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HYDROCHEMISTRY AT IH: A REVIEW

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## HYDROCHEMICAL RESEARCH AT IH

### INTRODUCTION

In February of this year I was given the task of surveying and commenting on the chemical work being undertaken at IH; this report presents my findings. I show that the chemical studies and interest in water quality are extensive, diverse and uncoordinated, while chemical expertise is very limited. Three important points are made: firstly, given the staff and chemical expertise available, IH has done remarkably well to set up and carry out a considerable number of projects having a hydrochemistry component; secondly, there is considerable overlap of interest both between IH sections and with our IGS colleagues on site; and thirdly, we need improved communication between sections. The report concludes that given senior management's intention of extending its support for water quality work, IH is ill-equipped for this change.

### HYDROCHEMISTRY AT IH: THE PRESENT

#### 1.1 Existing projects with some hydrochemical component

There are 18 projects on the IH Project List at present which can be described as having some hydrochemical/water quality component; they are listed in Appendix 1 and described in more detail in Appendix 2. Funding is approximately 75% science vote and 25% repayment. Within these projects, studies are undertaken by workers from most IH sections (Appendix 3) with expertise in wide and separate disciplines (eg Earth Sciences, Chemistry, Geology, Hydrology, Engineering). The projects have widely diverging objectives from the "pure" to the "applied" ends of the scientific spectrum, and the waters studied vary from ultrapure snowmelt and rainfall to hypersaline groundwaters and

polluted river waters: methods used vary from pure thermodynamics to black box modelling. The projects listed vary from those having a very limited hydrochemical component (eg Projects 33, 122) to pure hydrochemical research (eg Projects 26, 55, 68).

Despite these differences, the projects can be broadly categorised into two areas: (i) "the impact of man on the chemistry of natural waters" and (ii) "the chemistry of hydrological processes". Thus, for example, in the first category much of the work of the Analytical, Soil Physics, and Catchment Sections and that of the Water Data Unit could be included. Their chemical studies primarily consider the effects of agricultural activity, land use change and pollutant discharge on the chemistry of natural waters with subsequent implications for the management of our water resources; more indirectly, the Instruments Section's interests in developing an automatic water quality station, can also be included. In the second category, much of the Hydrochemistry and Hydrogeology Sections' work can be included, since they undertake both fundamental studies on the nature of some of the dominating chemical reactions in the hydrosphere and environmental studies of chemically active systems; more indirectly, the Overseas Section and dilution gauging work can be included here, since chemical determinands are primarily being used as a tool for identifying the direction or the size of water flow.

In many of these projects - those that have had their origins outside the Hydrochemistry and Hydrogeology Sections, and where there has been little or no contact between the project staff and the IH Hydrochemists - the chemical component is at a fairly low level, being pursued by workers with limited knowledge of hydrochemical processes and possibly with limited feel for the worth of the data they are using. This is not a criticism of the project

staff, who in some cases may have been unable to get help in the Hydrochemistry Section or who may have merely responded to customers' requests that consideration be given to hydrochemical aspects of projects that they were funding; these customers may themselves have had limited understanding of hydrochemistry, being more intent on avoiding possible criticism from their assessors than in funding work leading to positive advances in hydrochemistry. The point is that some projects have come into being through the external stimulus of a customer (such as Project 67: "Leaching of  $\text{NO}_3$  in a practical agricultural catchment", and much of the water resources work done by the Overseas Section) (App 4)); others have come into being because IH staff members guessed correctly that customers would be prepared to put money into work having a particular hydrochemical/water quality component (such as Project 94: "Water quality modelling for design and operational management"; Project 103: "The effect of upland land use on water quality"; Project 122: "Water quality monitoring control and telemetry instrumentation"). Other projects have come into being through particular interests of staff members within the Hydrochemistry Section (Project 26: "Hydrochemical Process Studies"; Project 68: "Clay Modelling") and in other sections (Project 124: "Pollution in Snow"; Project 39: "Hydrogeology of shallow alluvial aquifers").

Words that can be used to describe the state of hydrochemistry at IH are "extensive", "diverse" and "uncoordinated"; the lack of coordination, and the extent and diversity of the IH projects having hydrochemical/quality components, has largely come about as a result of the way in which projects have been initiated (vide the preceding paragraph); there is, as yet, no recognized procedure either for giving a seal of approval to proposed new projects, or for terminating those that are moribund or unproductive

of results. Criticism was voiced, during the survey, to the effect that there was a "lack of direction" not only within the Hydrochemistry Section but within IH as a whole; that there was a "lack of communication", and that the "roles of hydrochemists were not defined". These comments can be interpreted either as a criticism of IH management (for not having defined a direction and set course along it) or as a criticism of IH staff members themselves, for having been unable to define their own directions based upon personal interests and abilities and commitment to get results.

#### 1.2 Existing IH staff expertise and laboratory facilities in hydrochemistry

By comparison with the number of projects having some hydrochemical component, there are few IH staff members who are either trained in chemistry or who, through experience, have acquired a facility in the interpretation of hydrochemical data. Having lost its head of Hydrochemistry, IH now has only two environmental chemists (Colin Neal (SSO), Alun Thomas (HSO)) trained to PhD level; one other (Christopher Smith (SSO)) has training in chemistry to the equivalent of degree level and one (Tony Debney (PSO)) has extensive experience in environmental applications, whilst two others (Gareth Roberts (SSO); Paul Whitehead (SSO)) had advanced training in specialist fields of chemistry other than for hydrochemical applications. The strength of hydrochemical expertise within IGS at Wallingford is considerably greater with several workers in the Hydrogeochemistry and Groundwater Flow and Pollution Sections having established high reputations in their fields.

Regarding facilities, IH has a good analytical chemistry capability for the determination of the major ions, nutrients and total organic carbon contents of natural

waters. Over a 10 year research period, the Hydrochemistry Section has gained particular expertise with analytical colorimetric techniques using autoanalyser systems following the pioneering work of Vic Truesdale, Christopher Smith and Steve Jones on iodine speciation and silicate analysis in natural waters. Indeed IH can probably boast of having one of the best facilities for  $\text{IO}_3^-/\text{I}^-/\text{total}$  iodine analysis in natural waters. IH has three main laboratories which are well equipped with 1 atomic absorption spectrometer, 3 autoanalysers, 2 ultraviolet/visible spectrometers, 1 total organic carbon analyser, 1 autotitrator and a polarograph. The laboratories are mainly run by Christopher Smith assisted by James Walls who provide an analytical facility for the rest of the Institute, although there are also other users such as the remaining hydrochemists on site (IH and IGS) as well as some university departments. Complementary to these laboratories IH also has an X-ray diffraction facility, housed in two further laboratories, for mineralogical analysis and run by Christopher Smith and John Raynor. Christopher Smith also supervises Adrian Brunsdon, who works mainly in the joint IGS/IH stable isotope facility.

The IGS hydrochemists also have a well equipped analytical facility on site capable of determining major ions, nutrients, trace metals and the stable hydrogen, carbon, nitrogen and oxygen isotopic contents of natural waters. Over many years the group has gained particular expertise in the analysis of trace metals following the main interests of the "analytical chemist" in the group (Doug Miles). They have 4 main laboratories, two equipped with very major items, an inductively coupled plasma emission spectrometer and a VG micromass dual inlet ratio mass spectrometer, and the rest by major items of equipment such as 4 atomic absorption/emission spectrometers with flameless attachments, 2 ultraviolet/visible spectrometers, 1 autotitrator, 1 dual

channel autoanalyser and a gas chromatograph.

Between the IH and IGS hydrochemistry groups the analytical facilities and capabilities are fairly substantial; for example, the joint group has two very capable analytical chemists, albeit with only a relatively small back-up staff, and equipment whose value at present day costs will be around £500K. Although there is some overlap the groups seem to complement each other well, particularly with regard to routine and specific analytical functions as well as with regard to expertise on autoanalyser techniques, flameless/plasma induced atomic absorption/emission techniques, X-ray diffraction and mass spectrometry. Unfortunately, although there is some joint work and considerable goodwill between the two groups, there is not a very effective pooling of resources.

At present the IH laboratory facilities are under-used and there is a need to overcome the lack of appreciation amongst other IH groups of what is or is not practicable. There is also a communication barrier between the "chemists" and "non chemists" over identifying needs, areas of overlap and scientific priorities: in the past, and to some extent even now, this has led to considerable friction between the Hydrochemistry Section and other IH sections as well as with senior management. While these problems are not insurmountable, the following points must be stressed to avoid in future the feeling that the Hydrochemistry Section is being uncooperative:

- (a) If demand for analytical services increases substantially, there will be staffing problems, particularly if IGS equipment is used by IH staff.
- (b) The involvement of the analytical chemistry part



of the IH Hydrochemistry Section on a project from another section would need to be more than just provision of a service function if the outcome is to be satisfactory.

- (c) The analytical capabilities, while good, must be restricted mainly to existing on-site techniques since the development of new (or the introduction of established but unfamiliar) analytical techniques is often very time-consuming; indeed the development of new techniques may take years (eg the silicate work of Vic Truesdale, Christopher Smith and Peter Smith).

