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Development of PRAIRIE™ Dispersion Modelling

AEA Technology plc

R&D Technical Report P69

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Development of PRAIRIE™ Dispersion Modelling

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Statement of Use
This report contains a comparison of the DYNUT dispersion model incorporated within PRAIRIE™ (Pollution Risk from Accidental Influxes to Rivers and Estuaries) with the alternative ADZ (Aggregated Dead Zone) model. The report is intended for specialist modellers wishing to understand how PRAIRIE™ functions and proposes a method of determining dispersion coefficients that might significantly reduce the effort needed to determine this key input parameter.

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EXECUTIVE SUMMARY

A number of aspects associated with the physical modelling currently used within PRAIRIE have been evaluated, namely:

1. Examination of the advection-diffusion model, paying special attention to the prediction of longitudinal diffusion coefficients (LDCs);
2. Identification of improvements that could be made to deterministic and probabilistic modelling, again with an emphasis on LDC's.
3. Examination of the ADZ (aggregated dead zone) model, to see how it compared with PRAIRIE's ADE (advective dispersion equation) model and to assess how easily the model might be incorporated into PRAIRIE.

The LDC is an important parameter which, for present versions of PRAIRIE, must be supplied by the user, either directly as an LDC or indirectly using Elders/Manning's parameterization. There is presently little advice that the user can refer to regarding selection of LDC. Present advice is that the user should directly input the dispersion coefficient rather than use a Mannings constant. This would avoid the need for the user to manually correct for a numerical error in the code discovered during this project; the error is in practice of little significance.

Studies of empirical approaches showed that the Fischer parameterization predicts the LDC better than Elder's parameterization. It was therefore recommend that the Elder's parameterization in PRAIRIE is either replaced or supplemented by Fischer's parameterization.

Time was also spent time investigating whether it might be possible to use dye-tracer experiments to derive correlations between more easily measured parameters (such as flow and velocity) and the LDC. Using a relatively small set of dye-tracer data for the Rivers Dee and Wharfe we identified that there might be a correlation between velocity and LDC. If this could be substantiated there would then be sense in producing correlation matrices for all UK rivers of interest since this would then provide an improved way for the PRAIRIE user to select appropriate hydrological inputs.

Approaches by which improvements may be made to PRAIRIE's deterministic and probabilistic calculations were identified and briefly discussed.

Finally, we looked at the ADZ model (which adopts a different modelling approach to the ADE model) to see how the approaches compare and how the ADZ model might be incorporated into PRAIRIE.

The elemental ADZ model was assessed using dye tracer experiment data for moderately long ($\approx$ 15 km) stretches of the River Wharfe and the River Swale in Yorkshire. The elemental ADZ model was shown to provide good estimates of the peak concentrations at most downstream sites. However, the skewed profiles produced by the ADZ model were found to be increasingly inappropriate as the pollutant moved downstream.

The ADE and ADZ models were then compared for the Wharfe. The comparison showed that the ADE model is capable of producing predictions of the downstream peak concentrations at least as good as the elemental ADZ model. Further, whilst in the near field the skewed nature of ADZ's predicted concentration profiles better matched the measured profiles, at distances further downstream the measured profiles were found to be broadly Gaussian in shape and thus better represented by the ADE model.

Whilst it was recognised that the accuracy of the ADZ model could be improved by the use of multiple ADZs rather than an elemental ADZ, it was also noted that this would require considerably greater effort (and ideally more experimental data) to calibrate the model to the river. Additionally, for ADZ there remains a problem of how to estimate the first peak profile - ADZ modelling usually depends upon adjusting parameters to the first profile, and then making further downstream predictions based on the adjusted parameters. We have indicated in this report how the first peak might be approximated by an analytical solution. However, whilst the analytical solution of the elemental ADZ for a spike release was shown to produce reasonable estimates of the peak concentrations, the profiles downstream become excessively skewed.

The comparison of the ADE and ADZ models led us to conclude that:

1. Given the reservations regarding the (elemental) ADZ model and the relatively high level of accuracy obtained using the ADE, it is suggested that further research and more conclusive evidence is required before implementation of the ADZ methodology into PRAIRIE could be justified.

2. The assessment of the ADE model also demonstrated that the longitudinal dispersion coefficient may be successfully estimated from the Fischer parameterization with the Manning's coefficient being estimated from the river bed gradient. Since the river bed gradient can be reasonably approximated from contour maps, this represents a simple, easy to implement, method for the estimation of the dispersion coefficient.

1 INTRODUCTION

There has been considerable development of the PRAIRIE code within the last few years following the release of PRAIRIE 2.2 in 1992. Much of the work concentrated on refinement of PRAIRIE's appearance and feel to the user; one of the main objectives was to produce a programme that was useable, friendly, and that would encourage potential users to begin to perform risk assessments.

With the release of the windows version of PRAIRIE, and the conclusion of the Dee Water Protection Zone Public Enquiry, the impetus to refine the appearance of PRAIRIE diminished. This breathing space presented an opportunity to revisit some of the more technical aspects of PRAIRIE where it was believed (either from a developer's perspective or from user feedback) that it might be sensible to reconsider how PRAIRIE models the release of pollutants within a river.

The project reported here, further development of dispersion modelling within PRAIRIE, has been run in parallel to two other PRAIRIE development projects. One of the other projects sought to extend the chemical database (increased from 89 to 250 entries) whilst at the same time taking the opportunity to examine the adequacy of chemical removal mechanisms. The other project was directed at checking and extending the water quality database.

This project has allowed us to re-evaluate the physical models within PRAIRIE and to consider whether there are improvements which might be made to PRAIRIE so that pollution transport within a river might be more accurately modelled. Such modelling improvements should not, however, unduly add to the complexity of the modelling process since it is believed that one of the strengths of PRAIRIE is its ability to model pollutant spills with confidence but in a way that is intuitive and not overly complicated from the perspective of an intelligent but not specialised user.

The longitudinal diffusion coefficient is an important input parameter used by the DYNUT dispersion code (see, for example sensitivity study). All releases of PRAIRIE have so far provided the user with two options for the input of this coefficient, by either: (i) entering an appropriate longitudinal dispersion coefficient (LDC); or (ii) entering a Manning's coefficient which can then be used by PRAIRIE to determine the dispersion coefficient. Either approach demands choices which a user would often find difficult to make because, whilst flow data can be obtained with relative ease from the Environment Agency (EA), dispersion is rarely measured directly. The relationship between flow and longitudinal dispersion is complex, changing as a function of river and position within the river. It was therefore felt that PRAIRIE users could benefit from more assistance in the selection of the diffusion coefficient.

The probabilistic PRAIRIE mode presents even more difficulties to the PRAIRIE user. The Hydrological Database contains, for each river within the database, historical flow records and, for each gauging station, a record of the river's cross-sectional area and depth. PRAIRIE's probabilistic mode of operation automatically selects the flow station which will give the most conservative prediction of pollutant concentration. However, the user is presently required to select just one

LDC or Manning's constant which will be applied for all flows and at all reaches within the simulation. This is clearly a simplification which can effect the PRAIRIE predictions.

