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Using transient tracers: the regularization problem

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ABSTRACT

The generic problem of deducing fluid properties, velocity, mixing, and boundary conditions from realistic tracer observations is formulated and attacked. The focus is on oceanic transient tracers, but the same problem elements appear in many other fields including meteorology, medicine and chemical engineering. It becomes clear that use of tracers, transient or otherwise, requires at some stage the solution of the advection/diffusion equation either upstream, or backwards in time, or both, a situation notorious for its instability because diffusive processes progressively destroy information in the "forward" direction. We consider an example in simple finite difference form for one space dimension and time. The problem is run "backwards", but regularized by solving it through linear programming. Linear programming is shown also to have several potential advantages for stable and unstable forward problems, and the inverse problem: knowledge of the form of the answer is easily used; data uncertainty is accommodated; the positivity constraints on concentrations are implicit; sparse system software is available; questions of best observational strategy are addressed by the dual solution; and the strong instabilities of the inverse and backwards problems are suppressed.

1. Introduction

Passive tracers, whether stable, decaying steady-state or transient, are used in a wide variety of fields including oceanography, meteorology, chemical engineering and medicine (Nauman and Buffham, 1983; Buffham, 1985; Deuflhard and Hairer, 1983). One observes large-scale distributions of "dyed" fluid, either changing with time, or inferred to be in a steady-state. From the patterns, one tries to infer fluid properties, often rates of advection and of mixing. In oceanography at least, the inferences range from the purely qualitative (e.g., "that the flow must go that way", in Wüst's core-layer method), to the semi-quantitative, as in various box models (e.g., Bacastow and Björkström, 1981).

But it seems fair to conclude that we lack a general theory for the use of tracers. Such a theory if it could be constructed, would tell us a number of things: exactly which fluid properties, are determinable by what types of observation? What accuracy is required? When we are dealing with transient tracers, and are faced with designing an observational strategy while the signals are decaying, where should the effort be focussed? Are extended time series at a comparatively small number of places a more useful strategy than an attempt at complete geographical coverage in as short a time as possible?

The subject of the best use of tracers is a difficult one and a discussion could go in a number of different directions. Here the focus is on problems suggested by oceanic transient tracer observations, especially those of the tritium (^{3}H)/helium-3(^{3}He) pair, the chlorofluoromethanes (Freons), and radiocarbon (^{14}C). To become specific, consider Fig. 1, the Östlund and Fine (1979) classical picture of the tritium distribution along a section down the western North Atlantic at the time of GEOSECS ($\sim$1972). The qualitative import of Fig. 1 is reasonably clear. Most of the tritium seen was injected into the ocean through atmospheric nuclear weapons testing in the early 1960's (see Fig. 2) which was then rained out into the ocean in a very few years. The near surface maximum in Fig. 1 is interpreted as

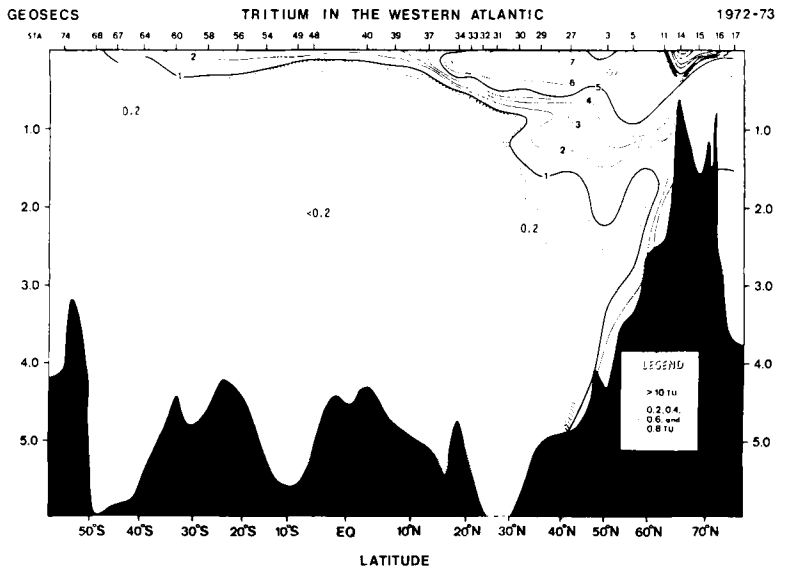

Fig. 1. Tritium concentration during GEOSECS, 1972 (Östlund and Fine, 1979) along a section in western Atlantic Ocean.

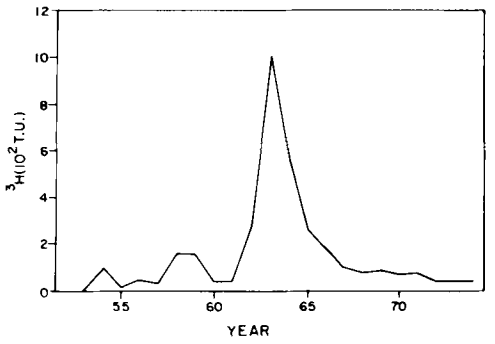

Fig. 2. Estimate of injection of tritium into North Atlantic Ocean surface through bomb tests (after Dreisigacker and Roether, 1978). Values are ^3H in precipitation at Valentia, Ireland.

the direct injection into the ocean from near-surface driving (Ekman fluxes and mixed layer formation). The bottom maximum is thought to be the result of convective injection in wintertime at high latitudes carrying the high surface tritium values deep into the ocean, spilling over the northern sills onto the floor of the Atlantic.

But Figs. 1 and 2 raise a number of questions. Can the rates at which the overflow waters carried the high tritium onto the deep Atlantic floor be quantified? To what extent can one distinguish between advective processes and diffusive ones, as a function of position, in Fig. 1? Is there any information in Fig. 1 concerning the actual rates of injection of tritium by Ekman-like processes? Is there information about the nature and strength of the unobserved high latitude deep-injection process?

The purpose of this paper is to begin the process of finding practical procedures for handling transient and other tracer data in a systematic, quantitative way. Tracer data involve a discussion of observational realities in the context of modelling needs, leading to a somewhat unorthodox set of issues. So the paper has two basic themes: to try to establish a mathematical context for discussing tracer data and, to suggest at least one method that may prove to be a practical procedure for making inferences about the ocean from data.