### 1.3 The framework of existing Hydrochemical projects

In general IH has achieved much given the limited resources available, whilst the Hydrogeology Catchment, Analytical and Soil Physics Sections have effectively extended these resources by getting hydrochemical support (both through direct funding and through assistance in kind) from organisations such as the river authorities and IGS (Appendix 5). Nevertheless, consideration must be given to developing the potential that already exists. Going through the sections individually:-

The Analytical Section (particularly Enda O'Connell and Paul Whitehead, Projects 94 and indirectly 122) has developed a good reputation in the field of modelling for water quality management and in the development of predictive water quality models. However, to achieve further major development in this area a far greater hydrochemical component needs to be added to allow identification and predictions to be made for important element partitioning and fluxes in the systems studied,

particularly when new pollutants (eg trace metals and organics) are considered. This requires help from the Hydrochemical Section for theoretical, field experimentation and laboratory simulation studies to be undertaken. Moreover, the work could probably be extended to consider reactions not just in rivers but also in the unsaturated and saturated zones, as well as hydrochemical modelling in general (cf project 121, "Modelling of hydrochemical systems"). Under these headings valuable overlap of interests would be gained, not only with the IH Soil Physics, Groundwater and Overseas Sections but also with our IGS colleagues on site.

Besides the work of the Analytical Section described above, which is directed principally at methods for managing the quality of water resources, other work by Liz Morris is directed more at the study of processes, particularly the quality of snowmelt water (Project 124). This work has good and sufficient collaboration with the Hydrochemistry Section through the active participation of Alun Thomas. Liz Morris also has strong interests in the study of acid precipitation, which could well be a growth area for IH Hydrochemistry (despite the shortsighted unwillingness of DOE to fund it).

The Catchment Section (Jimmy Blackie and Gareth Roberts: Project 67 and Project 103) have gained considerable experience in water quality work for upland catchments and has obtained good contacts with various organisations such as the Forestry Commission, ITE, FBA and the river authorities. While their work is essentially self-contained and separated from that of other IH sections, nevertheless their field activities and contacts might form the basis of much more intensive and wide ranging studies of water quality behaviour in catchments (eg with the IH Hydrochemistry and Hydrogeology as well as the IGS Hydrogeochemistry

Sections). On the shorter term, collaborative work with the Instruments and Hydrochemistry Sections on field monitoring of water quality might be of value; problems encountered are related to sample deterioration on storage, the high cost of chemical analysis and difficulties in undertaking a field sampling programme.

At Plynlimon studies are undertaken (Kevin Gilman) on the application of chemical dilution gauging techniques (Project 24) as well as on the hydrology and plant ecology of peat bogs and wetlands (Project 72). In addition work is undertaken by the Catchment Section, described previously, with Jim Hudson on site. The dilution gauging work, for studies of mixing, flow and times of travel in streams and rivers, is or has been fairly widely used not only by Kevin Gilman but also by various workers in the Analytical, Urban Hydrology and Catchment Response Sections. Since he (at Plynlimon) and Christopher Smith (at Wallingford) have specialist knowledge in this area, while the techniques used are often difficult to apply, perhaps they could act as consultants for other projects. The peat bog and wetlands work could perhaps be valuably extended to build on the original chemical work by Vic Truesdale at Plynlimon and to link with the Hydrogeology and IGS' Hydrogeochemistry Sections' interests in chemical cycling of major and trace elements.

The Soil Physics Section (John Bell, Steve Wellings and David Cooper (Projects 50 and 58)) has studied the movement of nitrate and chloride through the unsaturated zone using simple, possibly oversimplistic, ion conservative models; they assume that ions move through the unsaturated zone without loss to the solid phase and at the same rate as

water. To extend the work, allowance would have to be made for diffusion/dispersion and chemical reactivity. In addition, other aspects of the section's interests might be expanded to study changes in water quality following change in agricultural practice (eg change in crop type or irrigation methods); this might link in with the agricultural hydrologists. To do either extension effectively, considerable and wide-ranging expertise from outside the Soil Physics Section would have to be brought to the problems. This would require inputs from IH's Hydrogeochemistry and Analytical Sections as well as from IGS's Hydrogeochemistry and Groundwater Flow and Pollution Sections.

The Instrument Section (Ian Strangeways, Roger Wyatt) has been interested in work on field systems for water quality monitoring. Here the aim is to develop an automatic water quality station, which is both inexpensive and self-contained, for use in third world countries. The study will complement IH's involvement (Paul Whitehead and Roger Templeman) in the development of a more elaborate water quality monitor for the Anglian River Authority. The station, while being of particular value to the Overseas and Catchments Sections, will, like the automatic weather station, be of commercial value. However, given that the Instruments Section has little chemical background and a very limited knowledge of the potential of analytical methods that might or might not be useful, then the input of a hydrochemist, although perhaps short term, is desperately needed. This input could possibly be supplied by the IGS or IH analytical chemists (Doug Miles or Christopher Smith).

The Hydrogeology Section (Tony Debney and Colin Neal; Projects 25, 33, 39, 55 and 121) and linked to it the Water Resources Section (see below), has undertaken a wide variety

of chemical studies ranging from computer simulations of dispersion/diffusion effects and chemical reactions, to environmental studies of surface and groundwaters. Thus Roy Wikramaratna has developed a steady state model to describe saline intrusion into an aquifer; Colin Neal and David Cooper (from the Analytical Section) have developed a model describing the ion exchange properties of clays based on electrostatic theory; Tony Debney and John Davey have been studying variations in water quality as part of their work on groundwater movement in the Thames flood plain; Tony Debney and Adrian Brunson have begun stable isotope studies of rain and stream waters at Plympton; Tony Debney and Colin Neal have for several years been studying the evolution of highly alkaline springs from partly serpentinised rocks in Northern Oman; Tony Debney and John Finch (from the Overseas Section) have been developing a field conductivity probe for use on a new water resources study in Libya; Tony Debney, and to a much lesser extent Colin Neal, have studied the hydrochemistry of groundwater aquifers as part of several Water Resource Projects; John Davey has been studying groundwater chemistry in the Permian aquifer of Southern England as an extension to his PhD work. At present there seems to be a great overcommitment to science and technology studies within the section with pressure to expand its research activities and links with the Water Resources Section. This overcommitment is worrying but could be solved either (a) by establishing much closer contacts with the IH Hydrochemistry Section and IGS Hydrogeochemistry Section on environmental, research and stable isotope studies and with the IH Analytical Section on groundwater modelling; or (b) by a redefinition of its priorities. If this overcommitment problem were solved, in the longer term the Hydrogeology Section could form the basis of a much greater hydrochemical activity.

The Water Resources Section (Steve Pond, Dick Bradford and John Bromley) have been and are involved in water quality work in relation to most of their water resources studies (Project 33). Although the chemical provenances they study are diverse there is little chemical expertise within the Section. To overcome this limitation, chemical expertise has been introduced by members of the Hydrogeology Section (mainly Tony Debney and to a lesser extent Colin Neal); however the Section probably needs additional or new chemical support to capitalise on both potential repayment markets and new scientific research areas identified from their ongoing studies. It is difficult to see in the short term how the additional work could be supported given that the hydrochemists' present commitments are high. Further, even at present levels the Hydrogeology Section's assistance has significantly weakened its ability to carry out or complete its own research. Possibly much closer links with the IGS Hydrogeochemistry and Overseas Sections might form the basis for a solution.

Support for active hydrochemistry research at IH came from both the Visiting Group and Preparatory Group D; hydrochemistry is also an important component of the IH Forward Look. The Hydrochemistry Section at present is mainly working on studies of the cation exchange behaviour of clays (Alun Thomas and Colin Neal (Project 68)), the effects of acid rains on the environment (Alun Thomas and Liz Morris (Project 124)), and the development of an analytical chemistry and mineralogy facility (Project 26)). The group is at present in a state of upheaval following the loss of its Head of Section (Vic Truesdale) and the introduction of much firmer managerial ties with IGS Hydrogeochemistry Section. The situation is not helped by incessant pressure both to increase repayment and

collaborative work and to change scientific direction. In one sense, the resources are greatly stretched since the only environmental chemist in the Section (Alun Thomas) is heavily committed for the next two years to writing up his work on the cation exchange behaviour of clays, undertaking a joint study with Liz Morris (Analytical Section) on acid rains and snowmelt, and undertaking an ODA funded project based in Bangladesh. In another sense, the analytical facility is underused, as was discussed in page 6.

Mineralogical studies are undertaken in the Hydrochemistry Section mainly in relation to IH's floodplain (Project 39) and overseas repayment work (Project 33). These studies could perhaps be extended to most IH hydrochemical studies involving water quality-sediment interactions (eg for IH's Analytical, Hydrogeology and Hydrochemistry Sections), to fluvial geomorphological studies of fine-grained river sediments and rates of erosion (Plynlimon), and to rock-water interactions (eg IGS Hydrogeochemistry and IH's Hydrogeology Sections).