Issues regarding the selection of the dispersion coefficient and probabilistic modelling are inter-related. The report has therefore been structured as follows:

1. A discussion of the advection-diffusion equation (ADE) currently employed within PRAIRIE. In this section we discuss: (i) the general ADE model; (ii) a review of empirical methods to predict the longitudinal dispersion coefficient - to see if and how use of the Manning's coefficient within PRAIRIE might be improved; and (iii) an evaluation of how correlation matrices based upon dye tracer experiments might be used to estimate the longitudinal dispersion coefficient.

2. Discussion of an alternative approach to dispersion modelling, namely the Aggregated Dead Zone (ADZ) model. An enhancement to PRAIRIE would be the provision of models other than DYNUT. This would allow the user greater flexibility and would also provide a way of checking the reliability of predictions - greater confidence could be placed in a result if two independent calculations gave similar predictions. The ADZ model has been under development in the UK for some time and it has been suggested at PRAIRIE Development Group meetings that its inclusion within PRAIRIE would be beneficial.

3. Comparison of the ADE and ADZ models with experimental data. This section draws together sections 2 and 3.

4. Improvements to the deterministic and probabilistic modes of diffusion modelling.

5. Conclusions and Recommendations.

2 THE ADVECTION-DIFFUSION (ADE) MODEL

2.1 Current Implementation In PRAIRIE

PRAIRIE currently utilises Taylor's classical one dimensional advection-diffusion model for the dispersion of pollutants released in to rivers which, ignoring sources and sinks, may be given as (see *e.g.* [1])

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + K\frac{\partial^2 C}{\partial x^2} \tag{1}$$

where C is the pollutant concentration (kg/m^3),
t is the time (s),
u is the cross-sectional average of the longitudinal flow velocity (m/s),
x is the downstream distance (m), and
K is the (effective) longitudinal dispersion coefficient (m^2/s).

PRAIRIE currently either allows the user to input the dispersion coefficient, K, directly or calculates K from a user supplied value of the Manning's coefficient (n). For the latter option the method employed by PRAIRIE to estimate the dispersion coefficient is based on Elder's formulation [2]:

$$K = 5.93 \cdot d \cdot u^* \tag{2}$$

where d is the depth of the river and u^* is the friction velocity (m/s) which may be found from [3]:

$$u^* = \sqrt{g \cdot R \cdot S} \tag{3}$$

where g is the acceleration due to gravity (m/s^2),
R is the hydraulic radius (m), and
S is the energy gradient (dimensionless).

The slope may be related to the mean longitudinal velocity u by Manning's empirical formulation [4]:

$$u = \frac{R^{2/3} \cdot S^{1/2}}{n} \tag{4}$$

where n is Manning's coefficient (m$^{1/6}$).

Substituting (4) and (3) in to (2) yields :

$$K = A \cdot R^{5/6} \cdot n \cdot u \qquad (5)$$

where A is a non-dimensional constant of value 18.56.

The value of the hydraulic radius tends towards the d when the width of the stream is much greater than the depth (*i.e.* $R \approx d$ when $W >> d$). This assumption was made during the early development of PRAIRIE and the current parameterization of the LDC is:

$$K = A \cdot d^{5/6} \cdot n \cdot u \qquad (6)$$

Thus PRAIRIE models K from the user input values of n,u and d.

It was noted, when reviewing the PRAIRIE implementation of the parameterization for this project, that equation (6) has not been correctly implemented and that a value for A of 83.7 was assumed, rather than the correct value of 18.56. K is therefore overestimated by a factor of 4.51. To ensure that K is correctly calculated the user should therefore adjust the input value of n by dividing by a factor of 4.51.

This error is not large in the context of performing risk assessments. Moreover, in view of the reservations discussed below we would suggest that the user directly inputs estimates for the LDC rather than rely upon the empirical estimation based on Elder's formulation and the Manning's constant.

Perceived limitations and bounds of applicability of the ADE model are:

1. The model is strictly only applicable to:
    - time periods, t, where t is greater than the transverse mixing time, T. (T depends on the width of the river and the transverse eddy diffusivity and may be shown to extend to over 24 hours for very wide rivers [1] - however, this is probably less critical for UK rivers);
    - situations where the velocity field is statistically steady - this implies that equation (1) is not applicable to non-passive (*i.e.* buoyant) contaminant clouds (this is implicitly assumed in PRAIRIE);
    - periods where the cross-sectional area is both spatially and temporally constant
2. The model predicts Gaussian concentration profiles, whilst it has been shown (see *e.g.* [1] and [5]) that in practise these profile are often non-Gaussian with extended 'tails' after the peak. This skewed feature of the profiles is usually most noticeable in the near field and tends to diminish at distances far downstream from the injection site;
3. The ADE model tends to 'spike' the predicted concentration profiles, resulting in over-estimation of the peak concentration and under-estimation of the plume passage time [6] - this is despite the current implementation error which over-predicts Elder's formulations for K. It should be noted that this 'spiked' profile does not necessarily always lead to conservative consequence estimates;
4. The predicted concentration profiles appear to be relatively insensitive to variation of the Manning's coefficient within its expected bounds [7]. This problem is compounded by the difficulties involved in the estimation of the Manning's coefficient.

The above reservations/limitations have led to the present investigation in to potential development of PRAIRIE's dispersion modelling methodology. The limitations of applicability highlighted above in point (1) and, to a lesser extent, point (2) may only be tackled by a fundamental revision to the dispersion modelling approach adopted by PRAIRIE. One alternative approach which attempts to resolve some of these problems is the Aggregated Dead Zone, and this is discussed later in Section 3.

The problems due to the limitations of the ADE described above in points (3) and (4) can be, however, approached from consideration of alternative methods of estimation of the longitudinal dispersion coefficient. Two approaches to the estimation of K are now considered. First, alternative parameterizations for the empirical estimation of K are discussed in Section 2.2. Second, the possibility of using measured values of K from, for example, dispersion coefficient-flow-velocity correlation matrices is investigated in Section 2.3.

2.2 Empirical Estimation Of The Diffusion Coefficient

Empirical methods for the determination of suitable values of the longitudinal dispersion coefficient, K, have been discussed by a variety of authors (see *e.g.* [2], [3] and [8]). The approach of Elder, which lead to the formulation of equation (2) used in PRAIRIE, was based on the von Karman logarithmic vertical velocity profile. However, as reported by [3], this approach has been shown (see *e.g.* [9]) to be inadequate for natural streams. In particular it may be noted that Elder's parameterization tends to (often considerably) under-estimate K, thus leading to narrow, 'spiked' concentration profiles. This effect has been noted by PRAIRIE users (despite PRAIRIE's currently erroneously high prediction of K) and this has been one of the driving forces behind the investigation in to the development of the PRAIRIE dispersion modelling methodology.

