by El Nino verses La Nino years. However, it would also have been interesting to look at the sensitivity to the main drivers of the numerical Lagrangian calculation, namely the underlying flow fields from MSL ROMS, the choice of the diffusion coefficient K in the random walk, and the scale lengths involved in the kernel bandwidth method. Such calculations would indeed burden the process; nevertheless, such a measure would serve to estimate the sensitivity of the numerical solutions to the parameter choices.

The major concern, however, is associated with the important final step to accumulate the concentration plots and statistics for each of the contaminants based on the distributions of the Lagrangian test particles. The critical section describing the volume concentration calculation is rather opaque, and leads to some confusion in interpreting and understanding how the outputs have been produced. The techniques appear well merited in the literature, and it may just be in the application or explanation that issues have arisen.

1 Introduction

A report on the dispersal of pollutants associated with the wreck of the Rena at Astrolabe Reef was prepared by MetOcean Solutions Limited in September 2013 for the purposes of evaluating options for the removal or partial removal of the wreck of the MV Rena. The Ministry for the Environment has commissioned NIWA to provide an external review of that report. That review is presented below.

2 Summary of the report

The report describes the dispersal of potential contaminants from the Rena wreck at Astrolabe Reef using a Lagrangian particle model. The main results are summarised in terms of contour plots of contaminant concentrations derived from numerical simulations using the following techniques:

- A MSL ROMS model for 3D hindcast flow fields:
- Lagrangian integration of test particles in the hindcast flow fields, with an added random walk term dependent on a scaled diffusion coefficient;
- A "kernel bandwidth" method to produce concentration distributions as a function of space and time, dependent on kernel bandwidths and a specific kernel bandwidth function (namely that of Epanechnikov), and a grid of receptors on which to accumulate the concentrations;
- Specific parameterised time decays for one of the contaminants associated with its anticipated properties in the marine environment.

The MSL ROMS model simulations have been described in an accompanying report, and separately reviewed.

3 Review comments

The methods used are in general suitable, and the results presented are appropriate for the stated purpose. Some improvements can be suggested, however, as indicated below. In particular, the final step in transferring the information from the Lagrangian particles to the receptor grid to obtain the final set of results in terms of concentrations needs to be tidied up; this will improve its readability and help in explaining this important calculation component to the reader.

Verification

The MSL ROMS flow fields have had verification in an accompanying report using in-situ ADCP data. As noted in the review to that report, extra confidence in these flow fields would have been obtained from perhaps some more comparison with other historical records. The methods were, however, entirely appropriate.

Numerical methods: Trajectory modelling

The applied techniques are appropriate. In equations (3.1a) and (3.1b) the 3D flow fields

 $\tilde{u}(x, y, z, t)$ and $\tilde{v}(x, y, z, t)$ are not fully defined; they will arise from the MSL 3D ROMS solutions, but they are not specified in terms of mean fields (and thence what meaning period

has been used) or instantaneous fields (and what time intervals they are extracted at). This needs to be detailed.

In terms of the Lagrangian integration, the time step used Δt is not defined (but is presumably variable and dependent on the values of the diffusion coefficients $k_{u,v}$ and k_w used during the integration?). Also, the values used for $k_{u,v}$ and k_w are presented, but the reasons for their particular choices are not presented; in the context of trajectory modelling, the aim of the random walk process is to add back the turbulent motions not represented by the 3D model fields, so that the combination of model fields and random walk indeed matches that expected in reality. It is a difficult assessment to make, but some explanation for the particular choices made here would be helpful, particularly so as no mention is made of the sensitivity (likely or realised) of the concentration calculations to such parameters.

Numerical methods: Concentration calculation

The kernel bandwidth method to extract concentrations from the Lagrangian particle distributions seems to be familiar to the atmospheric modelling community (as evidenced by the reference to Vitali et al.,2006), but there seem limited (if any) applications in the oceanographic field known to these reviewers; this does not reflect on the validity of the method, rather the lack of familiarity of the reviewer with this technique. Certainly the discrete nature of Lagrangian particles (as opposed to the distributed properties of an integrated tracer field) means something like this method needs to be applied to obtain the maps of concentration.

Presumably the decision to not use a tracer field to represent the contaminants is based on experience, and perhaps the relative cost of numerical integration within the full MSL ROMS model. Perhaps a comment on this would be appropriate, and further establish bounds on the relative accuracy anticipated.

As noted for the trajectory calculations, it would be interesting to know how sensitive the concentration calculations are to the parameters chosen, viz the number of Lagrangian particles, the kernel bandwidths λ_x and λ_y , and the choice of the kernel function. Given that the trajectory modelling is described as "a post-processing trajectory scheme", it suggests that fields saved from the MSL ROMS 3D simulation are being used, in which case it should be possible to conduct multiple sensitivity studies in an off-line fashion to get some estimates of the solution variance.

Numerical Methods: Volume concentrations

This section is critical to understanding how the final plots are produced.

In each 13 month period of continuous simulation, it is noted that one particle per minute is released, i.e.,

the information to base the concentrations of each of the 4 contaminants of interest comes from a *single distribution of particles* that in themselves do not know which contaminant they represent. (Statement 1).

If Statement 1 is true (and would appear to be so from the text) then it would appear that there are only certain aspects of the accumulation of volume concentrations that can result in different accumulated concentrations (as plotted), namely particle decay with time, and the

so-called "grid size" associated with the "40 x 40 pixel grids centred on the release site". In terms of particle decay, this only impacts scenario c for milk powder in terms of accumulating concentrations, but, as far as we can tell, will not at all affect the trajectories of each individual Lagrangian particle. However, the pixel grid sizes were adjusted based on the "maximum excursion of the different pollutants" and this needs to be clarified and defined, because it seems;

- (i) that the maximum excursion will be determined by the particles, and there is only one distribution of those, and;
- (ii) that the change in the pixel grid sizes will have a marked impact on how the concentrations are accumulated, even though the particle distributions are the same for each pollutant.

Each of these points needs to be addressed to get a fuller understanding of the numerical process used.

As an example, consider the concentration figures for contaminants b (TCCA) and d (CCM) in Figures 4.5 to 4.8, and Figures 4.13 to 4.16, respectively. Apart from the value for their respective contaminant loadings, the concentration statistics are both accumulated on the same 30 km wide grid of pixels. Comparison of each respective Figure for each contaminant suggests strongly that indeed the distributions are the same, the only difference being the scale on which the plots are made; this is particularly evident for Figure 4.6 compared to Figure 4.14 in the lower frame, where remarkably similar patterns of concentration are evident.

Conversely, scenario a for NO₃ results in a much broader distribution of material (at least based on the relative concentrations and the size of the grid of receptors) and yet if Statement 1 is true then the same set of particles have been used to produce the estimates.

If Statement 1 is false, then this needs to be made clearer in the report. This would then lead on to provide clear explanations for the differences found in the accumulated concentrations, and lead to greater confidence in this final step in the numerical process.

However, if Statement 1 is true, then critical aspects of the volume concentration calculation need to be much more clearly explained. Firstly, why different maximum excursions are established? Secondly, why scenarios b and d that only differ by the particle loading (that could be normalised anyway) results in concentrations relative to the source that are different for contaminants b and d?



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4 References

1. Vitali L., Monforti F., Bellasio R., Bianconi R., Sachero V., Mosca S. and G. Zanini (2006). Validation of a Lagrangian dispersion model implementing different kernel methods for density reconstruction. Atmospheric Environment 40: 8020-8033.