The Water Data Unit and the Flood and Low Flow Prediction Sections both have a keen interest in aspects of water quality. For example, the former has for several years collated data from the harmonised monitoring network in the UK while the latter has considered studying the effects of regional and temporal variations in determining cost-effective water quality sampling. I recognise that IH could and perhaps should play a role in such fields; however, since the chemical expertise within the sections is very limited, it would seem from my limited view as a hydrochemist that little progress could be made without much greater input from an environmental chemist. It is hard to see at the moment how such an involvement could be achieved; however, discussions with the IGS Hydrogeochemistry and IH's Analytical and Hydrogeology Sections might be of value.

#### 1.4 Improving communication

One important point raised in the survey was the lack of communication between sections. During the survey it became apparent that sections tended to be isolated from each other's work and that few appreciated the extent of the analytical chemistry facilities; there was, however, an awareness of this isolation of sections. As a start towards overcoming some of these difficulties, Nick Mandeville has begun a series of across-the-Institute seminars, whilst within the Analytical Section Enda O'Connell has also initiated project seminars to which others are invited as appropriate. These approaches could be extended to across-the-Institute discussions of chemical topics and might form the starting points for future collaborative research. Topics that might be considered are:-

- Chemicals/isotopes as tracers of pathways of water movement through hydrological systems;
- Arid and semiarid zone hydrochemical research;
- Catchment scale hydrochemical research in the UK;
- Freshwater conservation;
- The uses of isotopic studies in hydrology;
- 6. Chemical transport models for hydrological systems;
- The chemistry of water-rock/sediment interactions;
- 8. Automatic water quality stations;
- 9. Chemical transport through the unsaturated zone;
- 10. The use of thermodynamic models in hydrology;
- 11. Erosion and sediment transport;
- 12. Environmental impact studies;
- 13. Groundwater hydrochemistry.



In addition to these a chemical laboratory Open Day might be considered to advertise the scope of the analytical facility.

#### 1.5 The role of IH hydrochemists

A strong feeling expressed during the survey is that the role of IH hydrochemists has either never been properly defined or not universally agreed. The problem is that while the Hydrochemistry Section deserves to exist in its own right primarily for hydrochemical studies the need of a "service/consultancy role" to supply chemical expertise and analytical facilities to cater for other sections' needs is large. It has always been assumed (by those outside the section) that the Hydrochemistry Section is the natural home for such a service/consultancy. However, it has never properly been recognised (without meaning to be derogatory in any way) that much of the work involved with such a "service/consultancy" would be of little interest to, and outside the scientific expertise of, the "hydrochemists". Despite this uncomfortable disparity of view, the Hydrochemistry Section should fulfill both requirements. Possible roles that the hydrochemists might fill are as follows:-

- (a) That of doing research into the processes by which the chemical composition of water changes as it proceeds through the land phase of the hydrological cycle ("chemical process work");
- (b) That of acting as consultants for those projects manned by staff with limited chemical competence ("Consultancy");
- (c) To act as a service facility providing chemical

analyses of samples submitted to them ("Analytical Chemistry Service").

NB: The word "service" is perhaps a poor "label" for the role of the analytical chemistry facility; as expressed earlier in the report, to make this "service" work there must be close liaison between the user and the analytical chemist in the planning, implementation and interpretation stages of the projects.

(d) To provide some mixture of (a), (b) and (c).

Role (d) is that which best serves IH interests, and it then remains to determine what the mixture should be. In the past, the Hydrochemistry Section has been criticised because it placed too great an emphasis on certain areas under (a) that while scientifically production, the research appeared to have marginal relevance to the chemistry of fresh waters; nevertheless, it is work under (a) which offers the greatest stimulus to "prime mover" chemists, and it may be argued that an understanding of chemical processes occurring at the interface between water and solid is so fundamental to many practical water quality problems that such work should have the highest priority. A significant proportion of hydrochemists' time should therefore be devoted to chemical process work.

Consultancy work ((b) above) also clearly might be considered an important activity for the IH Hydrochemistry Section, particularly since we have many projects with hydrochemical components that are staffed by scientists with limited chemical knowledge. In the past, it has been assumed that contact between such project staff and the specialist hydrochemists would take place at an informal level, and certainly these informal contacts have sometimes worked. At other times, however, such informal contacts

between project staff members diffident of revealing their ignorance of chemistry and hydrochemists diffident or revealing ignorance of hydrological terminology and objectives, have been unsuccessful, with both "consultant" and "patient" entering a paralysing state of frustration through the inability of each to understand what the other is about.

Informal contacts between project staff and hydrochemists can only work if both participants are not ashamed to reveal the limitations of their own knowledge; if, for whatever reason, the climate of research within IH is not conducive to allow such revelations, then a more formalised contact between hydrochemical consultant and hydrological patient may be a solution, however distasteful formality may be. It is here that the Task Force idea, or some variant of it, would find application, since it would require participants to talk together before a project had even begun, when contact between them is essential.

The consultancy aspect of the IH hydrochemists' work therefore is of an importance secondary only to their chemical process work (possibly first equals with it?). It must be borne in mind, nevertheless, that any increase in consultancy activity by the IH hydrochemists can only be at the expense of their chemical process work. This paper suggests that, as a desirable target, the work of the Hydrochemistry section should be divided equally between chemical process work and consultancy work.

The analytical chemistry service aspect (c) of Hydrochemistry Section activities is clearly of great importance, and IH can count itself fortunate in having a dedicated and highly experienced chemist who finds satisfaction in the contacts

with project staff that this work provides - even though it is not used to anything like its full capacity at the present time.

## THE FUTURE

### 2.1 Chemical studies at IH

The future of IH chemical research could be an exciting and very productive one providing we can establish first good communication between Sections and secondly a managerial system which can cope with their joint needs. Because of limitation in staffing and expertise at present progress might be slow, although a much closer tie with the IGS workers on site would alleviate some of the difficulties (remember that on site we probably have the largest grouping of hydrochemists in the UK). In all the sections I approached there were potentially clear growth areas, eg connected with "Chemical modelling of hydrological systems", "Chemical cycling of elements in catchments", "Chemical transport through the unsaturated zone".

For the Hydrochemistry Section perhaps it is appropriate for me (given my strong ties with it) to make some comment on the direction I would like to see it develop. This I do in the following section (2.2).

## 2.2 Hydrochemistry studies at IH

We have seen (i) that existing IH projects with a hydrochemical component can be classified under the two headings impact of man on the chemistry of natural waters and chemistry of hydrological processes; (ii) that the present large number of diverse projects with some hydrochemical component have "just grown" rather than having been consciously undertaken as part of a planned progress; (iii) that hydrochemical expertise at IH is very limited. The section attempts to define a course that IH can chart through the field of hydrochemistry, taking account of the several constraints on progress which include the following:-

- (i) The need to accommodate the interests of the hydrochemists themselves, and of their hydrological colleagues;
- (ii) The need to exploit the talents, experience and enthusiasms within IH;
- (iii) The need to avoid starting late in a race along a course which other research institutes began long ago, and on which we have no chance of catching up (an earlier paper by Enda O'Connell, written in about 1979 and given as Appendix 6, defines the distinction between IH interests and those of WRC).
- (iv) The need to ensure that the hydrochemical work that we do in future is complementary to that already being done by our IGS colleagues;
- (v) The impossibility of securing any expansion of hydrochemical staff beyond what IH has had in the past;

- (vi) The need to recognise and cater for the fact that while there is a strong movement towards studies on water quality rather than quantity, IH is profoundly unprepared for such a change given that only a handful of staff have a knowledge of chemistry above A-level standard.

Before going further, a definition is given of the branch of hydrochemistry IH workers generally consider appropriate for IH objectives; we take hydrochemistry to be the study of processes by which the chemical composition of water changes as it proceeds through the land phase of the hydrological cycle from precipitation (either as rain or snow), through temporary or longer-term storage, within soil, aquifers, lakes and glaciers, to flow in river channels. We recall that changes in chemical composition may be brought about either by decay processes within water itself (for example, by radioactive decay of an unstable isotope); by chemical action where water comes into contact with soil, rock, sediment, plant roots and air; and by the mixing of waters of different chemical compositions. This definition embraces work having both more practical objectives (impact of man ...) and less immediately practical ones (chemistry of hydrological processes).

Within the subject area Impact of man on the chemistry of natural waters, new work that IH may wish to consider is studies of the geochemical cycling type within different climatic-vegetation regimes. At the PSO meetings held at IH last year, there was a consensus that greater emphasis should be placed on work within the arid and semiarid tropics; geochemical cycling work within these regions is also extremely attractive to some of our IGS colleagues (Mike Edmunds in particular, who already has contacts with personnel at possible sites). Similar geochemical cycling studies could also be undertaken in the humid tropics,

possibly as a complement to Jim Shuttleworth's project on energy partitions, and Robin Clarke/David Cooper's study on isotopic fractionation, within the Amazon. Work in the humid tropics may be logistically and administratively more difficult to set up than work in the semiarid tropics, however, since the latter could be undertaken as a collaborative venture with IGS colleagues using shared facilities. If this work is to be done, however, there must be a positive commitment by IH and IGS local management to support the contact and to develop a joint programme of work. A commitment to an arid-zone hydrochemical research project would be particularly attractive because, through their consulting services, both IH and IGS staff members are given opportunities to visit many countries within the zone for short periods, when additional observations and measurements could be taken to supplement more intensive work carried out at one or two specialist sites.