Fischer argues [3] that the inaccuracy of equation (2) in modelling longitudinal dispersion in natural streams is due to the neglect of the transverse velocity profile. Extending Elder's parameterization to unidirectional shear flow Fischer has shown that the longitudinal dispersion coefficient is proportional to the square of the distance over which the shear profile extends. Now, as the width to depth ratio of natural streams tends to be large, the longitudinal dispersion coefficient will generally depend very much more on the transverse shear profile (which may extend up to the entire width, W, of the stream) than it does on the vertical profile (which only extends over the depth, d, of the stream). This has again been emphasised within the context of PRAIRIE, by the apparent insensitivity of the code's predicted concentration profiles to variation of the Manning's coefficient within its expected range. However, it should be noted that the assumed dominance of the transverse shear over the vertical shear is not always justified and depends on the relative depth, width and shear forces (and hence friction velocity) of the river. In particular, for wide, relatively smooth (*i.e.* low Manning's coefficient) rivers, the transverse velocity shear may only affect the fringes of the river and it is likely that in such instances the vertical shear will play a more important role in the longitudinal dispersion.

Following the above theory, and utilising laboratory experiments, Fischer proposed that the longitudinal dispersion coefficient may be better parameterized for real streams by:

$$K = \frac{0.011 \cdot u^2 \cdot W^2}{d \cdot u^*} \qquad (7)$$

(On first inspection the inverse relationship between K and u^* may appear to be counter-intuitive. However, this apparent anomaly disappears when the relationship between u^*, u, W and d is considered.)

Table 1 provides a comparison of estimates of K from equations (6) and (7) with experimental values for a variety of measurements in open channels presented in [3] (and reassessed in [4]).

In Table 1, the PRAIRIE values are as calculated by the current parameterization of equation (6) with A erroneously set to 83.7, the Elder values are those as calculated from equation (6) with A = 18.56, and the Fischer values are calculated from (7). For each parameterization, the ratio of the measured value of K to that predicted is also presented in Table 1. These ratios demonstrate that both PRAIRIE and equation (6) always under-estimate the longitudinal dispersion coefficient and that the under-estimate can be by several orders of magnitude. However, Fischer's parameterization is shown to predict the measured values of K to within a factor of about ±5.

Table 1 Comparison of Experimental to Predicted Values of K for Open Channels

Depth, d	Width W	Mean vel u	Shear vel, u*	disp coef, K	PRAIRIE		Elders		Fischer	
m	m	m/s	m/s	m2/s	predicted K	obs/pred	predicted K	obs/pred	predicted K	obs/pred
0.85	34	0.15	0.055	9.5	1.250095	7.599422	0.2772275	34.26788	6.12	1.552288
0.4	19	0.16	0.116	9.9	1.240736	7.979135	0.275152	35.98011	2.19089655	4.518698
0.58	36	0.21	0.049	8.1	0.7599508	10.65858	0.1685306	48.06249	22.1213793	0.366162
0.035	0.4	0.25	0.0202	0.123	0.01890518	6.506153	0.0041925	29.33803	0.15558699	0.790555
0.49	16	0.26	0.08	9.5	1.048208	9.063087	0.232456	40.86795	4.85616327	1.956277
0.49	16	0.27	0.08	20	1.048208	19.08018	0.232456	86.03779	5.23689796	3.819055
8.07	48.8	0.27	0.0191	3	4.12162338	0.727869	0.9140324	3.282159	12.3894765	0.242141
0.85	47	0.32	0.067	14	1.522843	9.193331	0.3377135	41.45526	43.691266	0.32043
0.94	26	0.34	0.067	33	1.6840852	19.59521	0.3734714	88.36018	13.6488028	2.417794
0.43	16	0.37	0.05	14	0.57491	24.35164	0.127495	109.8082	17.9307163	0.780783
0.91	37	0.4	0.067	39	1.6303378	23.92142	0.3615521	107.8683	39.5184517	0.986881
2.35	70	0.43	0.1	110	6.2839	17.50505	1.39355	78.93509	42.4089787	2.59379
0.035	0.34	0.44	0.0348	0.25	0.03256932	7.675936	0.0072227	34.6129	0.20211967	1.236891
0.021	0.33	0.45	0.0328	0.4	0.01841851	21.71728	0.0040846	97.92919	0.35217008	1.135815
0.035	0.4	0.45	0.0351	0.415	0.03285009	12.63315	0.007285	56.96633	0.29010989	1.430492
0.047	0.43	0.45	0.0359	0.253	0.0451184	5.607468	0.0100057	25.28562	0.24409693	1.036474
0.021	0.19	0.46	0.0388	0.22	0.02178775	10.09742	0.0048318	45.53203	0.10312514	2.133331
2.04	104	0.58	0.05	315	2.72748	115.4912	0.60486	520.7817	392.387514	0.802778
0.85	18	0.6	0.1	21	2.2729	9.239298	0.50405	41.66253	15.0945882	1.391227
4.75	127	0.64	0.08	670	10.1612	65.93709	2.2534	297.3285	191.239006	3.503469
0.76	64	0.67	0.27	35	5.487048	6.378658	1.216836	28.76312	98.5654893	0.355094
1.56	24	0.71	0.043	9.6	1.7937192	5.352008	0.3977844	24.13368	47.6144544	0.201619
3.84	72	0.76	0.13	260	13.348608	19.47769	2.960256	87.83024	65.9796923	3.940606
2.47	34	0.82	0.18	65	11.888604	5.467421	2.636478	24.6541	19.2313054	3.379906
2.1	53	0.83	0.107	47	6.008478	7.82228	1.332471	35.27281	94.7321811	0.496136
1.1	59	0.88	0.12	42	3.52968	11.8991	0.78276	53.65629	224.640533	0.186965
2.1	60	0.94	0.104	54	5.840016	9.24655	1.295112	41.69524	160.213187	0.337051
0.58	25	1.01	0.14	14	2.171288	6.447786	0.481516	29.07484	86.3693042	0.162095
2.16	69	1.55	0.17	160	9.818928	16.29506	2.177496	73.4789	342.650674	0.466948
2.7	200	1.55	0.074	1500	5.342652	280.7594	1.184814	1266.022	5483.18318	0.273564

(The values for K predicted using equation (7) and presented in Table 1 (inexplicably) do not match those presented in [3]. However, the values do agree with the re-assessment values presented in [4])

The inability of Elder's equation (2) to adequately model scenarios with large dispersion coefficients has been noted for PRAIRIE (see [6]). To illustrate this point, consider the

VRDEE9A case in [6] where the measured velocity of the Dee was 1.21 m/s and the dispersion coefficient was measured as 63.8 m^2/s. Assuming an estimated depth of 2 m and PRAIRIE's maximum guidance value for n of 0.15, the maximum value for K that can be predicted from Elder's equation is 6 m^2/s. Fischer's parameterization, however, produces values of K which broadly equate to the measured value using intermediate values of n ($\approx$ 0.06).