2. Forward and inverse problems

Consider any passive tracer C, stable, unstable, steady, or transient in any combination of

stable/unstable with steady/transient. All such tracers satisfy an equation like

$$\frac{\partial C}{\partial t} + \boldsymbol{u}\cdot\nabla C - \boldsymbol{\alpha}\cdot\nabla\nabla C = Q(\boldsymbol{x}, t), \tag{1}$$

where C represents sinks, as in radioactive decay of ^{3}H, or sources as in nutrients, or even boundary conditions if that is convenient. (Eq. (1) is not the most general possibility, as it does not address the possibility of significant gradients of the diffusion coefficients $\boldsymbol{\alpha}$, nor of diffusion laws more complex than the simple one used. Nonetheless the issues raised by (1) are adequately general.) To reduce the discussion to its simplest possible elements, consider a one dimensional version of (1)

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - \alpha\frac{\partial^2 C}{\partial x^2} = 0 \tag{2}$$

without interior sources in sinks, and with u, α constant in space and time. Although one can solve this reduced equation analytically, we rewrite it in simple finite differences as

$$\frac{C_i^{t+1} - C_i^t}{\Delta t} + u\left(\frac{C_{i+1}^t - C_{i-1}^t}{\Delta x}\right) - \alpha\left(\frac{C_{i+1}^t + C_{i-1}^t - 2C_i^t}{\Delta x^2}\right) = 0, \tag{3}$$

or

$$C_i^{t+1} + C_i^t[-(1-2d)] + C_{i+1}^t(\tfrac{1}{2}\bar{c} - d) + C_{i-1}^t[-(\tfrac{1}{2}\bar{c} + d)] = 0 \tag{4}$$

$$\bar{c} = \frac{u\Delta t}{\Delta x}, \quad d = \frac{\alpha\Delta t}{\Delta x^2},$$

$$t = 0, \Delta t, 2\Delta t \ldots, (T-1)\Delta t$$

$$x = 0, \Delta x, 2\Delta x \ldots, (I-1)\Delta x$$

in a simple explicit scheme which Roache (1976) denotes FTCS (forward in time-centered in space). The usual stability requirement (Roache, 1976) requires $d \leqslant 0.5$, $\bar{c}/d = R_{ep} = u\Delta x/\alpha \leqslant 2$. (The Péclet number, $P_e = uL/\alpha$.)

To the finite difference system (4) we append the initial conditions

$$C_i^0 = \overline{C}_i^0, \quad 0 \leqslant i \leqslant I-1. \tag{5}$$

The upstream boundary condition

$$C_0^t = \overline{C}_0^t, \quad t = 0, \Delta t, \ldots, (T-1)\Delta t \tag{6}$$

and the downstream boundary condition

$$C_{I-1}^t - C_I^t = 0. \tag{7}$$

With $u > 0$, eq. (7) is essentially passive. We will generally assume Δx, $\Delta t = 1$.

In modelling a real flow and tracer, one needs to decide whether the finite difference representation is an accurate model of the fluid properties, and perhaps whether the solution to the finite difference equations is an adequate approximation to the supposed underlying partial differential equation. For present purposes however, the finite difference scheme can be regarded as a simple analogue to more complex representations which might prove necessary with realistic problems. As will be seen, even the simple form (4) raises difficult issues.

What we will call the "forward" problem is simply the conventional system defined either by (1), (2) or (4), with their appropriate initial and boundary conditions. The "inverse" problem could take many forms, but would usually involve a variant of specifying that C was known over some domain of space and time sufficient to define its derivatives in the above equations. The values of u, α which best satisfy the governing equations are sought.

Munk's (1966) determination of u, α (his w, k) can be thought of as an inversion of the steady form of eq. (2) in which a scale assumption about the solution was made, such that u, α did not vary with depth. The derivative terms were fit to exponentials and u/α determined. A second unstable tracer was used to separate u, α. Wunsch (1985) discussed the two dimensional steady problem in finite difference form.

More commonly, the problem is solved in the forward direction, often in conjunction with a dynamical model for the construction of the u, or $\boldsymbol{u}$ fields. Consider the forward problem, for which Sarmiento's (1983) calculation is a good example. The modeller takes an oceanic general circulation model (gcm), providing a full determination of $\boldsymbol{u}$, $\boldsymbol{\alpha}$ in three dimensions. To determine the field of C, a three-dimensional version of eqs. (4–7) is used together with the boundary conditions for C. The model is then integrated forward in time to t_1, the integration is stopped, and the computed field, $\hat{C}$, is examined. The distribution of $\hat{C}$ is usually compared with some set of interior observations

$$C(\boldsymbol{x}_i, t_1) \pm \varepsilon_i,$$

where ε_i represents the observational error. If $\hat{C}$ agrees with the observations within the estimated error, then one stops, because there is nothing in the tracer observations to suggest any deficiency in the model. Alternatively, such a result suggests that the tracer observations contain no new information.

Such a simple outcome will be recognized as not only disappointing, but also as exceedingly rare. The usual result is that the model reproduces some aspects of the observed tracer distribution, and fails to reproduce others.

If the modeller wishes to modify the results of his forward problem, to bring $\hat{C}$ in closer accord with observation, there is an awkward number of choices. Many things in any model are subject to uncertainty. The purely dynamical part driven by dynamical and thermodynamical boundary conditions, is subject to serious questions about accuracy (heat transfers and windstress-curls are poorly known). Parameterizations or simplifications of various dynamical and thermodynamical effects will have been made too. There are thus usually considerable ranges over which one might plausibly modify $\boldsymbol{u}$, $\boldsymbol{\alpha}$ as a function of position. Which, if any or all, of these things the modeller is best advised to modify to improve agreement with the observed C is difficult to determine.

Consider next the forward problem for the tracer alone, with $\boldsymbol{u}$, $\boldsymbol{\alpha}$ specified from the dynamical model. As already noted, the solution of the advection/diffusion equation is dependent upon specification of the tracer boundary condition. For ^{3}H, Freons, and other tracers, these boundary data are also obtained from observations and contain errors. Errors in the boundary data for (1) may lead to serious discrepancies in the computation of $\hat{C}$, even if the underlying dynamical model were perfect. Were infinite computer capacity available, one could simply keep re-solving the forward problem, over and over again, each time with a different combination of perturbations to the uncertain problem parameters, ultimately mapping out the domain of all acceptable model runs. But computer capacities are finite, and the number of combinations and permutations of potentially acceptable perturbations is astronomical.

Given all the possibilities for changes, dynamic and kinematic, it is unsurprising that most comparisons of tracer forward computations with data cease at the stage where the comparison is made, with no attempt to go back and recompute with modifications to the original specifications.

The situation suggests that the inverse problem should be attempted, with the observed tracer field used to help determine the dynamical variables. Doing this is indeed our ultimate goal, but there are several serious difficulties which must be addressed first, and which arise from the plethora of uncertainties involving tracer distributions, tracer boundary conditions, tracer initial conditions, dynamical model specifications, and dynamical boundary conditions.

Part of the problem of using tracers quantitatively evidently involves, as an important subproblem, the difficulty of separating errors in the forward computation owing to flaws in the circulation model, from flaws in the specification of the tracer boundary conditions. This *piece* of the transient tracer problem is the particular concern here.

3. Using tracers

For most of the transient tracers in use for studying the ocean circulation, ^{14}C, ^{3}H/^{3}He, Freons, the boundary conditions are known crudely. For example, the North Atlantic ^{3}H injection rate as a function of space and time has been estimated by Weiss et al. (1979) from concentration measurements in precipitation at a few coastal stations, estimates of over-ocean precipitation rates and humidity, etc. The results are undoubtedly qualitatively correct, but it would be rash to confuse the boundary data available for the ^{3}H/^{3}He advection/diffusion calculation with conventional mathematically precise specifications for solution of a parabolic system. For other tracers, the boundary conditions might be better known, but in all cases one must admit the likelihood that the specification is in error by varying amounts in any given place in any given year.