In the area of the chemistry of hydrological processes, possible areas of research activity include study of the changes in chemical composition brought about by contact between water and soil in the unsaturated and saturated zones; between water and the rock matrix of an aquifer; between soil water and plant roots; between intercepted water and plant canopies; between river water and sediments; between snowpack and atmosphere; between water in lake or reservoir storage and the atmosphere. Some of these areas for possible study are already under occupation by other research teams: in studies of chemical interactions between lakes and atmosphere, for example, IH Hydrochemistry would be competing with the expertise of FBA, ITE and WRC, whilst areas such as chemical interactions between water and rock matrices - and between water and soil in the unsaturated zone - are already being worked by IGS colleagues on site. If staff time allows, there would still be scope for contributions in these areas from IH

Hydrochemistry, provided that there is good liaison between IH and IGS personnel to ensure that research projects are complementary rather than competitive.

However, of the areas listed above, those areas of the chemistry of hydrological processes that (i) appear most appropriate for IH specialization, (ii) appear best adapted to IH staff interests, (iii) appear to offer the best prospects for intersectional bridge building are:

- (a) Changes in chemical composition of water brought about by the interception of rain and snow by plant canopies;
- (b) Changes in chemical composition of soil water brought about by contact with soil and plant roots;
- (c) Changes in chemical composition of river water brought about by its contact with sediment and with the river bed, particularly in upland streams;
- (d) Changes in chemical composition of groundwater brought about by its contact with the aquifer matrix;
- (e) Changes in chemical composition of snowpack brought about by contact with the atmosphere.

In summary, therefore, one "scenario" for the development of IH Hydrochemistry would be the following:-

- (i) a substantial commitment (40%?) to the above five topics (a) to (e), supplemented as necessary by others (eg in the unsaturated zone) where IH workers are already active and productive (all of these



topics coming under the heading "chemistry of hydrological processes");

- (ii) a substantial commitment (20%?) to a joint IH/IGS initiative for a research programme of the geochemical cycling kind, probably in the semiarid tropics;
- (iii) a substantial commitment (40%?) to "consultancy" and "service" work to assist IH project staff with limited hydrochemical knowledge (the latter two commitments coming under the heading "Impact of man on the chemistry of natural waters").

It will be clear that this partitioning is not one with clearly defined boundaries; the work in a semiarid environment would have a large "process" component, for example.

### 2.3 Implications for staffing within the Hydrochemistry Section

As stated above, IH has but two environmental chemists (Colin Neal, Alun Thomas) trained to PhD level and whose time is already heavily committed (indeed one, Colin Neal, is not even in the Hydrochemistry Section); these are backed by Christopher Smith, John Raynor and James Walls in charge of "Analytical Chemistry services". The above scenario for hydrochemistry development at IH can be undertaken with only very limited effect with such few personnel, and the question of a replacement for Vic Truesdale then arises.

Of the above three possible areas (i) to (iii) for future hydrochemical work, that in the arid zone (ii) could be supervised by Mike Edmunds (assuming that the IGS/IH project

came into being at a site or sites available through Mike Edmund's contacts); for the "service/consultancy" work (iii) within IH, the level of chemical competence required probably does not warrant the appointment of a PSO chemist (although the volume of work will greatly overburden the chemists that we have). If, however, any serious hydrochemistry is to be done under the heading (i) "chemistry of hydrological processes" (vide the topics (a) to (d) above) then it seems improbable that Mike Edmunds or any other of our IGS colleagues will have time to involve themselves deeply with it. The appointment of another chemist (who, in the light of the Visiting Group's comments on the importance of chemistry at IH, would have to be an established research chemist) would therefore be necessary.

#### HYDROCHEMISTRY/WATER QUALITY STUDIES AT IH: A FORWARD LOOK

While (a) the Visiting Group recognised that a broad hydrochemical programme is an integral part of IH's programme and (b) there is a strong feeling within IH senior management that water quality research should constitute about 50% of the total (cf 5 to 10% at present) while (c) chemical research at IH could be scientifically exciting in both a "pure" and "applied" sense, little attention has been given to the implications either in terms of the logistics of continuing or enlarging on IH's chemical programme. The facts that we have lost the Head of Hydrochemistry and an SO chemist without even seriously considering replacement, that the major hydrochemical resource at Wallingford (namely IGS) is largely untapped, that our chemical expertise is very thin on the ground, that IH's areas of interest are large, diverse and uncoordinated, all attest to this contention. If IH wishes to have a major water quality research programme within the next ten years, the implications must be fully understood; while this report can describe the

state of hydrochemical/water quality research at IH and  
can identify problems, clearly executive decisions on  
staffing are needed to solve them.

CN/RTC/SJB

APPENDIX 1

Hydrochemical/Water Quality Research at IH

<u>Project</u>	<u>Title</u>	<u>Workers</u>	<u>Section</u>	<u>Funding</u>
	<u>Large chemical component</u>			
24	Application of chemical tracer dilution methods	<u>KG</u>	<u>Plynlimon</u>	NERC
25	Environmental isotopes in the water cycle	<u>AGPD</u> <u>APB</u>	<u>Hydrogeology</u>	NERC
26	Hydrochemical process studies	<u>(VWT)</u> <u>CN</u> <u>CJS</u> <u>JW</u>	<u>Hydrochemistry</u>	NERC
39	Hydrogeology of shallow alluvial aquifers	<u>AGPD</u> <u>CN</u> <u>JCD</u> <u>EJR</u> <u>AJD</u> <u>RSW</u>	<u>Hydrogeology</u>	NERC
50	Measurement of unsaturated soil moisture fluxes in chalk to derive NO <sub>3</sub> fluxes beneath arable plots treated with inorganic fertilizer	<u>SRW</u> <u>JPB</u>	<u>Soil Physics</u>	NERC
55	Evolution of alkaline groundwater	<u>CN</u> <u>AGPD</u> <u>EJR</u>	<u>Hydrogeology</u>	NERC
68	Clay modelling	<u>AGT</u> <u>(VWT)</u> <u>CN</u>	<u>Hydrochemistry</u> <u>and Hydrogeology</u>	NERC

(The major workers/sections on the projects are underlined)

APPENDIX 1 (continued)

<u>Project</u>	<u>Title</u>	<u>Workers</u>	<u>Section</u>	<u>Funding</u>
121	Modelling of hydrochemical systems	CN AGPD DMC RSW AGT	<u>Hydrogeology Hydrochemistry and Analytical</u>	NERC
67	Leaching of nitrate in a practical agricultural catchment	GR JMS JRB	<u>Catchment</u>	MAFF
72	Hydrological survey of two wetland conservation sites in Wales	KG	<u>Plynlimon</u>	NERC
94	Water quality modelling for design and operational management	PGW RJW RC PEOC KB	<u>Analytical</u>	EEC/AWA/ TWA/NERC
103	The effect of upland land use on water quality	GR JH JRB	<u>Catchment</u>	WRC/FC/DOE/ UTCAA
124	Pollution in snow	EMM AGT	<u>Analytical and Hydrochemistry</u>	NERC/NSHB
<u>Small chemical component</u>				
58	Groundwater recharge - Fleam Dyke	JDC DC JPB SB	<u>Soil Physics</u>	NERC/DOE

APPENDIX 1 (continued)

Project

	Instrumentation	<u>ICS</u>	RW	Instruments	NERC/ODA
28/90	Instrumentation				
33	Short-term repayment projects at home and overseas	AGPD SFP	RBB CN	Overseas Hydrogeology Hydrochemistry	Private sector NRPB Various Government Agencies
122	Water quality monitoring control and telemetry instrumentation				
		RFT		Instruments	AWA

APPENDIX 2

Hydrochemical/water quality project descriptions

## APPLICATION OF CHEMICAL TRACER DILUTION METHODS

OBJECTIVES:

Development and use of chemical methods in

- (i) Hydrometry. Investigation of dilution gauging as an alternative to the velocity/area method, particularly where flow is non-uniform and turbulent;
- (ii) Modelling of solute transport. Accurate simulation of solute transport in rivers, using detailed information on residence times and dispersion obtained from tracer experiments.
- (iii) River channel survey. Use of tracer dispersion experiments to characterize the large-scale form of river channels, for ecological and flood-routing applications.

Construction of a theoretical framework for studies of the behaviour of conservative and adsorbed tracers in natural streams.

METHODS:

Exploration of the limitations of chemical dilution gauging, to determine its usefulness, particularly when compared with other spot gauging methods. Use of the technique in 'difficult' circumstances where a comparison is possible. Theoretical and field studies of sources of error, both systematic and random. Maintenance of contacts with WA, WRC and overseas hydrometric teams, through BSI and ISO.