Analysis of the data presented in Table 1 (performed as part of the current study) suggests that a relationship exists between the 'accuracy' of Fischer's predictions of K and the relative values of u and u^*. It has been found that a sample correlation of about -0.5 exists between (observed K)/(predicted K) and u/u^*. This is shown in Figure 1.

It can be seen from Figure 1 that as the value of u/u^* increases, Fischer's parameterization of K becomes increasingly more likely to over-estimate rather than under-estimate the measured values (though there is no evidence to suggest that the actual levels of over-estimation increase with u/u^*). As u/u^* is largely dependant on $1/n$, this means that for small values of the Manning's coefficient, n, Fischer's equation is likely to underestimate peak concentrations. This result is not unexpected because, as noted earlier, at small n, the transverse velocity shear will not necessarily be the dominant driving force for the longitudinal dispersion.

Analysis of the Elder's predictions of K, when applied to the above experimental measurements, suggests that equation (2) appears to become increasingly accurate (though still over-estimating K by roughly an order of magnitude) when n is large. This is also true when the depth, d, becomes large relative to the width, W. This latter result is expected as, in this situation, the vertical velocity shear becomes increasingly important to the longitudinal dispersion coefficient.

Implementation of Fischer's parameterization into PRAIRIE would be relatively straightforward. The width of the river may be either input by user via an extension to the hydrological information input interface, or estimated within PRAIRIE assuming a rectangular cross-section from:

$$W = \frac{Q}{u \cdot d} \tag{8}$$

The dispersion coefficient may then be calculated from (7) by input of the Manning's coefficient n in the current manner where n may be estimated, for example, using the PRAIRIE guidance which is based on [4] or from information on bed material following [10].

Alternatively, the energy gradient, S, may be input and the dispersion coefficient calculated from substituting equations (3)and (4) into (7).

The energy gradient across an open river reach may be expressed as [11]:

$$S = \frac{\Delta h + \Delta h_v - k(\Delta h_v)}{L} \tag{9}$$

where Δh is the change in height of the water surface across the reach (m),

k is a constant generally taken to range between 0 (for a uniform or contracting river reach) and 0.5 (for an expanding reach),
L is the length of the reach (m), and
Δh_v is the change in velocity head (m) where h_v is defined by :

$$h_v = \frac{\alpha \cdot u^2}{2g} \tag{10}$$

where the velocity head coefficient α can be assumed to be unity [11].

For uniform flows or flows in steeply sloped channels where changes in velocity head and water depth across the reach are small compared to the channel bed gradient, the energy gradient, S, is equivalent to the river bed gradient. As the river bed gradient may be readily estimated from contour maps, this option would be an attractive alternative in the situations prescribed above, particularly if direct estimates of the Manning's coefficient are not readily made.

Further assessment of the Fischer parameterizations and the methods for estimating n is provided in Section 4 where the methods are evaluated against experimental dye tracer measurements for the River Wharfe.

2.3 Correlation Matrices For The Estimation Of The Diffusion Equation

One of the assumptions central to the PRAIRIE risk assessment methodology is that the concentration of a pollutant accidentally released into a river is highly correlated to flow. This assumption is borne out by dye tracer experiments and indicates that dilution is the most important mechanism for reducing the concentration of a pollutant. (The other main assumption in PRAIRIE is that the concentration is directly related to the amount of chemical released into the river.) Sensitivity studies have shown that whilst the concentration is related to the LDC this correlation is less significant than the correlation with flow.

Predictive risk calculations such as those made by PRAIRIE require the user to provide a certain amount of hydrological information; all hydrological information must be supplied if PRAIRIE is run in deterministic mode whilst less information is required if PRAIRIE is run in probabilistic mode. The behaviour of UK rivers varies from catchment to catchment and even within a catchment. It is therefore difficult to suggest generic or typical input data from which a user could start to build a release scenario. The user must therefore consult with the various Environment Agency regions to find out from local hydrologists what types of hydrological conditions might be suitable for a PRAIRIE simulation. The Environment Agency will be able to provide information regarding typical daily flows (minimum, maximum and average) at their gauging stations and probably advise upon velocity. However, the user will find it more difficult to obtain information on LCD's.

In recent years there has been a reasonably extensive programme within the EA to characterise the behaviour of the UK's rivers by dye tracer experiments. This experimental programme allows an understanding to be drawn of the relationship between flow, velocity and LDC.

Table 2 details LDC estimates for a sub-set of dye tracer experiments made on the Rivers Dee and Wharfe.

Correlations between the various parameters, namely flow, depth, velocity, and dispersion coefficient were studied. For the Dee the correlations between flow and velocity were weak (Pearson correlation coefficient of -0.17). There was also only a moderate correlation between flow and dispersion (correlation coefficient of -0.42). These correlation coefficients were determined omitting the experiments with very high dispersion (9a and 9b) since these data tend to distort the results; the correlation is at first sight better when these points are included but this is likely to be an artificial distortion caused by the internal correlation between experiments 9a and 9b rather than the good correlation between either flow vs. velocity or flow vs. dispersion coefficient throughout the full range of the data. Figure 2 shows plots for the Dee of flow against dispersion coefficient for the restricted dataset.

Table 2 LDC Estimates for Dye Tracer Experiments on the Rivers Dee and Wharfe

Dye Tracer Experiment distance (m) (and expt. identifier)	Measured Flow m^3s^{-1}	Calculated Velocity ms^{-1}	Estimated Dispersion Coefficient m^2s^{-1}
River Dee data - all distances in m from tidal limit			
43600 (2a)	13.44	0.12	4.25
42900 (2b)	13.39	0.09	3.16
40300 (2c)	13.4	0.1	5.84
39000 (2d)	13.42	0.09	3.36
348100 (3a)	12.34	0.16	6.09
43600 (3b)	12.41	0.14	5.45
58900 (4a)	6.57	0.31	34.08
48100 (4b)	7.52	0.26	12.19
95000 (6b)	9.26	0.39	35.47
80700 (6e)	10.07	0.34	34.02
95000 (6b)	16.19	0.36	18.88
80700 (6d)	13.47	0.32	28.49
118700 (7a)	11.78	0.38	23.2
108600 (7b)	10.44	0.39	32
128300 (7c)	14.57	0.49	27.09
118700 (7d)	13.53	0.42	24.7
95000 (12b)	10.57	0.51	30.12
80700 (12c)	11.4	0.44	32.16
95000 (9a)	94.92	1.21	63.8
80700 (9b)	95	1.1	62.52

Table 2 (continued) LDC Estimates for Dye Tracer Experiments on the Rivers Dee and Wharfe

River Wharfe data - distances in m relative to release point			
1800 (case 1)	1.3	0.09	2.19
8100 (case 1)	2.8	0.14	9.14
15650 (case 1)	3.34	0.16	9.38
1800 (case 2)	10.03	.4	9.88
8100 (case 2)	11.72	.51	33.63
15650 (case 2)	12.91	.50	45.54
1800 (case 5)	3.99	.28	8.8
8100 (case 5)	5.11	.33	17.86
15650 (case 5)	4.61	.33	24.07
20850 (case 5)	5.99	.3	23.23

The correlation between velocity and dispersion coefficient, however, was strong (0.87 for the reduced dataset, 0.93 for the full Dee dataset). The correlation between velocity and dispersion coefficient was fair for the more limited Wharfe dataset (0.83).