Similarly, the problem of appropriate initial conditions can be very difficult. For some tracers like ^{3}H, prior to the bomb injections which began in the 1950's, the natural background vanished and setting an initial condition of zero is reasonable. For ^{14}C, the situation is uncertain

because radiocarbon occurs naturally. The "pre-bomb" concentrations are not well known (see Stuiver et al., 1981) deriving from measurements in corals and the rare measurements made in the 1950's and 1960's. For ^{3}He, the situation is intermediate between ^{3}H and ^{14}C; although ^{3}He occurs in nature (e.g., Lupton and Craig, 1981), its distribution appears to be localized and predictable. Similarly the Freon problem is partly confused because of leakage from refrigerators on sunken ships, although this is a minor nuisance.

So one must conclude that quantitative use of tracers requires accounting for uncertainty in both boundary and initial condition data and their use in "forward" problems *may lead to computed interior distributions which disagree with measurements only because of their mis-specification* and not necessarily because the ocean circulation is poorly modelled.

By virtue of great efforts over many years, the tracer chemistry community has accumulated a large number of different observations from the world oceans. The realities of work at sea mean however, that at best the observations are widely scattered in space and time. Ships are adequate for two distinct modes of measurement—the large scale survey at one time, as was done in the GEOSECS and Transient Tracers program, or more rarely, the generation of a time series of tracer concentration by periodic return to a given location. These practical constraints mean that if a survey has been done, one can compute spatial derivatives of a transient tracer field for the inverse problem; but then it is usually impractical to compute the time derivatives. If the time derivatives are computable because a time series has been generated, then one usually cannot compute the space derivatives. Furthermore, any measurement has errors in it. For many of the tracers, the important error is not the analytical uncertainty, which is usually small, but rather the sampling error owing to eddies and other noise features in the ocean. If the inverse problem is tackled head-on, and one attempts to compute diffusive terms, then the Laplacian, appearing in eqs. (1–4) demands second-derivatives of the observations, a notoriously unstable calculation.

The use of steady tracers is enormously simplified compared to that of transient ones: distribution and boundary condition measurements made at arbitrary times can be combined to yield a complete spatial picture, in a way that is impossible with transients. Deciding whether the intuitive belief that transient tracers contain enough additional information to warrant their use, despite the evident problems, is one of our goals (no verdict is rendered here however).

Going back to the one-dimensional problem, suppose an initial estimate, u, α, of the flow and diffusion in the ocean exists. Let there exist a number of measurements/estimates of the boundary conditions of the generic tracer C: $C_0^j = \overline{C}_0^j \pm \varepsilon_j$, $j = 1$ to J. In addition, we have a set of "interior" measurements $\overline{C}_{i_p}^{t_p} \pm \varepsilon_p$, $p = 1$ to P at different positions and times within the fluid. For temporary simplicity, the initial interior conditions $C_i^{t=0}$, all i, are supposed known perfectly, and for convenience are taken to be identically zero. Only one space dimension is considered initially.

Two questions are posed as necessary preliminaries to full transient tracer use: (a) are the initial estimates of the u, α field and the boundary data with their error bars consistent with the extant interior observations? (b) Can the interior observations be used to improve the estimates of the boundary conditions?

That question (a) is germane should be readily apparent. The importance of the second question may not be so clear. It is posed here because the boundary data may themselves be of primary interest (e.g., the question of how much ^{3}H or carbon was taken up by the ocean are fundamental issues in their own right), and because improved boundary conditions are a necessity for any reasonable forward calculation of the type of Sarmiento (1983) for testing their models. We postpone the central question of improving the initial estimates of u, α until these two preliminaries have been resolved.

In the forward problem of (4) the exact boundary conditions, (6), are "connected" to the interior field C_i^t at any point i, t through the finite difference equations; that is, the finite difference equations permit us to map the boundary data onto any interior point. One can ask naively whether the set of interior measurements $\overline{C}_{i_p}^{t_p}$ could replace some or all of the boundary conditions and be used equally well to generate the complete C_i^t field including, as a special case, the boundary values C_0^t? The replacement of boundary data by interior observations is in

many ways the heart of the transient tracer problem. Unfortunately it takes us away from the familiar territory of well-posed boundary value problems in the Cauchy sense, and it will be immediately recognized that the general answer to the question as just posed is a clear "no".

For, consider the purely diffusive case, $u = 0$. Then it is well-known (e.g., Morse and Feshbach, 1953, eq. 7.4.13) that a Green's function solution to the one-dimensional diffusion equation for a semi-infinite bar, $0 \leqslant x \leqslant \infty$, is

$$G(x, x_0, t, t_0) = \frac{2\pi^{1/2}}{\alpha^{1/2}\sqrt{t - t_0}} \times (e^{-(x - x_0)^2/4\alpha(t - t_0)} - e^{-(x + x_0)^2/4\alpha(t - t_0)}), \quad (8)$$

where $G(x_0 = 0) = 0$. The decaying exponentials reflect the great stability of the forward problem: small errors in boundary (or initial) conditions are strongly damped as time or distance from the boundary increase. But it is obvious that the system is grossly unstable if one tries to proceed in the opposite direction. Attempts to compute the tracer field at times preceding the observations involves a sign reversal in (8) and a rapid amplification of any slight errors in the data. The usual wisdom is that one cannot solve diffusive systems backwards or upstream. But that would seem to be the requirement in the transient tracer problem we posed.

To examine the difficulty in a slightly different way, consider that the problem (4 to 7) can be viewed as a set of IT simultaneous algebraic equations in IT unknowns C_i^t. The count of equations includes those specifying the initial conditions (5) and the boundary data (6, 7). We can formally write this collection as

$$\underset{\sim}{A}\boldsymbol{q} = \boldsymbol{d}, \quad \boldsymbol{q} = \{C_i^t\},$$
$$i = 0 \text{ to } I - 1, \; t = 0 \text{ to } T - 1. \quad (9)$$

Solving this conventional problem by direct matrix inversion would be grossly inefficient compared to the usual procedure of marching forward in space and time from the boundary data. The latter procedure is an efficient recursive matrix inversion method (see Twizell, 1984) which takes advantage of the special structure of $\underset{\sim}{A}$. It is conceptually useful however, to contemplate a direct approach to (9) in which the entire domain of the system, $0 \leqslant x \leqslant (I-1)\Delta x$, $0 \leqslant t \leqslant (T-1)\Delta t$ is solved simultaneously rather than through progression. We choose, out of many methods for obtaining a solution, to write the answer to (9) in terms of the singular value decomposition (SVD), described by Lanczos (1961), Lawson and Hanson (1974), Noble (1969), Wunsch (1978) and many others as

$$\boldsymbol{q} = \sum_{j=1}^{IT} \left(\frac{\boldsymbol{U}_j \cdot \boldsymbol{d}}{\lambda_j} \right) \boldsymbol{V}_j \quad (10)$$

where the λ_j are the singular values and the U_j, and V_j are the corresponding eigenvectors of the SVD of $\underset{\sim}{A}$. The dot denotes the vector dot product. If one computes the singular values of the $\underset{\sim}{A}$ matrix of the forward problem, it is found that they are all finite, and do not change markedly in magnitude from the largest to the smallest; there are of necessity IT such finite singular values.