Literature survey of stream dispersion, and comparison of various models of dispersion with tracer experiments. Attempts to derive a conical form for dispersion in natural streams, as opposed to regular laboratory channels.

Investigation of effects of extreme form roughness on longitudinal dispersion.

APPLICATIONS:

An alternative gauging method for non-uniform flow.

Models of flow and dispersion in natural channels, using parameters measured in the field.

Criteria for assessing the effectiveness of river engineering in maintaining an efficient river channel without sacrificing ecological diversity.

DATES: Ongoing

Funded by: NERC

STAFF:

K Gilman                      SSO

COSTS:

1980/81 (£K)	1981/82 (£K)	Estimated staffing 1981/82 (man years)
13.0	11.2	0.4



## ENVIRONMENTAL ISOTOPES IN THE WATER CYCLE

OBJECTIVES:

Combined development of the use of tritium, oxygen 18 and deuterium to assist in field surveys and determine the significance of dominant hydrological processes.

METHODS:

- (i) Stable isotopic variations with altitude in Plynlimon rainfall.
- (ii) Isotopic variations in streamflow (Plynlimon and Thames areas)
- (iii) Isotope tracing of flood plain exchanges between rivers and alluvial groundwaters in the Thames floodplain.

APPLICATIONS:

- (i) Support for overseas repayment studies in arid zones
- (ii) Use of stable isotopes in UK hydrological studies.

DATES: Ongoing

Funded by: NERC

Project is co-ordinated with parallel IGS investigations and with joint operation of the Wallingford Isotope Laboratory.

STAFF:

A G P Debney	PSO	(L)
A Brunson	ASO	

COSTS:

1980/81	1981/82	Estimated staffing 81/82
(£K)	(£K)	(man years)
12.5	7.4	0.1

## HYDROCHEMICAL PROCESS STUDIES

OBJECTIVES

To discover and quantify mechanisms that control the chemistry of natural waters.

METHODS

The problem is approached through both laboratory simulation of reactions and modelling of entire natural systems. The former approach gives clues as to whether an equilibrium or a kinetically mediated system is under study. The latter approach involves biological, physical and sometimes other chemical processes and facilitates evaluation of the importance of a given reaction mechanism. One of the more difficult problems is to identify the species of a given element that are present in a natural water. This problem, in the case of silicon and iodine, is being investigated using a "comparison of analytical methods" approach; discrepancies between methods being attributable to interfering substances or the presence of different species.

APPLICATIONS

1. The analytical (chemical) work is of general value to all other laboratories dealing with the same elements, while the silicate chemistry will be of much wider interest owing to the occurrence of silicate in natural water, rocks, steel, etc.
2. Information about the mobility and pathways of chemicals in our natural environment is of obvious importance, especially after Japanese experience with mercury. The iodine work is valuable in considerations of the potential problems of release of radio-I from radioactive waste.

DATES: Ongoing.

Funded by:- NERC

STAFF

V W Truesdale	PSO	(L)
C J Smith	HSO	
C Neal	HSO	

COSTS

1980/81 (£K)	1981/82 (£K)	Estimated staffing 81/82 (man years)
25.0	31.2	1.2

## SPECIAL INSTRUMENTS PROJECT

OBJECTIVES:

To develop new instrument techniques, not directly linked with current research.

METHODS:

As appropriate, and by keeping abreast of current technology.

APPLICATIONS:

Future hydrological instrument requirements.

DATES: Ongoing

Funded by: NERC

STAFF

T J Dean	PSO	(S)
I C Strangeways	PSO	
G P Brunsdon	SSO	
M Turner	SSO	
A J Baty	HSO	
D J Harris	ESO	
M T H Key	HSO	
R G Wyatt	PTO3	
S J Edwards	PTO4	
W S Insell	PTO4	
M R Stroud	PTO4	
J Cross	(Contract)	

COST:

1980/81	1981/82	Estimated staffing 1981/82
(£K)	(£K)	(man years)
170.0	120.4	4.9

## SHORT TERM REPAYMENT PROJECTS AT HOME AND OVERSEAS (SEE ALSO APPENDIX 4)

OBJECTIVES:

To provide a specialised consulting service in all aspects of hydrology so as to put into practice rapidly the results of the Institute's research programme. Also, to build up a large body of experience and data relating to problems in the major climatic zones of the world to assist in the development of a broadly based research programme.

METHODS:

As appropriate

DATES: Ongoing

Funded by: Private Sector

STAFF

A G P Debney	PSO
D T Plinston	PSO
S F Pond	PSO
R B Bradford	SSO
F A K Farquharson	SSO
B S Piper	SSO
	SSO
D S Biggin	HSO
J Bromley	HSO
J W Finch	HSO
C S Green	HSO
C Neal	HSO
Y P Parks	HSO
R Wikramaratna	SO
J Ridler	ASO
Various other staff from time to time	

COSTS:

1980/81	1981/82	Estimated staffing 1981/82
(£K)	(£K)	(man years)
250.0	240.0	10

## HYDROGEOLOGY OF SHALLOW ALLUVIAL AQUIFERS

OBJECTIVES:

Understanding of groundwater occurrence and flow in superficial deposits and the relationships with surface waters particularly in the alluvial tracts of major UK rivers.

METHODS:

- (i) Instrumentation of shallow boreholes in Thames Valley with the analysis of geological and water level data to determine the interdependence of surface and groundwaters.
- (ii) Field and laboratory studies of groundwater temperature, stable isotopes and major-ion chemistry as tracers of underground and surface connections.
- (iii) Laboratory testing of geological samples to examine variations in aquifer composition and assess their effects on hydraulic properties.
- (iv) Modelling of the Thames system to test hydrological and hydro-geological concepts and examine management options.

APPLICATIONS:

Environmental management and water resources evaluation, especially with regard to conjunctive-use schemes. The effects of sand and gravel extraction, and waste disposal on the flood plain environment.

DATES: Ongoing

Funded by: NERC

STAFF:

J C Davey	ESO	(L)
A G P Debney	PSO	(S)
A J Dixon	ESO	
R Wikramaratna	SO	
A Neal	ESO	
S Rainer	ESO	
	Student	

COSTS:

1980/81	1981/82	Estimated staffing 81/82
(£K)	(£K)	(man years)
78.0	88.4	3.75

MEASUREMENT OF UNSATURATED SOIL MOISTURE FLUXES IN CHALK TO DERIVE  
NITRATE FLUXES BENEATH ARABLE PLOTS TREATED WITH INORGANIC FERTILIZER

OBJECTIVES:

To provide measurements of vertical soil water movement in the upper 3 metres of chalk profiles beneath arable plots treated with known rates of inorganic fertilizer.

To combine soil moisture flux data with measurements of the nitrate nitrogen and chloride concentrations of pore water samples taken from beneath the same plots in order to estimate the direction and magnitude of solute fluxes in the chalk.

METHODS:

The experimental site comprises treated arable plots and an adjacent grass plot on the chalk at Bridgets Experimental Husbandry Farm, near Winchester. The soil physical project has been superimposed on an established MAFF (ADAS) experiment on the contamination of drainage water by farm effluents.

Measurements of soil moisture content and potential profiles are made twice weekly in the upper 3 m of the chalk beneath the plots using a neutron probe, mercury and pressure transducer tensiometers, and electrical resistance blocks. The zero flux plane technique is used to measure the upward and downward soil water fluxes throughout the year. Water samples for chemical analysis have been collected using manual destructive coring of the chalk every two months, followed by centrifugation. This method has proven reliable for obtaining pore water chemistry profiles down to 3 m depth on a routine basis.

APPLICATIONS:

Groundwater pollution studies: movement of solutes in the unsaturated zone. Measurement of actual evaporation from agricultural crops and aquifer recharge from chalk downland soils.

DATES: End: Fieldwork April 1981;  
Analysis 1981/82

Funded by: NERC

STAFF

S Wellings	ESO	(L)
J P Bell	PSO	(S)
Student		

COSTS:

1980/81	1981/82	Estimated staffing 1981/82
(£K)	(£K)	(man years)
27.5	28.2	0.98

## EVOLUTION OF ALKALINE GROUNDWATER

OBJECTIVES:

To determine the chemical and mineralogical changes associated with the origin of extremely alkaline groundwaters in ophiolitic rocks. This project is nearing completion. New material has been received from Oman to allow closer examination through isotopic studies of the origin of the waters as opposed to their chemical evaluation.

METHODS:

- (i) Chemical and isotopic studies of the spring waters and the associated gas and sediment components.
- (ii) Mineralogical studies on sediment and rock weathering components.

APPLICATIONS:

- (i) To explain the origin of alkaline groundwaters in other basic and ultramafic areas.
- (ii) To advance understanding of the process of serpentinisation.
- (iii) To explain the hydrochemical and hydrogeological relationships between alkaline and other groundwaters in Oman.