These results, albeit on a restricted set of dye tracer experiments, seem to indicate that, for above rivers, the LDC can be calculated relatively simply from the velocity, and that one regression equation can be applied for all reaches of a river (*cf* Equation (7)). For the Dee, the data that visually appear to be furthest from the regression line all seem to have dispersion coefficients in the range 30-35 m^2s^{-1}; further investigation shows that apart from experiment 4b just two experiments (6b &6e and 12b & 12c and which were conducted as pairs) are responsible for the apparent lack of agreement. It might therefore be possible that experimental difficulties account for the lack of agreement rather than the fact that artificial correlation's have been introduced due to the availability of a restricted statistical sample. Moreover, the results would seem to hold for a fairly wide range of conditions since the Dee dye tracer data cover both upstream stretches (which are shallow, tortuous and fast flowing) and downstream stretches (which are deeper and more sluggish).

This suggestion of a good correlation between LDC and velocity leads towards two important implications. First, it would help the user to input realistic dispersion coefficients with greater confidence than at present, since users often have a better intuitive feel for velocity than LDC. Secondly, the findings could be used to improve the accuracy of probabilistic modelling since at present, for reasons of simplicity, the user supplies one LDC which is used for all stretches within a simulation. Inputting the LDC as a function of velocity could be easily implemented with only minor modifications to the PRAIRIE interface and the DYNUT dispersion code. Possible improvements to PRAIRIE's ADE modelling are discussed in Section 5.

3 THE AGGREGATED DEAD ZONE (ADZ) MODEL

3.1 Development Of The ADZ Model

The existence of storage or dead zones within natural rivers and the effect that these zones have on the dispersion of pollutants within rivers has been acknowledged for some time (see *e.g.* [1]). Following the recognition of this feature of dispersion within natural rivers, it has been suggested [12] that these dead zones in fact dominate the turbulent shear flow dispersion of the ADE model to the extent that most of the dispersion could be attributed to the aggregated effect of the dead zones.

Assuming steady flow and complete and instantaneous mixing, a single dead zone may be described by a simple dynamic mass balance as (ignoring sinks) [5]:

$$\frac{dC_d(t)}{dt} = -\frac{Q}{V_1}C_d(t) + \frac{Q}{V_1}C_o(t) \tag{11}$$

where C_d is the concentration in the single dead zone (kg/m^3),
t is the time after release (s),
Q is the discharge of the dead zone flow field (m^3/s),
C_o is the concentration entering the dead zone (kg/m^3), and
V_1 is the volume of the single dead zone (m^3)

Equation (11), which describes a single dead zone within a river reach, may be extended to describe an entire river reach using the assumption that the aggregated effect of all the dead zones within the reach may be treated as a single dead zone with an effective (much larger) volume V_e [5].

Finally, the advective properties of the channel can be considered by the introduction of a simple time delay, τ. This leads to :

$$\frac{dC_d(t)}{dt} = -\alpha \cdot C_d(t) + \beta \cdot C_o(t-\tau) \tag{12}$$

where $\alpha = \beta = Q/V_e = 1/T_r$ where T_r is the ADZ residence time.

The number of ADZ elements required to model long stretches of rivers varies according to the variation in the hydrological characteristics of the river along the reach. To enable the use of multiple ADZ elements Wallis *et al* [5] consider the discrete-time version of the elemental ADZ of Equation (12) where, for a sample interval of Δt :

$$C_d(t_k) = -aC_d(t_k - 1) + b_oC_o(t_k - \delta) + b_1C_o(t_k - \delta - 1) \tag{13}$$

where k denotes the variable value at the kth time interval,

δ is the advective delay time in sampling intervals and is the nearest lower integral value of $\tau/\Delta t$.

Equation (13) thus enables the concentration profile at the end of the elemental ADZ to be calculated from the concentration profile at the entrance to the ADZ.

When the initial arrival time τ is an exact multiple of the sampling interval (*i.e.* $\tau/\Delta t$ is equal or very close to an integral value), then equation (13) simplifies with $b_1 = 0$. In this case the discrete time parameters a and b_o can be related to the continuous time parameters α and β by:

$$\begin{aligned} a &= -\exp(-\alpha \cdot \Delta t) \\ b_o &= (1 + a) \end{aligned} \tag{14}$$

A fundamental property of the elemental ADZ model is that the mean travel time $\bar{t}$ (*i.e.* the travel time between the centroids of the downstream and upstream concentration profiles) is given by:

$$\bar{t} = T_r + \tau \tag{15}$$

Now, as $\alpha = 1/T_r$, this means that Equation (14) may be re-written as:

$$\begin{aligned} a &= -\exp\left(\frac{-\Delta t}{\bar{t} - \tau}\right) \\ b_o &= (1 + a) \end{aligned} \tag{16}$$

Thus the concentration profile at the end of an ADZ may be estimated from the concentration profile entering the ADZ provided that $\bar{t}$ and τ are known.

The elemental ADZ equation (13) may now be generalised to model multiple ADZ elements in series or parallel via use of transfer functions following [5].

3.2 Implementation Of The ADZ Model

Wallis *et al* have shown that the elemental ADZ model provides excellent results when calibrated to measured data for short river sections and propose that it is a simple and accurate dispersion model and, as such, is an attractive alternative to the ADE methodology. One of the aims of the present study was to assess the applicability and implementation of the ADZ model for potential usage within PRAIRIE.

Section 3.1 showed how the elemental ADZ model may be used to estimate the downstream (*i.e.* end of aggregated dead zone) concentration profile from a given upstream (*i.e.* aggregated dead zone entrance) concentration profile from the ADZ time parameters $\bar{t}$ and τ. However, in order that this model be used within predictive dispersion applications three issues need to be resolved, *viz.*:

1. how are the time parameters $\bar{t}$ and τ to be estimated ?;

2. how can the upstream concentration profile be generated in a predictive scenario ?; and
3. what is the range of applicability of the elemental ADZ model ?

The applicability of the elemental ADZ model (issue 3) is assessed by evaluation with experimental dye tracer measurements over long reaches of the River Wharfe and River Swale and also by comparison with the ADE model. This assessment is detailed in Section 4. The feasibility of the implementation of the elemental ADZ methodology in to PRAIRIE is reliant on the resolution of issues 1 and 2 and these are now discussed.