If we now modify the forward problem by replacing in eq. (9) some or all of those rows of the $\underset{\sim}{A}$ matrix defining the boundary conditions, by a new set of equations defining the interior values instead, we may still have an $\underset{\sim}{A}$ matrix consisting of IT equations in IT unknowns. But it is then found that the values of the smaller singular values decline markedly from those in the forward problem. When in the system (9), the boundary conditions were replaced by defining values of $C_i^8 = \overline{C}_i^8$, $i = 0$ to 4, it was found that 4 of the singular values vanished altogether.

We can thus identify the instability in trying to solve "backwards" as representing the tendency of many system eigenvalues (singular values) to become very small and perhaps vanish altogether. The further difficulties that occur when the number of available interior data are fewer than the number of formally required boundary data, and when all the data contain errors can be understood immediately in terms of the behavior of the solution form (10).

Once the problem is identifiable as one with small singular values, in the presence of generally inadequate, noisy data, it is obvious that there is a strong formal connection with inverse problems. The solution of ill-posed problems is called "regularization" by mathematicians (e.g., Tikhonov and Arsenin, 1977). Much of the machinery for inverse problems, which are usually ill-posed, inevitably duplicates that of regularization.

The regularization procedures applied by Beck et al. (1985) to the backwards solution of the heat equation are identical to the ridge analysis/tapered least-squares inverse methods used by Wunsch (1978), Menke (1984) and others. All of the procedures employed in these problems (and there is a wide choice possible depending upon the particular problem and the investigator's convenience) are directed at distinguishing the components of the solution which are stable and determinable, and identifying and thereby suppressing the components which are not determinable. In the present problem, a naive solution, e.g., direct matrix inversion of (9), attempts to resolve small scale components for which the necessary defining information has been destroyed by diffusion.

But diffusion does not destroy large-scale information and the inability to determine everything about the solution should not preclude determining what we can, and describing the parts that remain indeterminate. The rest of this paper is directed at showing how to carry out this prescription.

The least-square methods to which the SVD is intimately connected are an attractive regularization procedure, just as they are in inversions. Their straightforward use is difficult because the dimensions of the matrix $\underset{\sim}{A}$ grow very rapidly in realistic geometries and time-spans. Nonetheless, I believe they can be made practical: $\underset{\sim}{A}$ is a very sparse matrix, and methods exist (e.g., Bunch and Rose, 1976) for efficient inversions and eigenvalue problems. Furthermore, approximate inverse methods exist that are essentially search procedures. As will be discussed presently, the idea of searching for a solution rather than computing it directly has certain attractions.

In what follows however, I have proceeded using the techniques of linear programming. There are advantages to this method over least-square ones, but there are also disadvantages and it is not claimed that linear programming is necessarily the best choice.

4. Regularization by linear programming

4.1. The canonical problem

There are several ways of stating a canonical linear program. In one form it is:

find the minimum of $H = \boldsymbol{b}\cdot\boldsymbol{q}$

subject to,

$$\begin{aligned} \underset{\sim}{A}_1\boldsymbol{q} &= \boldsymbol{d}_1, \\ \underset{\sim}{A}_2\boldsymbol{q} &\leqslant \boldsymbol{d}_2, \\ \underset{\sim}{A}_3\boldsymbol{q} &\geqslant \boldsymbol{d}_3, \\ 0 &\leqslant \boldsymbol{q}, \end{aligned} \tag{11}$$

where $\boldsymbol{b}$, $\boldsymbol{d}_i$ are constant vectors, and $\underset{\sim}{A}_i$ are constant matrices. The objective function, H, is any linear function of the parameters q_i. Maximization is handled by multiplying H by -1. Many problems which do not have this precise form, e.g., those with non-zero lower bounds, perhaps negative, on q_i can be manoeuvred into it (see Luenberger, 1973; Wagner, 1969). Here the non-negativity constraint is natural, corresponding to the demand that tracer concentrations always be positive.

At first sight, the numerical problem of linear programming appears just as serious as direct matrix inversion: one must invert a series of matrices of dimension of order of the smaller dimension of the defining constraint matrix. There are a number of saving features, however. In an inverse context, one normally explores a series of "nearby" solutions. Because the usual numerical procedure for solution, the Simplex method, is a search procedure, the system can be restarted from any previous solution, with nearby solutions found extremely rapidly. A starting solution can even be found by conventional forward time-stepping, and then fed into the Simplex algorithm as an initial estimate for a modified problem. In the oceanic case, one often has a reasonably good idea of what the solution should be like. If this information is quantifiable, it can be used to narrow the search, thus greatly speeding up the computation. Furthermore, the constraint matrix is band-structured and very sparse. The heavy use of linear programming techniques in management and elsewhere has led to the development of a number of efficient software packages for sparse systems, one of which (Center for Computational Research in Economics and Management Science, 1975) we use here. Descriptions of the linear programming problem in general can be found in a very large literature; Luenberger (1973) has a clear account.

4.2. Some examples

We use the one space dimension plus time problem as an example. To exaggerate the issues, a highly diffusive forward problem was defined in terms of the boundary condition at $x = 0$ as shown in Fig. 3. The interior initial data were all zero: $C_i^0 = 0$, $d = 0.2$, $c = 0.1$, $R_p = 0.5$, $P_e = 7.5$. This conventional initial value forward problem has a solution, *computed by linear programming*, as shown in Fig. 3. (The stability criterion stated above is now irrelevant, as the algorithm used for solution can be regarded as a completely implicit one.)

Now consider a backwards problem. The boundary conditions used to generate Fig. 3 (eq. 6) were replaced by the conditions $C_4^t = \bar{C}_4^t$, $t = 0$ to $T - 1$ where the values were taken from those computed in the forward problem. In this initial trial, the new data were made "perfect", i.e., equal to the values computed to within machine accuracy.

From the discussion in Section 3, we must anticipate the possibility that the problem will no longer be well-posed, i.e., there may be one or more zero singular values present. The problem can no longer be assumed at the outset to have a unique solution. To the contrary, it can be shown that three situations can occur: no solution; a unique solution; an infinite number of solutions. If the third possibility occurs, it is necessary to shift from seeking *the* answer to a different set of questions.

If no solution exists, it means that the set of constraints is contradictory (said to be "infeasible"). Should this be the case, the collection of interior plus boundary data are not consistent with the assumed model—here the values of u, α being used. When the Simplex algorithm is used in the so-called two-phase version, it first seeks *any* solution consistent with the constraints (said to be a "feasible" solution). If it is determined that no such solution exists, the constraints being contradictory, then the algorithm will attempt to minimize the infeasibility, producing a solution $\hat{C}$, satisfying the collection of constraints as nearly as possible. The use of this solution will be taken up later.