DATES: Ongoing

Funded by: NERC

STAFF:

C Neal	HSO	(L)
A G P Debney	PSO	(S)
S Raynor	HSO	

COSTS:

1979/80	1980/81	Estimated staffing 80/81
(£K)	(£K)	(man years),
26.0	14.5	0.3

## GROUNDWATER RECHARGE - FLEAM DYKE

OBJECTIVES:

- (1) Development of soil physical methods for measuring recharge to aquifers.
- (2) Comparison of these recharge estimates with those from a large undisturbed monolith lysimeter operated by IGS.
- (3) To study the small and large scale variability of recharge over a single soil/geology/land use unit to assess the representativity of a single site.
- (4) Application of measured hydraulic properties of the unsaturated zone to nitrate movement.

METHODS:

In summer conditions, tensiometers are used to identify a depth in the soil across which there is no water flow, the zero flux plane. Changes in soil water content above this depth, measured by neutron probe, are attributable to rainfall and evaporation. Changes below the zero flux plane are due to drainage which eventually appears as aquifer recharge.

During the winter, direct solution of Darcy's Law is being attempted using unsaturated hydraulic conductivities measured in situ.

APPLICATIONS:

Measurements of groundwater recharge. Crop water use studies. Groundwater pollution and movement of solutes in the unsaturated zone. Irrigation management.

DATES: Start: 1977

End: Present comparison between lysimeter and soil physical methods - March 1982.

Funded by: Initially DoE, now NERC (with possibility of minor DoE contribution) EEC funding being sought for continuation of other aspects of study.

STAFF:

J D Cooper	SSO	(L)
J P Bell	PSO	(S)
R J Raynor	SC	
S A Boyle	SO	
Sandwich student		
B J Burton	ASO	(b time)

COSTS:

1980/81	1981/82	Estimated staffing 1981/82
(£K)	(£K)	(man years)
47.0	48.7	2.26



## LEACHING OF NITRATE IN A PRACTICAL AGRICULTURAL CATCHMENT

OBJECTIVES:

- (1) To determine the variations in nitrogen concentrations with time and discharge rate in Shenley Brook.
- (2) To determine relationships between these variations and rainfall, fertilizer applications and agricultural practices within the catchment.

METHOD:

- (1) IH continue the existing hydrological measurements, to organize and maintain the collection of rainfall and discharge water samples and to transport these samples to MAFF, Reading, for analysis and to make the data available to MAFF.
- (2) MAFF to negotiate with the farmers to continue recording the agricultural practices being carried out on the catchment.
- (3) IH to participate in the analysis and interpretation of the data collected.

APPLICATION:

To provide information on the effects of land use management on the levels of nitrogen in streams.

DATES: Ongoing

Funded by: MAFF

STAFF:

G Roberts	SSO	(L)
J R Blackie	PSO	(S)
J M Smith	ASO	
Student		
Driver		

COSTS:

1980/81	1981/82	Estimated staffing 1981/82
(£K)	(£K)	(man years)
5.0	6.3	0.23

## CLAY MODELLING

OBJECTIVES:

To improve understanding of the mechanisms and importance of cation exchange upon clays in the environment. This project originated as a study of ion-exchange in the estuarine environment, in collaboration with MBA, and this remains the short-term objective.

METHODS:

So far, the work has mostly been of a theoretical nature with the rationalisation of the entire literature upon this complicated subject as the prime objective. Subsequent practical work involves laboratory simulation experiments in which the behaviour of a range of clays in waters of various salinities is studied. Field sampling in the estuary is to be performed in conjunction with MBA staff as part of their Tamar estuary programme. X-ray diffraction will be used to characterise the mineralogy of estuarine sediments and to investigate the structuring of adsorbed water near the clay surface.

APPLICATIONS:

The knowledge gained in this project is applicable to a whole range of subjects as well as the particular problem of the estuary. These subjects include ceramics, the environmental sciences and various aspects of engineering (eg, dam construction, dredging, etc.).

DATES: Ongoing

Funded by: NERC

STAFF:

C Neal	ESO	(L)
V W Truesdale	PSO	(S)
A G Thomas	ESO	

COSTS:

1980/81	1981/82	Estimated staffing 81/82
(£K)	(£K)	(man years)
36.0	48.1	2.5

## HYDROLOGICAL SURVEY OF TWO WETLAND CONSERVATION SITES IN WALES

OBJECTIVES:

A detailed understanding of the hydrology of wetland sites and their interaction with surrounding 'reclaimed' land, and the provision of criteria for evaluating possible threats from peripheral drainage.

METHOD:

- (i) installation of climatological and hydrological instruments on two neighbouring fen sites on Anglesey, one of which has been considerably altered by agricultural practice, and the evaluation of water balance components over a two-year period;
- (ii) 'process' studies, including a detailed survey of water courses, measurements of the permeability and specific yield of the peat, and intensive microclimate measurements;
- (iii) collection of available data from related areas, and of climate data for the surrounding area, to evaluate possible climatological reasons for wetland deterioration.

APPLICATIONS:

Better management of wetland nature reserves, which are widely endangered by activities on surrounding land. Evaluation of strategies both for conservation of sites which are in a satisfactory condition, and for restoration of sites which have already undergone some deterioration.

DATES: End mid-1981

Funded by: NERC

STAFF:

K Gilman	SSO	(L)
M D Newson	PSO	
R T Clarke	SPSO	(S)

COSTS:

1980/81	1981/82	Estimated staffing 80/82
(£K)	(£K)	(man years)
14.0	7.0	0.2

## SIMPLE INSTRUMENTS

OBJECTIVES:

To design and develop a new style of instrument, particularly for 3rd World countries, which is both cheap and also requires minimal maintenance. A range of such instruments is to be developed to cover all of the common variables (rain, river level, etc.).

METHODS:

The re-thinking of instrument design philosophies so as to allow cheap manufacture coupled with a throw-away design. The development of such techniques to the production stage. A programme of field testing to prove the new instruments.

APPLICATIONS:

While originally conceived with 3rd World users particularly in mind, the new style of instrument can also be used in the more developed countries where maintenance effort, while available, is costly.

DATES: Ongoing

Funded by: ODA

STAFF:

I C Strangeways	PSO	(L)
W S Insell	PTO4	

COSTS

1980/81	1981/82	Estimated staffing 1981/82
(EK)	(EK)	(man years)
9.6	6.6	0.25

## WATER QUALITY MODELLING FOR DESIGN AND OPERATIONAL MANAGEMENT

OBJECTIVES:

To provide integrated dynamic stochastic models of flow and water quality for the design and operational management of water resource systems.

In the case of the Anglian Water Authority it is intended to provide real time operational models using telemetered data from flow gauging stations and automatic water quality monitors located on the Bedford Ouse River System.

For the Thames Water Authority the objective is to provide simulation models (particularly for nitrates) which may be used to assess future development schemes within the TWA region.

METHODS:

Reduction, storage and analysis of telemetered data using mini/micro computers. Modelling flow and water quality using statistically based techniques to update models and forecast future water quality behaviour. Development of methodologies for the design of water resource systems from the viewpoint of water quality.

APPLICATIONS:

Provision of reliable, telemetered water quality data and forecasts for operational managers.

Provision of integrated models of flow and water quality for assessing design problems in river basins.

DATES: Ongoing

Funded by: EEC/AWA/TWA

STAFF:

P G Whitehead	SSO	(L)
P E O'Connell	PSO	(S)
R J Williams	SO	
	ASO	

COSTS:

1980/81 (£K)	1981/82 (£K)	Estimated staffing 1981/82 (man years)
60.0	40.5	1.8

## THE EFFECTS OF UPLAND LAND USE ON WATER QUALITY

OBJECTIVES:

To study the effects of four land use changes: clear felling, tree planting, aerial fertilizer applications to forests, and grassland improvement, on water quality in upland areas.

METHODS:

Two small catchments (about 100 ha) are to be used for each study, one as a control and the other being subject to the land use change after a suitable calibration period. Each catchment will be instrumented to measure rainfall, runoff and the measurements required to estimate evaporation. Samples of the discharge and the rainfall will be collected for chemical analyses. If necessary, traps will be constructed to measure sediment loss.

Only two of the eight required catchments have been identified. These are at Great House EHF and will be used to study the effects of grassland improvement. These will be instrumented in the spring/summer of 1981.

APPLICATIONS:

An assessment of any increase in nutrient, particularly nitrogen and phosphorus, concentration due to the land use change. Also an assessment of change in water yield.

DATES Start: 1980

Funded by: WRC, FC, DoE

STAFF:

G Roberts	SSO	(L)
J R Blackie	PSO	(S)
J A Hudson	HSO	

COSTS:

1980/81 (EK)	1981/82 (EK)	Estimated staffing 1981/82 (man years)
6.0	25.8	1.05

## MODELLING OF HYDROCHEMICAL SYSTEMS

OBJECTIVES

To investigate the potential of computer modelling of primary physico-chemical processes as an interactive tool for interpretation of sparse chemical data and to test hydrological models for water resource studies.