It has been shown (see *e.g.* [5]) that both $\bar{t}$ and τ may be regressed from the discharge Q for short channels (for [5] the channel lengths were < 150 m). This point has been verified for longer river reaches within the current study using dye tracer data for the rivers Wharfe (a 21 km reach between Hebdon and Hollins) and Swale (a 27 km stretch between the Whiske tributary and Myton). Five separate tracer experiments were performed for each river with concentration measurements taken at time intervals at various points along the two river stretches. The measured concentration profiles were used to used to calculate $\bar{t}$ and τ (in minutes) for each tracer experiment and these were regressed with the discharges (in m^3/s) recorded at the nearest gauging station using inverse relationships of the form:

$$\bar{t} = A + B \cdot Q^{-1} \tag{17}$$

where A and B are the regression coefficients.

The analysis showed that both $\bar{t}$ and τ may be accurately regressed from Q using the above inverse relationship and the results are summarised in Table 3.

Table 3 Summary of $\bar{t}$ and τ regression with Q for the Swale and Wharfe

River	Time interval	Regression Coefficients		Coefficient of Determination
		A	B	
Swale	τ	166.5	11790	0.994
Swale	$\bar{t}$	233.3	12379	0.993
Wharfe	τ	167.3	3941	0.984
Wharfe	$\bar{t}$	160.3	5008	0.965

Thus, once a river stretch has been analysed and the four regression coefficients evaluated (two each for $\bar{t}$ and τ) all the required elemental ADZ parameters can be inferred from the just the discharge. For implementation in to PRAIRIE, the ADZ time parameters may be taken from the discharge Q, which would be input in the usual manner, and from the four regression coefficients which may be input either via database or through additional user input windows.

This still leaves the problem of the upstream concentration profile. The problem may be overcome by solving Equation (12) assuming that the input concentration profile (C_o) can be specified as a Dirac (spike) function (scaled according to the mass of pollutant injected) and that the reach between the injection point and the site at which the first profile is required may be treated as an elemental aggregated dead zone. Under this assumption the concentration profile at this first point is given by :

$$C_d(t) = 0 \qquad t < \tau$$
$$C_d(t) = \frac{M}{Q} \cdot \beta \cdot e^{-\alpha(t-\tau)} \qquad t > \tau \tag{18}$$

where M is the mass of pollutant injected.

As mentioned in [5], dispersion in the reach immediately after the injection is not *necessarily* well modelled by an elemental aggregated dead zone. However, good results for the predicted initial peak values have been obtained as part of this study in comparison with dye tracer experiment data for the rivers Wharfe and Swale (see Section 4). This solution is of course inappropriate for finite duration releases. In this latter situation, the user input profile may be used as the entrance concentration profile, though in practical application the concentration profile will be sensitive to the mesh size assumed for the model and the concentration may therefore be dominated by the initial numerical dispersion.

This problem may be surmounted by using an ADE model to generate the first profile. However, in practise this is unlikely to provide greater accuracy as an initial profile close to the injection point is always prone to the problems of numerical dispersion and, further, would give a Gaussian profile - the main objection of supporters of the ADZ model. Alternatively, the problem may be tackled by the use of multiple aggregated dead zones. The difficulty with multiple dead zones is the complexity of calibration. Wallis *et al* [5] used sophisticated regression techniques to determine the optimum ADZ combinations (either in series and/or in parallel) and it is unlikely that this approach would be generally feasible in the context of a generic tool such as PRAIRIE. Additionally, this approach requires significant amounts of data to drive the necessarily sophisticated regression analysis.

It is likely that the analytical solution may represent the best approach to the resolution of the impulse injection problem. However, it is recommended that the accuracy of the method should be further assessed with experimental data before implementation in to PRAIRIE is considered.

4 Assessment Comparison Of ADZ And ADE Methods

4.1 The Elemental ADZ Model

In order to assess the applicability of the elemental aggregated dead zone model to longer reaches, the model has been calibrated and applied to dye tracer experiments for the River Wharfe and River Swale.

For the River Wharfe data was available from five separate dye tracer experiments and the elemental ADZ model was calibrated and compared with the measured concentration data for three of these experiments (cases 1, 2 and 4 were selected in order to cover a range of different discharge rates). The stretch of river considered was from the injection site at Hebdon to a site at Lobwood located 15.65 km downstream. Periodic concentration measurements were taken at Lobwood and two intermediary points at Burnsall (1.8 km downstream from Hebdon) and Barden (8.1 km downstream from Hebdon). For each of the three cases the elemental ADZ model was calibrated on the measured Burnsall concentration profile and the model was then used to predict concentrations at Barden and Lobwood.

The predicted concentrations at Barden were estimated from the measured Burnsall data assuming that the river stretch between Burnsall and Barden may be treated as an elemental ADZ and that the coefficient b_1 of equation (13) may be neglected. Similarly the Lobwood concentrations were predicted from Burnsall data assuming that the Burnsall to Lobwood stretch is considered as an elemental ADZ. Thus, the Barden predictions assume an elemental ADZ of length 6.3 km, and the Lobwood predictions assume an elemental ADZ of length 13.85 km and hence these analyses test how well the elemental ADZ model works over large reaches. In each instance the ADZ time parameters $\bar{t}$ and τ were inferred (using equation (16)) from the measured concentration profiles at each of the various monitoring sites.

The pertinent hydrological data for the three cases is summarised in Table 4 together with a comparison of the measured and predicted peak concentrations at the monitoring sites.

Table 4 Comparison of the Elemental ADZ Model Experimental Data for the River Wharfe

Case	Mass Injected (mg)	Discharge (m^3/s)	ADZ Time Parameters from Burnsall (min)				Peak Concentrations (mg/m^3)				
			Barden		Lobwood		Burnsall	Barden		Lobwood	
			τ	$\bar{t}$	τ	$\bar{t}$	(Measured)	Measured	ADZ	Measured	ADZ
1	14	2.8	420	605	1025	1285	1.4	0.30	0.53	0.19	0.42
2	20	12.485	158	200	372	457	1.28	0.37	0.43	0.23	0.26
4	14	3.74	347	396	712	866	0.87	0.23	0.53	0.17	0.27

The measured and predicted concentration profiles at the three monitoring sites are plotted in figures 3 to 5. It can be seen for these dye tracer experiments that the elemental ADZ model overestimates the peak concentrations by a factor of up to about 2. A similar investigation using dye tracer experiments for the River Swale has also been performed and this yielded similar levels of accuracy for the predicted peak values over river reaches of several km in length. To illustrate this the ADZ predictions are compared with the measured values for one of the Swale tracer experiments (case 5) in Figure 7. Comparisons between the Wharfe and

Swale dye tracer experiments suggest that the elemental ADZ model does indeed represent a simple and broadly accurate method for estimating peak concentrations within large river stretches. Whilst comparisons over large reaches for just two rivers not does imply such accuracy for all rivers *per sa* it is worth noting that, despite their close proximity, the Wharfe and Swale are physically different rivers ; the Wharfe is more meandering and runs in a much steeper gradient than the Swale for the reaches of interest.