The case of a unique solution corresponds to the fully posed forward problem and is equivalent to the conventional solution (as shown in Fig. 3). No more needs to be said.

When the system is feasible, but with an infinite number of solutions, one can lump the most common strategies for proceeding into three categories: (a) Determine the extremal properties of all solutions, such as the maximum and minimum fluxes of interesting quantities, like heat, or of C. (b) Determine the "best-estimate" solution, usually from a maximum likelihood principle. Such a procedure is especially appeal-

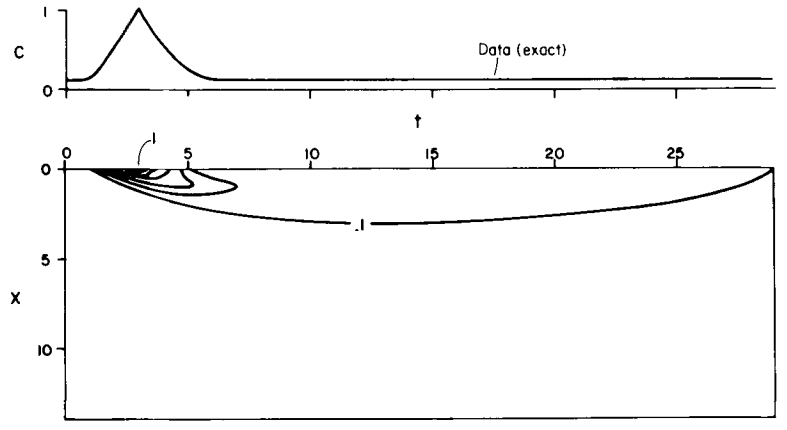

Fig. 3. A forward problem solved by linear programming methods. The overall Péclet number, P_e, was 7.5. The boundary condition at $x = 0$ is shown at the top. An x–t diagram of the solution is shown; contouring here and later is sometimes incomplete. Time and space units are Δx and Δt and are taken = 1.

ing if *a priori* statistical properties are available. (c) Find the simplest solution consistent with the data. The three strategies differ only in their choice of an objective function H.

In the present case, strategy (a) leads for example, to questions such as "what is the maximum and minimum injection at the boundaries,

$$H = \sum_i C_0^i, \tag{12}$$

of tracer into the flow that is consistent with the data?" In some examples to be shown, equation (12) was employed as the objective function. Strategy (b) works best with linear programming methods, if one is willing to use exponential probability densities (see Arthnari and Dodge, 1981). But here main use is made of (c), which is particularly simple and elegant.

There is a slight complication in using (c). In so-called L_2 norm problems (e.g., least-squares), discussed in Wunsch (1978), or Menke (1984), there is a powerful and compelling choice of "simplest". The vector space interpretation of the L_2 norm problem permits one to identify the null-space of the coefficient matrix of the defining constraints as the undeterminable components. Exclusion of the null-space from the solution is an intuitively appealing process for choosing a unique simplest solution. Linear programming uses L_1 norms (absolute values), and no such vector space interpretation is available; a somewhat different procedure must be used. Here "simplest" is defined as the solution with the smoothest boundary condition

$$\min H = \sum_{i=0}^{T-2} \left| C_0^i - C_0^{i+1} \right| \tag{13}$$

consistent with the "data". Such a choice is somewhat arbitrary, and nature may not cooperate by producing the smoothest solution as the right one. Nevertheless, in this precise sense, we can be assured that whatever solution is obtained will have no more *variation* in time (or later, space) than is demanded by the "data"; it is related to an extreme entropy principle. Equivalently, it may be regarded as the correct solution filtered so as to remove any unobserved structures. The examples worked here involve objective functions written only in terms of the boundary conditions. But nothing prevents choosing H in terms of interior values, e.g., finding the globally smoothest solution.

Objective function (13) is not canonical; it can easily be placed in that form. See the Appendix.

Once H is chosen, the Simplex method will automatically handle the three possible outcomes for solution numbers. When the perfect data C_4^i (shown in Fig. 3) were used to solve for C_0^i, the forward solution of Fig. 3 including C_0^i was *perfectly* reproduced (Fig. 4a). This perfect reproduction is partly fortuitous. Physically, it is clear that information about the boundary condition at $x = 0$, for times $t = 26$ and later has not had time to extend to $x = 4$; in effect, four pieces of information are missing from the system, implying the vanishing of four singular values. In the present case, the fully correct boundary condition is recovered because by happenstance, it corresponds to the smoothest condition. In some of the later examples, the lack of information for late times will be more obvious. The present point is that the system can be solved "backwards" in well-behaved fashion.

But when the "data" were stipulated as uncertain by $\pm 10^{-4}$, written as $\overline{C}_4^i - 10^{-4} \leqslant C_4^i \leqslant \overline{C}_4^i + 10^{-4}$, where $\overline{C}_4^i$ is the exact value, to reflect the uncertainty of real data, the system determined the boundary conditions as depicted in Fig. 5. Some of the extreme structure of the correct boundary data is no longer required—given the errors present in the "observations". But the demand for minimum structure does a very efficient job at controlling the components of the solution which are no longer determinable from the available information. The best way to state the meaning of this result is that it shows the simpler, flatter, boundary data of Fig. 5 are adequate to fully explain the "observations".

Notice that although H depends only upon the boundary data, the solution $\hat{C}$ is necessarily computed over the entire domain $0 \leqslant t \leqslant T-1$, $0 \leqslant i \leqslant I-1$, and we have succeeded in connecting, as we desired, a set of noisy interior observations back to the missing boundary conditions.

Huestis (1979) set up the heat diffusion problem as a linear programming problem and used essentially the same objective functions as employed here. The fundamental difference is that with the Laplace/Poisson equation in simple geometry, he had an analytical Green's function