METHODS

Diffusion/dispersion and ion-exchange processes are currently being studied to assess the significance that water mixing and water/sediment interactions have on controlling water quality in aquifer systems. Diffusion/dispersion processes are being examined through finite element modelling of coastal saline intrusion. A model has been developed which is being compared with field data for the UK chalk aquifers to examine the validity of commonly used longitudinal and transverse dispersivity terms. Ion exchange processes are being studied by modelling clay-electrolyte systems based both on electrostatic and mass action type thermodynamic theory. The exchange models developed are being tested against laboratory based experimental evidence which simulates saline intrusion.

APPLICATIONS

Initially to develop better understanding of the nature of hydrogeological environments. If successful, the models could be developed to examine surface water and unsaturated zone problems.

DATES: Start: December 1981

Funded by: NERC

STAFF:

A G P D ebney

## WATER QUALITY MONITORING CONTROL AND TELEMETRY INSTRUMENTATION

OBJECTIVES

The design, development and supply of an intelligent river water quality monitoring station capable of controlling water quality monitors (by initiating calibration, cleaning and measurement operations) and of two way automatic data transmission to a central master station. The central master station to be capable of remote interrogation to allow access to stored data providing information in the form of computer generated system messages. The master station will also be linked to a DEC MINC minicomputer already controlling a water quality network by telephone telemetry.

METHODS

Microprocessors programmed in FORTH will be used as the intelligence in both the outstation and master station. They will be linked by telemetry over the public telephone network.

The outstations will handle up to 10 analogue inputs which will be sampled and averaged at defined periods. The stations will activate pumps, compressors and valves as required and will be controllable both by use of a keypad to enter data and commands, and automatically in preselected sequences.

The master station will be interfaced to a DEC MINC microcomputer system using RS232 protocol. It will scan outstations, store and display data from them and provide speech output to staff dialing in with a lost cost interrogator.

APPLICATIONS

Monitoring, control, forecasting of water quality on river systems. Provision of information to water authority staff to allow them to react in real time to changes in water quality. Similar ideas with small changes in system software and sensors would allow groundwater or river levels to be monitored in a similar way.

DATES: Start: November 1981 End: April 1982

Funded by: AWA

STAFF:

R F Templeman (L)



## POLLUTION IN SNOW

Description: When snow melts, the first meltwater appearing at the bottom of a snow column contains much of the total dissolved load of the snow. Thus, in areas where storage in a snowpack is an important stage in the passage of air-borne pollutants through the natural environment, the first meltwater may be highly contaminated relative to ambient concentrations. This surge of pollutants, such as trace metals and acids, which may represent the combined total of several weeks or months of pollution in precipitation, can have a seriously adverse effect for users of the water downstream.

Objectives: The aims of this programme are (i) to determine the characteristics of the flush-out mechanism in a seasonal snowpack in the Cairngorms, N.Scotland; and (ii) to investigate the processes of melting in a snowpack. Such a study should define the variation of the quality of meltwater with time.

Relevant Markets: Users of water in Scotland, Wales and the North of England who would be adversely affected by a sudden surge in the level of pollutants, eg. Water Authorities, River Purification Boards, Fisheries. Those especially affected will be users who need a constant supply of high priority water, eg. fish farmers.

Progress to date: A pilot project, funded from Science Vote money and consisting of two brief field trips, has produced evidence that a flush-out mechanism was certainly in operation in the Cairngorms: after melting had removed 60% of the snowpack, the remaining snow contained only 5% of its original concentration of pollutants. However, such a short study has only served to raise questions such as how big a surge was there, what process(es) caused it, is the surge time predictable.

Forecast Progress 83/83: Funds from sources other than DOE will be used to fund some field work during 83/83.

Proposed Work 83/84: It is proposed that a study be made of the melting of snow in a small catchment in the Cairngorms. Measurements of meteorological and streamflow data will be made throughout the whole winter season from before the first snow until after snowmelt finishes. The conductivity of the stream will be measured continuously and samples of snow and stream water will be collected for chemical analysis in the laboratory.

Future Years: It is envisaged that three seasons of field work will be necessary to define precisely the characteristics of melting snow. Therefore we will be seeking further funding in 84/85.

Application of Results: With the ability to predict the timing of a surge of pollutants, precautionary action may be taken to avoid taking any of this contaminated water. The developments necessary to reach this stage will also mean that continuous prediction of water quality during snowmelt will be possible.

STAFF

E M Morris  
A G Thomas

APPENDIX 3

Main IH workers on hydrochemical/water quality studies.

<u>Worker</u>	<u>Section</u>
A G Thomas	Hydrochemistry
C J Smith	
C Neal	Hydrogeology
A G P Debney	
S R Wellings	Soil Physics
G Roberts	Catchment
P G Whitehead	Analytical

Appendix 4

Overseas repayment projects 1970-1980 with a water quality/  
hydrochemistry component.

BOTSWANA

Pre-investment studies of groundwater availability in the  
north-eastern region

for Sir Alexander Gibb & Partners (Africa)

BOTSWANA

Assessment of the potential of existing boreholes around  
Molepolole and Mochudi, and the siting of new wellfields  
following geophysical survey.

for Sir Alexander Gibb & Partners (Africa)

BOTSWANA

Hydrogeological and geophysical investigation of the groundwater  
potential of the Cave Sandstone near Serowe to meet the demand  
for cooling water at Moropule power station. The study  
included the use of satellite imagery, and magnetic, resistivity  
and gravity surveys, as well as a programme of drilling to  
provide the necessary information for digital model studies.

for Sir Alexander Gibb & Partners (Africa)

IRAN

Investigation of the alluvial aquifer underlying Tehran: the  
development of analogue and digital models of groundwater  
movement and the selection of new wellfield sites.

for Sir Alexander Gibb & Partners

## JORDAN

Groundwater investigations for the water supply to the processing plant and township associated with the Arab Potash Project. Geophysical survey and aquifer modelling to define wellfield locations. Prediction of future levels of the Dead Sea to determine dyke and pumping station levels.

for Sir Alexander Gibb & Partners

## OMAN

Review of all water resource studies leading to recommendations on water conservation, development of additional resources, and improvement of supplies for irrigation.

for Turner Wright & Partners

## OMAN

Water resource survey of Northern Oman including setting up basic instrument networks, analysis of storm rainfall and runoff, recharge to the alluvial aquifers, groundwater fluctuations and quality, a survey of existing water sources and use, and estimation of the long term resources.

for Sir Alexander Gibb & Partners

## SAUDI ARABIA

Use of environmental isotopes to examine the groundwater processes in the Umm er Radhuma aquifer of Saudi Arabia and Bahrain.

for Groundwater Development Consultants

## SEYCHELLES

Groundwater exploration in the coastal plateau areas on several islands leading to preliminary water resource estimates.

for Ministry of Overseas Development

SOMALIA

Groundwater exploration and digital model studies to estimate recharge of the alluvial aquifer between the Schebelli river and the coast. Design and location of new wellfields to augment the water supply of Mogadishu.

for Sir Alexander Gibb & Partners (Africa)

Appendix 5

Publication list for IH research with a chemical component.

- Boulton, G.S., Morris, E.M., Armstrong, A.A. and Thomas, A.G. (1979). 'Direct measurement of stress at the base of a glacier'. *J. Glaciology* 22, 3-24.
- Bowie, S.H.U., Parker, A. and Raynor, E.J. (1979). Uranium reconnaissance survey of British Lower Palaeozoic shales: trace elements related to clay mineralogy. *Transactions/Section B of the Institution of Mining and Metallurgy*, 88, 61-64.
- Caddy, D.E. and Whitehead, P.G. (1981). Practical Techniques of River Monitoring and Pollution Forecasting, Part I. Continuous Quality Monitoring and Data Acquisition, *Effluent and Water Treatment Journal*. September, 407-416.
- Clarke, R.T. and Cooper, D.M. (1982 in press). Water recycling in tropical forests as a stochastic process. *Acta Amazonica*.
- Elderfield, H. and Truesdale, V.W. (1980). On the biophilic nature of iodine in sea water. *Earth and Planetary Sciences Letters*, 50, 105-114.
- Edwards, A., and Truesdale, V.W. (1981). The speciation of iodine in Loch Etive. NATO Fiord Workshop.
- Gilman, K. (1975). Application of a residence time model to dilution gauging with particular reference to the problem of changing discharge. *Hydrol. Sci. Bull.*, 20, 523-537.
- Gilman, K. (1977). Dilution gauging on the recession limb: I - Constant rate injection method. *Hydrol. Sci. Bull.*, 3, 353-369.
- Gilman, K. (1977). Dilution gauging on the recession limb: 2 - The integration method. *Hydrol. Sci. Bull.* 22, 4, 469-481.