The plots in figures 3 to 5 suggest that the skewness of the concentrations profiles is somewhat exaggerated by the elemental ADZ, particularly at the far downstream distances and especially for the River Swale (figure 7). This suggests that the non-Gaussian shape often claimed for concentration profiles (see Section 2) is not always significant. This somewhat undermines the rationale behind any potential switch to the ADZ model and it is interesting to compare the ADE and ADZ models for the dye tracers experiments (see Section 4.2).

The concentration profile measurements at the first monitoring site downstream has also been compared with the predictions of the analytical solution of the elemental ADZ model assuming the dye injection could be considered as a spike release using equation (18). The analytical solution of the elemental ADZ model is compared with the measured data for the initial monitoring site on the River Wharfe (*i.e.* Burnsall) for experiment cases 1, 2 and 4 in Figure 6. This figure shows that the analytical solution provides a reasonable estimate of the peak concentration at the initial site. A similar result is found for the River Swale, and the comparison for the initial monitoring site on the Swale (*i.e.* Skipton) is shown in Figure 8.

However, despite the goodness of fit for the initial site, if the analytically generated profile at this site were to be used by the elemental ADZ model to predict downstream profiles, then the predicted downstream profiles would retain the very skewed 'saw-tooth' shape of the initial profile. As has been mentioned above, this level of skewness has been found to be increasingly excessive as one moves downstream.

4.2 Comparison Of The ADE And ADZ Models

The ADE model has been assessed against the River Wharfe experimental dye tracer data described above. This has been performed by direct input of the longitudinal dispersion coefficient into PRAIRIE and by estimation of the required hydrological data for the simulations from the available tracer experiment data.

For the River Wharfe experiments the initial arrival times at each of five monitoring sites from the injection site has been measured. This information, combined with the known downstream distance of each site, has been used the estimate the flow velocity along each stretch of the river. Additionally, the measured concentration profiles were used to estimate the discharge at each monitoring site under the assumption of conservation of dye mass. From the velocity and discharge data, the cross-sectional area was inferred and thus, by assuming a constant ratio, the river depth and width were roughly estimated.

The longitudinal dispersion coefficient was estimated at each monitoring site using the Fischer parameterization (equation (7)) with the friction velocity u^* estimated from equation (3) assuming that the hydraulic radius R is approximated from the river depth and that the energy gradient S is equal to the river bed gradient. The river bed gradient was estimated from a

contour map of the region. Since PRAIRIE presently allows only a single value of the longitudinal dispersion coefficient may be input, a value of the coefficient that was representative of the required river stretch (Hebdon to Lobwood) was estimated.

Using the information above, PRAIRIE was run in order to assess the ADE model with the River Wharfe dye tracer data. The relevant hydrological data for three of the River Wharfe dye tracer scenarios is given in Table 5 together with a comparison of the measured and predicted peak concentrations at the monitoring sites.

Table 5 Comparison of the Fischer Parameterization of the ADE Model with Experimental Data for the River Wharfe

Case	Mass Injected (mg)	Discharge (m^3/s)	Estimated Dispersion Coefficient K (m^2/s)	Peak Concentrations (mg/m^3)				
				Burnsall (Measured)	Barden		Lobwood	
					Measured	ADE	Measured	ADE
1	14	2.8	4.52	1.4	0.30	0.40	0.19	0.31
2	20	12.485	35.8	1.28	0.37	0.36	0.23	0.25
4	14	3.74	7.53	0.87	0.23	0.32	0.17	0.28

The measured and predicted concentration profiles at three monitoring sites are presented in Figures 3 to 5. It can be seen that, like the elemental ADZ model, the ADE model with the Fischer parameterization tends to over predict the peak concentrations by up to factor of about two (and often by much less). The exceptions to this rule are the ADE predictions at the initial monitoring site at Burnsall, where the predicted peak concentrations underestimate the measured values. The reason for this lies in the varying nature of the River Wharfe over the first few kilometres downstream of the injection point. Analysis of the experimental data suggests that the dispersion coefficient over the stretch between the injection point and Burnsall is considerably smaller than it is over the Burnsall to Lobwood stretch. As PRAIRIE only currently allows a single value of the longitudinal dispersion coefficient a single representative value for the river had to be estimated for each of the cases considered. Now, as the stretch between Burnsall to Lobwood is very much longer than the stretch between the injection point and Burnsall, the estimated representative value of the dispersion coefficient was skewed towards its value for the former stretch. This means that the level of dispersion up to the Burnsall site has been somewhat overestimated. The solution to this problem is, of course, to develop PRAIRIE to enable the user to specify the dispersion coefficient at different stations along the river.

Comparison between the ADZ and the ADE models suggests that both models can produce reasonable predictions (to within a factor of about 2) of the peak concentration and that, for the particular scenarios studied, Figures 3 to 5 show that the ADE model produces slightly more accurate peak concentration predictions than the elemental ADZ model. Additionally, it is indicated that the shape of the concentration profile is best parameterized by the elemental ADZ model in the near field, where the profile has a tendency to be positively skewed, and by the ADE model in the far field where the profile becomes increasingly Gaussian in shape.

5 IMPROVEMENTS TO PRAIRIE ADE MODELLING

The work discussed in Section 2 immediately suggests improvements that could be made to PRAIRIE. Although the suggested improvements apply to both the deterministic and probabilistic modes of operation there are methodological differences between the two types of operation which demand slightly different approaches to the ways in which the improvements might be implemented.

The project has studied the correlations between flow, position and diffusion coefficient for the rivers Dee and Yorkshire Wharfe to see whether further information could be found to help the user input realistic LCD's. At present the advice to the PRAIRIE user is limited: they can either refer to hydrologists within the Environment Agency who would themselves refer to dye tracer data; or they can refer to tabulations such as that provided with PRAIRIE for advice regarding Manning's coefficients most suitable for the stretch of river they wish to simulate. We have shown here two ways in which the user might select the LDC with greater confidence: Section 2.3 discusses how the LDC seems to be correlated with velocity and shows that the correlation seems to be independent of position or river shape; this analysis would therefore suggest ways in which PRAIRIE modelling might be improved. Section 2.2 discusses how the dispersion coefficient might be better estimated using Fischer's parameterization rather than the current Manning's/Elder's parameterization.

The deterministic mode of PRAIRIE currently allows the user to either: (i) provide one LDC which will be applied for all distances within the simulation; or (ii) using Elder's parameterization, to provide one Manning's constant that will be constant for all distances within the simulation - because PRAIRIE allows depth to vary this means that it is possible that a different LDC might be calculated for all distances within the simulation.

Recommendations for improvements to deterministic modelling - data entry for LDC or Manning's constant should be moved from the River Specific Parameters screen to the Hydrological Stations Flow screen; the user could then: (i) enter one value (LDC or Manning's constant) for the upstream boundary which is replicated for all downstream stations; or (ii) enter a series of LDC or Manning's values for each station (and PRAIRIE would interpolate between points); or (iii) enter the correlation between velocity and LDC, allowing PRAIRIE to calculate the LDC from user inputs of velocity (should further studies confirm that the these parameters are sufficiently well correlated).