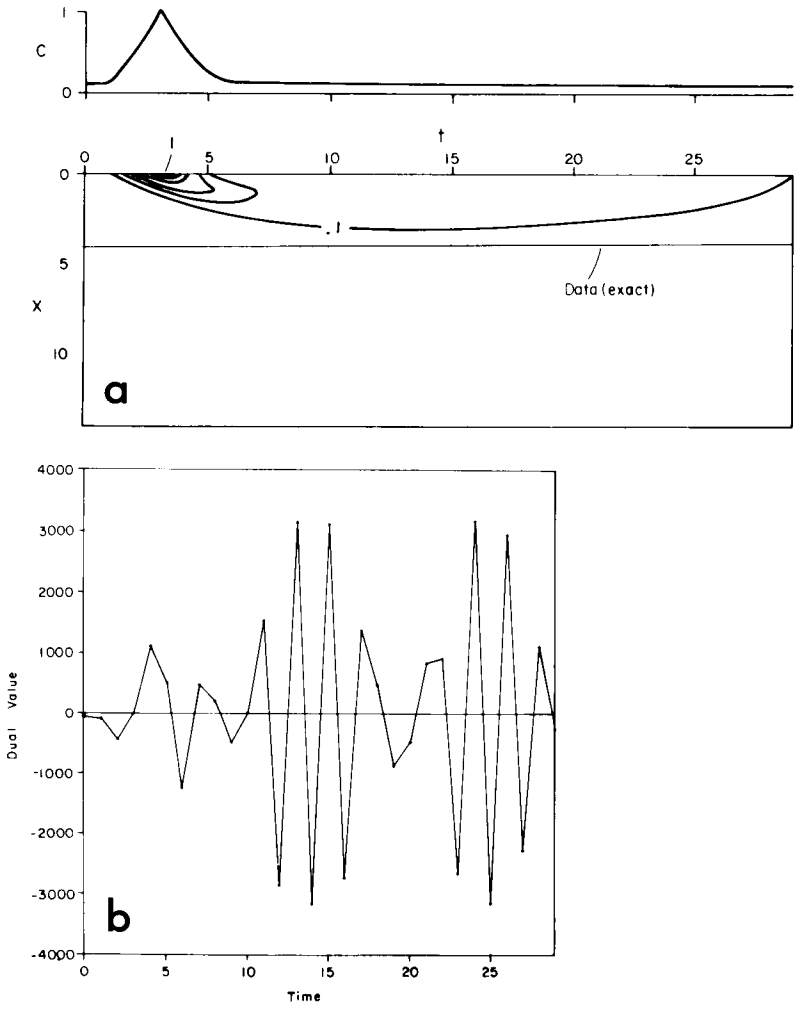

Fig. 4. (a) "Observed" time history at $x = 4$, used to solve the advection/diffusion problem upstream/backwards. Because the "data" were perfect, and the later history was a constant, the perfect boundary condition was recovered. (b) The dual of the "data". The different signs indicate whether the data would have to change upward or downward to effect the value of H, and the magnitude is the differential sensitivity of H to such a change.

available, and the problem is reducible to a much simpler set of relations than required by the finite differences.

4.3. The dual solution

One of the important by-products of the Simplex algorithm is the so-called dual solution (e.g., Luenberger, 1973). The dual corresponds to the Lagrange multipliers of the constraining equations of the system, and the magnitude of each element of the dual is a measure of the sensitivity of the extreme value of the objective function to perturbations in the value of the constraint bounds (cf. Schröter and Wunsch, 1986; Cacuci, 1981a, b). Given the change in $\hat{C}$ seen in the shift from Figs. 3 to 5, we can ask "which of the 'data' values were most important in the loss of structure"? The answer is plotted in Fig. 4b, showing the dual of the perfect data. The largest magnitudes show that the information

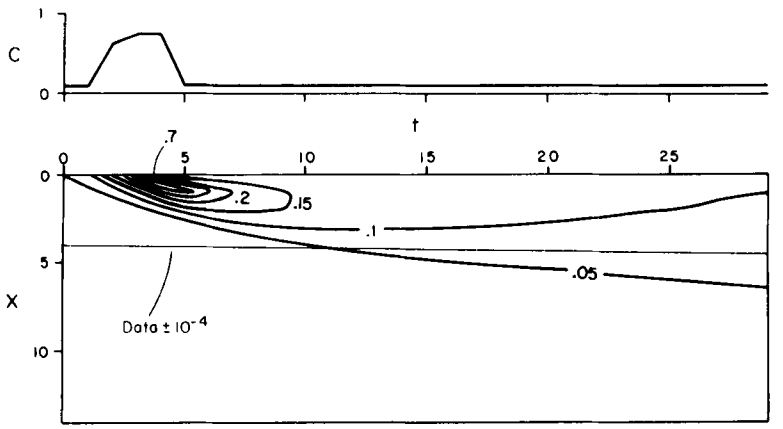

Fig. 5. Same as Fig. 3, except that the "data" at $x = 4$ were given an uncertainty of $\pm 10^{-4}$. As a result, the inferred initial condition has lost much of its structure.

content is (generally) greatest where the "observations" are changing most rapidly. The sign of the dual solution is determined by whether the corresponding inequality would need to be increased or decreased to effect the minimum of H, i.e., whether the inequality is binding from above of below. Use of the dual, and other properties of the linear program solution provide the elements of an observational strategy; they tell us *which of the observations is most important, and give us a numerical measure of that importance.*

We can of course ask other questions about the boundary data. Fig. 6a, b shows the boundary, and full field of $\hat{C}$ determined when we demanded the minimum and maximum of eq. (14), determining the largest and smallest injection of tracer C_0' that is consistent with the "observations". The maximum solution shows clearly that by having observations available only at $x = 4$, no information is available about what the boundary data would have been at late times, $t > 25$; this last data has not yet reached $x = 4$. The total true *average* injection was 0.16; the minimum average injection determined through (14) was 0.15. If the obviously indeterminate values of C_0' ($t > 25$) are excluded, the maximum average injection was 0.16. Despite the instability of the problem, the information we have been able to extract about the boundary data, namely the simplest structure, and the maximum and minimum possible injections, may still be useful.

The method is able to answer questions about potential observational strategies. Reference to Fig. 3 shows that the peak occurring in the boundary data has been diffusively removed from the internal solution beyond locations $x = 2$. One can pose the following question: to what extent is it vital to observe the interior at times and places where the peaked nature of the injection is visible, or is it sufficient to observe where the peak did occur, but had decayed before one arrived, or is it sufficient to observe downstream where only the general rise to the asymptotic mean value occurs?

No general answer is possible, because *it depends upon the accuracy of the data provided*, although it appears from experimentation that data taken during times of maximum rate of change is more useful than data from relatively stable times (see the dual solution in Fig. 4b).

Similarly, we can ask whether data taken at fixed t for all x is equivalent to data taken for all t for fixed x? Out of all the large number of possibilities to explore, a configuration was chosen to be somewhat like a real oceanographic case, in which neither time, nor place is fixed, but the data are acquired on a slice through the x–t plane as depicted in Fig. 7. The data were perfect, but only 12 observations were provided along the line depicted, instead of the 30 numbers necessary to fully specify the problem through the boundary conditions. Fig. 7 shows the smoothest boundary condition, the complete fields $\hat{C}$, and the maximum and minimum injection consistent

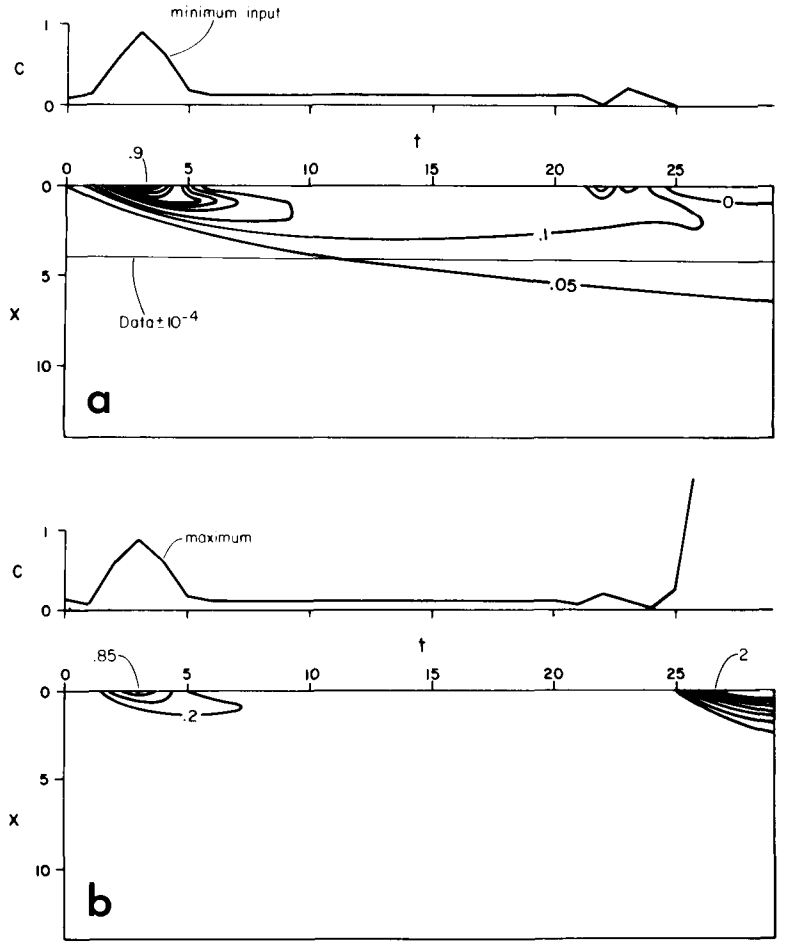

Fig. 6. (a) Same as Fig. 3, "data" were specified at $x = 4$, $t = 0$ to 29 with an uncertainty of $\pm 10^{-4}$, except that the objective function was changed to be the minimum tracer injection (eq. 14). (b) Same as Fig. 4a, except that eq. (14) was maximized (maximum injection). There was no useful information about the last boundary conditions in time, and hence they were maximized by going to the overall upper-bound stipulated for the problem ($C \leqslant 2$).

with the data. The last two points in time in the boundary data are again indeterminate and are restricted bounded only by an *a priori* upper bound set equal to 2.

5. Using the wrong model

We now have a method capable of connecting imperfect tracer observations made in any part of the domain with those made anywhere else, including the boundaries. Components of the flow which are indeterminate are suppressed, and components which are uniquely determinable are found. The mathematical procedure is sufficiently robust to operate automatically both on problems which are fully determined (the forward problem) or on those which are nearly totally indeterminate. We can therefore return to one of the original issues. Suppose the initial estimates of u, α are incorrect?

To explore this problem, the data, $\overline{C_4^t} \pm 10^{-4}$, were used to run backwards a model *deliberately chosen to have the "wrong" parameters*, $\bar{c}$, d. That

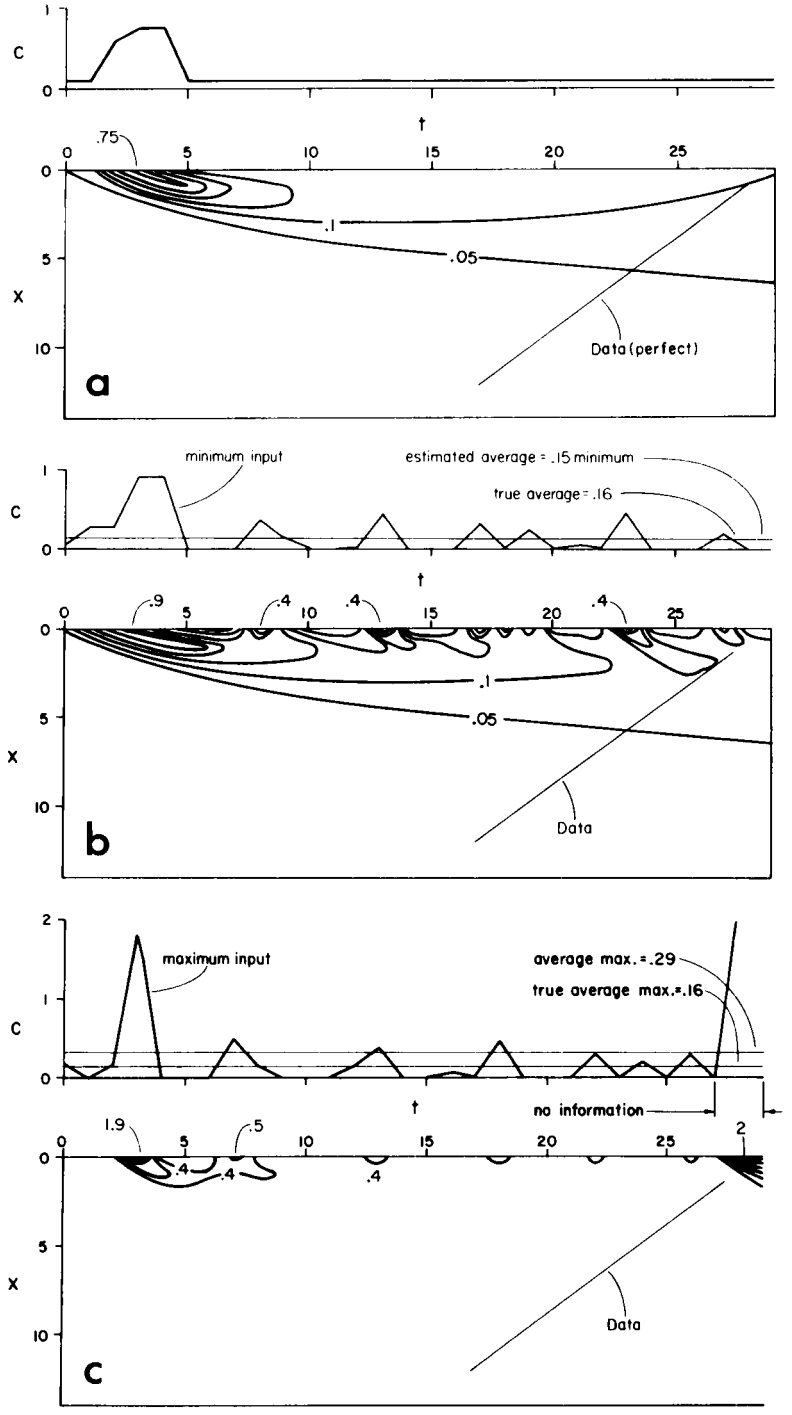

Fig. 7. (a) Smoothest boundary conditions determined from perfect data along the line shown (correct answer would be same as Fig. 3). (b) Same as (a), except solution is for minimum injection. (c) Same as (a) except for maximum injection.

is, the data were generated from Fig. 3, which had $\bar{c} = 0.1$, $d = 0.2$ ($P_e = 7.5$) and is the correct model; but the backwards model was made much less diffusive with $\bar{c} = 0.6$, $d = 0.2$ ($P_e = 45$). The determination of the smoothest boundary data and the full domain solution are displayed in Fig. 8. The strong peak in the boundary data of the correct model is not found in the high Péclet number model. Evidently the interior observations are quite consistent with the wrong model. But, when a single partially uncertain boundary value observation, $\overline{C}_0^4 = 1 \pm 0.05$, was added as an additional equation, the Simplex Method showed the system to be infeasible.