The probabilistic mode of PRAIRIE currently uses one, positionally independent, value for the longitudinal dispersion coefficient; the value is a user supplied input and it has been recommended, to ensure a conservative analysis, that the value chosen is the smallest expected within the simulation stretch. However, inspection of Table 2 shows that whilst the dispersion coefficient does not change markedly for one dye tracer experiment it is also unrealistic to expect that one value will be applicable to all positions within the stretch, especially if the simulation is over a long distance. Steps have therefore been taken to evaluate how PRAIRIE/DYNUT could be reconfigured to model diffusion coefficients as a function of distance for probabilistic analyses.

The probabilistic mode of PRAIRIE presently prompts the user to supply only the LDC with respect to hydrological input; flows are taken from the appropriate flow database and velocities are estimated by the code. Two enhancements are possible:

1. If further investigation confirms that velocity and LDC are indeed well correlated, then the user could be prompted to supply details of the correlation rather than input a fixed LDC. The LDC would then be calculated as a function of velocity for all meshes within the simulation;

2. Alternatively, the river database could be modified to include an empirical LDC adopting Fischer's parameterization (equation (7)) - depth data are already included in the database for each flow station and width data could be added with relative ease. The LDC would then again change as a function of velocity (which PRAIRIE already calculates) for all meshes within the simulation.

Recommendations for improvements to probabilistic modelling - a new screen should be created which is devoted to the dispersion coefficient. The user could then: (i) enter one position and velocity independent LDC - the current method of implementation; or (ii) enter the correlation between velocity and LDC, allowing PRAIRIE to calculate the LDC from user inputs of velocity; or (iii) be offered the chance to edit the empirical Fischer's parameterization that might be added to the river specific database.

Improvements to both deterministic and probabilistic approaches would offer either: (i) the option for the user to adopt a simple and robust approach (by entering one relatively simple parameter); or (ii) the option to provide more sophisticated data, and therefore gain more control over the simulation.

Either or both modifications could be implemented easily. Modifications to the code would centre around additions to the routines which read datafiles and to additional lines of coding to the QUICKEST routine which solves the ADE equation. Modifications would also be required to the user entry screens and to the checks which ensure that the user does not provide conflicting inputs.

6 CONCLUSIONS

At the beginning of the project we set out to examine a number of aspects associated with the physical modelling currently used within PRAIRIE, namely:

(1) Examination of the advection-diffusion model, paying special attention to the prediction of longitudinal diffusion coefficients;

(2) Identification of improvements that could be made to deterministic and probabilistic modelling, again with an emphasis on LCD's.

We also spent time studying the ADZ model, to see how it compared with PRAIRIE's ADE model and to assess how easily the model might be incorporated into PRAIRIE.

The LDC is an important parameter which, for present versions of PRAIRIE, must be supplied by the user, either directly as an LDC or indirectly using Elders/Manning's parameterization. There is presently little advice that the user can refer to regarding selection of LDC.

Our studies of other workers findings relating to empirical approaches showed that there is a small error in the current implementation of the Elder's/Manning's parameterization. This error causes the Elder's parameterization of the LDC to be overestimated, therefore producing potentially optimistic underestimates of the peak concentrations. However, it may be seen that this error has, in fact, generally led to more accurate estimates of the actual dispersion coefficient due to the excessive pessimism of Elder's parameterization.

- In the short term we recommend that the user overcomes this erroneous implementation by dividing the Manning's n by 4.51;
- In the longer term we recommend that the DYNUT dispersion code is corrected to eliminate the error.

Our studies of empirical approaches also showed that the Fischer parameterization predicts the LDC better than Elder's parameterization.

- We therefore recommend that the Elder's parameterization is either replaced or supplemented by Fischer's parameterization.

We also spent time investigating whether it might be possible to use dye-tracer experiments to derive correlation's between more easily measured parameters (such as flow and velocity) and the LDC. Using a relatively small set of dye-tracer data for the River's Dee and Wharfe we identified that there *might* be a correlation between velocity and LDC. Whilst the dye-tracer measurements for the Dee cover a range of conditions (fast flowing tortuous reaches to more sluggish meandering reaches) the results have been treated with caution due to the statistically small data set. However, if more extensive studies support the early findings then dye tracer experiments could be used to generate correlation's between velocity and LDC.

- We therefore recommend that further studies are made to investigate correlations for a range of dye tracer experiments. PRAIRIE could be modified with relative ease to improve LDC estimation if the correlations prove to be significant.

Approaches by which improvements may be made to PRAIRIE's deterministic and probabilistic calculations were identified and briefly discussed.

Finally, we looked at the ADZ model (which adopts a different modelling approach to the ADE model) to see how the approaches compare and how the ADZ model might be incorporated into PRAIRIE.

The elemental ADZ model was assessed using dye tracer experiment data for moderately long ($\approx$ 15 km) stretches of the River Wharfe and the River Swale in Yorkshire. The elemental ADZ model was shown to provide good estimates of the peak concentrations at most downstream sites. However, the skewed profiles produced by the ADZ model were found to be increasingly inappropriate as the pollutant moved downstream.

The ADE model was implemented for the Wharfe dye tracer data using the Fischer parameterization for the dispersion coefficient with the Manning's coefficient being estimated from the river bed gradient. The results for this implementation showed that the ADE model is capable of producing predictions of the downstream peak concentrations at least as good as the elemental ADZ model. Further, whilst in the near field the skewed nature of the ADZ predicted concentration profiles matches the measured profiles better, at distances further downstream the measured profiles were found to be broadly Gaussian in shape and thus better represented by the ADE model.

Whilst it should be stressed that the accuracy of the ADZ model could be improved by the use of multiple ADZs rather than an elemental ADZ, this would require considerably greater effort (and ideally more experimental data) to calibrate the model to the river. Additionally, the problem of the estimation of the first profile in the ADZ regime is unresolved. Whilst the analytical solution of the elemental ADZ for a spike release has been shown to produce reasonable estimates of the peak concentrations, the profiles downstream become excessively skewed. This solution is also, of course, inappropriate to finite duration releases.

With regard to the modelling of the dispersion coefficient within PRAIRIE, it is concluded that:

- Given the above reservations regarding the (elemental) ADZ model and the relatively high level of accuracy obtained using the ADE, it is suggested that further research and more conclusive evidence is required before implementation of the ADZ methodology into PRAIRIE could be justified;

- The assessment of the ADE model has also demonstrated that the longitudinal dispersion coefficient may be successfully estimated from the Fischer parameterization with the friction velocity u^* (and hence the Manning's coefficient) being estimated from the river bed gradient. As the river bed gradient can be reasonable approximated from contour maps, this represents a simple and easy to implement method for the estimation of the dispersion coefficient.

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