At this stage we would know that the collection of tracer observations, which happen to include one boundary datum, are inconsistent with the flow and diffusive parameters assumed in the first guess. If the error bars on the tracer data are believed to have been realistic, then the initial estimate of the u, α field must be modified. A simple and efficient procedure takes advantage of the search nature of the Simplex algorithm: modify u to $u + \Delta u$, α to $\alpha + \Delta\alpha$, and re-solve for the $\hat{C}$ field using the previous solution as starting point. Even through the preceding solution was infeasible, it should be close to one that is feasible with the new u, α field. The family of solutions lying within the neighborhood of the initial estimate can be explored until one or more are found that are feasible with the observed data.

An alternative procedure is to solve the inverse problem directly. We can take the infeasible field $\hat{C}$ which is as close to feasible as possible, replace the values which do not agree with the observations $\overline{C}_i^t$, and invert for u, α in the inverse calculation. These new u, α are used to re-solve the backward problem, giving a new, perhaps still infeasible field $\hat{C}$, which is then used to re-invert. A process of iteration can be maintained until consistency is obtained (although the convergence properties of the scheme have not yet been explored).

6. Discussion

This paper is obviously incomplete, focussing upon the regularization aspect of the transient tracer problem. The complete problem involves a much more elaborate program, in which both forward and inverse problems must be solved as well, and eventually attention must turn to the dynamical model governing the flow field.

In its full definition, the problem is seen to be one of non-linear constrained estimation in which direct measurements of the tracer and flow fields are combined via the coupled dynamical and advection/diffusion equations. In the one large system, consistency is demanded within the specified limits of uncertainty of the measurement and model parameters. Methods exist for performing such non-linear optimizations (e.g., Tarantola and Valette, 1982; Mercier, 1986; Schröter and Wunsch, 1986), but the computational load for realistic problems appears to be so large as to overwhelm foreseeable computational facilities.

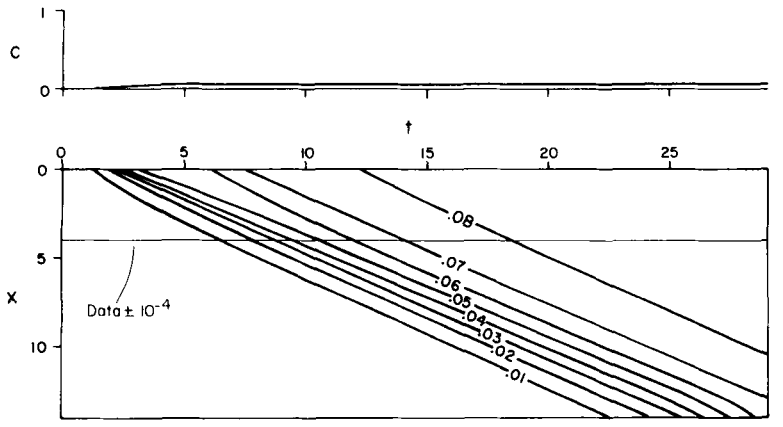

Fig. 8. Inferred boundary condition and C field when data at $x = 4$, $t = 0$ to 29 from a model with $P_e = 7.5$ and an uncertainty of $\pm 10^{-4}$ were used to drive a model with $P_e = 45$. The model is inconsistent with an additional stipulation that value at $t = 3$ is $C_0^t = 1 \pm 0.05$.

The present paper has outlined one procedure for solving the problem piecemeal, by iteration, with the emphasis upon the regularization subproblem. The demonstrated ability to connect interior observations backward to the tracer field at earlier times and positions, including the special case of boundary data, is of some interest in its own right. We can in principle stably estimate from the interior data alone the rates of injection of the tracer, even if no boundary data at all were available. The importance of such issues for CO_2 and other problems is apparent.

Much more needs to be done. Although the results are not shown here, the method has been used on problems with two space dimensions plus time. The linear programming method has some potential appeal even for solving ordinary forward problems because one often can make an oceanographically plausible estimate of the nature of the solution. These prior estimates speed the convergence of the algorithm to the final state. But as has already been said, the least-square methods also lend themselves to such search algorithms and no claim is made here that linear programming has a real computational advantage if efforts were made to truly optimize for large-scale realistic problems. A clear advantage of linear programming is however, the natural means afforded to incorporate inequality information, of which the non-negativity of tracer concentrations is an important type. Although inequalities can be dealt with in L_2 norm problems (Lawson and Hanson, 1974), the procedures are awkward.

In working with realistic data (an effort now underway), one must confront the general undesirability of the finite difference form as applied to observations. The computation of second derivatives of noisy data creates problems which to some extent can be avoided by writing the governing equations at least in part in integral form. Integral forms are used in box models, although most published ones represent either steady balances or rather simple time evolution—perhaps parametric—as in Wunsch (1984).

One attractive procedure to use in practice is the so-called compartments model described by for example Wen and Fan (1975) (called the "mammalian" model in the biomedical literature). Here one abandons the distinction between advection and diffusion and reverts to box balances in the (simplified) form:

$$\frac{dC_i}{dt} = -\sum_{j \neq i} u_{ij} C_i + \sum_{j \neq i} u_{ji} C_j + Q_i, \tag{16}$$

where u_{ij} represents the flux of C from box i to box j, and Q_i are sources/sinks. Because the distinction between turbulent fluxes and advection is often only one of a statement of the spatial scale over which the advective velocity is permitted to vary (Wunsch and Minster, 1982), the loss of the separate determinations is not necessarily of importance. Wen and Fan (1975) discuss the structure of the equation set (16). Owing to its linearity, all of the linear programming considerations used above can be invoked. Further discussion is postponed until it can occur in the context of real data.

7. Acknowledgements

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8. Appendix

The conversion of an objective function of the type (13) into the standard linear programming form is carried out by introduction of auxiliary variables (Wagner, 1969, p. 558). Put

$$C_0^l = \alpha^l - \beta^l$$
$$\alpha^l \geqslant 0, \quad \beta^l \geqslant 0. \tag{A1}$$

Eqs. (A1) are added to the constraining equation set, and the objective function, eq. (13), is then replaced with the new one

$$\min H = \sum_l (\alpha^l + \beta^l). \tag{A2}$$

Note added in proof

It has subsequently become clear that the problem described here, and its solution, are best viewed as special cases of the general problem of control theory with the missing boundary conditions corresponding to the need to find an optimal control variable. A full discussion will be published presently.

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