- Moore, R J. (1971). Dynamic aspects of water quality modelling, PTRC course on 'Modelling of Water Resource Systems', 14-18 November.
- Moore, R.J. and Jones, D.A. (1978). Coupled Bayesian-Kalman Filter estimation of parameters and states of a dynamic water quality model, in Chiu, C (Ed), Applications of Kalman filtering to hydrology, hydraulics and water resource Proc. AGU Chapman Conference, Pittsburgh, USA, 599-635.
- Moore, R.J. and Venn, M.W. (1979) The CAPTAIN package for recursive time series modelling, in Adey, A A (ed), Engineering Software, Proc. 1st Int. Conf., Southampton University, Pentech Press, Rendon.
- Moore, R.J. (1978). Recursive estimation procedures for dynamic water quality models, UNESCO workshop on Progress in the application of systems analysis to environmental management and engineering, Udine, Italy. 13-16 December.
- Neal, C. and Truesdale, V.W. (1976). The sorption of iodate and iodine by riverine sediments: its implications to dilution gauging and hydro-chemistry of iodine. J. Hydrology, 31, 281-291.
- Neal, C. (1977). The determination of adsorbed Na. K. Mg and Ca on sediments containing  $\text{CaCO}_3$ . Clay and Clay Minerals, 25, 253-258.
- Neal, C. and Jordan, P, (1978) Iodide and lithium tracers in chemical dilution gauging of storm sewers. IH report 50.
- Neal, C. (1979) Arsenic in sediments of the North Atlantic Marine Chem. 7, 207-219.
- Neal, C. (1979) Major exchangeable cations of rivers and marine clays. Inst. Int. Conf. on Cohesive Sediments, Cambridge, England, 1-10.
- Neal, C., Thomas, A.G. and Truesdale, V.W. (1982) in press. The thermodynamic characterisation of clay electrolyte systems. Clays and Clay Minerals.
- Roberts, G., Blackie, J.R., and Hudson, J., (1979). The effect of land improvement on the discharge from upland pastures. Interim Report by MAFF.



- Roberts, G., Blackie, J.R. et al. (1979). The effects of agricultural practices on the discharge from a lowland catchment. Interim Report to MAFF.
- Raiswell, R.W. and Thomas, A.G. (in press). Solute acquisition in glacial meltwaters. I. Fjallsjökull (SE Iceland): Bulk meltwaters with closed system characteristics. J. Glaciology.
- Smith, P.J. The numerical computation of streamflow and its error using constant rate injection method of dilution gauging. IH Report 38
- Smith, P.J., Gilman, K and Greenland, P.C. (1977). Measuring the flow of the River Avon using the constant rate dilution gauging method. IH Report 45.
- Thomas, A.G. and Raiswell, R.W. (in press). Solute acquisition in glacial meltwaters II. Argentière (French Alps): Bulk meltwaters with open system characteristics. J. Glaciology.
- Thomas, A.G., Truesdale, V.W. and Neal, C. (1982 in press). The heterogeneous distribution of anions and water around a clay surface with special reference to estuarine systems. Transfer Processes in Cohesive Sediment Systems.
- Truesdale, V.W. (1973). The factors controlling the natural chemical composition of rivers - a critical review. Proc. Challenger Soc., IV (5).
- Truesdale, V.W. (1975). "Reactive" and "Unreactive" iodine in seawater - a possible indication of an organically bound iodine fraction. Marine Chem., 3, 111-119.
- Truesdale, V.W. and Smith, C.J. (1975). The spectrophotometric characteristics of aqueous solutions of  $\alpha$  and  $\beta$  molybdosilicic acids. Analyst, 100, 797-805.

- Truesdale, V.W. and Chapman, P. (1976). Optimisation of a catalytic procedure for the determination of total iodine in sea water. *Marine Chem.*, 4, 29-42.
- Truesdale, V.W. and Smith, C.J. (1976). The automatic determination of silicate dissolved in natural fresh waters by means of procedures involving the use of either  $\alpha$ - or  $\beta$ - molybdosilicic acid. *The Analyst*, 101, 1931.
- Truesdale, V.W., Smith, C.J. and Smith, P.J. (1977). Transformation and Decomposition of  $\beta$ -Molybdosilicic Acid. *The Analyst*, 102, 73-85.
- Truesdale, V.W. (1978). The automatic determination of iodate and total iodine in sea water, 6, 253-273.
- Truesdale, V.W. (1978). Iodine in inshore and offshore marine waters. *Marine Chem.*, 6, 1-13.
- Truesdale, V.W., Smith, P.J. and Smith, C.J. (1979). The kinetics of molybdosilicic acid formation. *The Analyst*, 104, 897-918.
- Truesdale, V.W. and Smith, C.J. (1979). A comparative study of three methods for the determination of iodate in sea-water. *Marine Chem.*, 7, 133-139.
- Truesdale, V.W., Neal, C, and Thomas, A.G. (1982 in press). A rationalisation of several approaches to clay/electrolyte studies. *Transfer Processes in Cohesive Sediment Systems*.
- Waring, R.H. and Roberts, J.M. (1979). Estimating water flux through stems of scots pine with tritiated waters and phosphorus-32. *Jour. Expt. Bombay*, 30, 459-471.

- Wellings, S.R. and Bell, J.P. (1980). Movement of water and nitrate in the unsaturated zone of Upper Chalk near Winchester, Hants, UK. Jour. of Hydrology.
- Wellings, S.R. and Bell, J.P. (1980). Water and nitrate fluxes in unsaturated Upper Chalk at Bridgets Experimental Husbandry Farm, Winchester, UK. UNESCO Helsinki Symposium, June 1980.
- Wellings, S.R. (1982). The use of deuterium oxide as a water tracer in a study of the hydrology of the unsaturated zone of the English Chalk. Anal. Chem. Symp. Series, 11, 167-171. Elsevier, Amsterdam.
- Whitehead, P.G. (1977). Water quality models for waste water management. UNESCO Conference on Impact of Urbanisation on Water Resource Systems.
- Whitehead, P.G. (1977). Mathematical modelling and the planning of environmental studies. CRES Report AS/R15.. (to be published in Simulation of Land Air and Water Resource Systems) (ed Vansteenkiste) American Elsevier, North Holland.
- Whitehead, P.G. (1978). Modelling and operational control of water quality in river systems. Water Research, 12, 337-384.
- Whitehead, P.G., Young, P.C. and Michell, P. (1978). Some hydrological and water quality modelling studies in the ACT region. Australian Institute of Engineers Hydrology Conference Proceedings.
- Whitehead, P.G. and Young, P. (1979). Water quality in river systems: Monte-Carlo Analysis. Water Reserources Research, 15, 451-459.

- Whitehead, P.G. and O'Connell, E. (1979). Water quality modelling of water resource systems: A proposal for a collaborative project. IH Internal Report.
- Whitehead, P.G. and Caddy, D. (1979). Real time forecasting of water quality in river systems.
- Whitehead, P.G. (1980). Real time monitoring and forecasting of water quality in river systems. Hydrological Sciences Bulletin, IAHS, Publ. No. 129.
- Whitehead, P.G. (1980). Water quality modelling for design, UNESCO Helsinki Conference, Hydrological Science Bulletin, No 130.
- Whitehead, P.G. (1980). An instrumental variable method of estimating differential equation models of dispersion and water quality in non-tidal rivers. J. Ecological Modelling.
- Whitehead, P.G. (1980). Papers presented at Water Quality Modelling Workshop, Melbourne, Australia.
- (a) River Quality Modelling
  - (b) An Introduction to Time Series Analysis Techniques and Dynamic Modelling.
  - (c) Use of Time Series Analysis Techniques to Analyse Flow and Quality Data.
  - (d) Dynamic Modelling of River Water Quality.
  - (e) Application of Dynamic Water Quality Models.
- Whitehead, P.G. (1981). Operational Management of Water Quality in River Systems. First Report to EEC (Contract ENV 400-80 UK(B)).
- Whitehead, P.G. and Beck, M.B. (1981). A systems model of flow and water quality in the Bedford Ouse River system: Part II, Water Quality Modelling. Water Research, 15, 1157-1171.

Whitehead, P.G. and Williams, R.J. (1981). A dynamic nitrate-nitrogen balance model for river basins, IAHS Conference, Exeter 1982.

Whitehead, P.G. and Leck, T. (1981). UNESCO Book, Dispersion and Self Purification of Pollutants in Surface Water Systems.

Whitehead, P.G. (1981). A review of the Albert and Campine canals modelling study, University of Brussels Report.

Whitehead, P.G. and Caddy, D.E. (1981). Practical Techniques of River Monitoring and Pollution Forecasting, Part II: Data Processing and Modelling, Effluent and Water Treatment Journal, June 1982.

Whitehead, P.D., Beck, M.B. and O'Connell, P.E. (1981). A systems model of flow and water quality in the Bedford Ouse river system, II: Water quality modelling. Water Research Vol. 15.

Whitehead, P.G. and Williams, R.J. (1981). The River Thames water quality model - progress report to Thames Water Authority.

Whitehead, P.G. and Hornberger, G.E. (1981). Modelling algal behaviour in river systems. IFIP Conference Proceedings, Rome.

Whitehead, P.G. and O'Connell, P.E. (eds) (1982). Water quality modelling, forecasting and control. Proceedings of IH Workshop.

- Whitehead, P.G. (1982). Long term prediction and short term forecasting of water quality changes in river basins. UNESCO Workshop on Water Quality Modelling, Spain.
- Whitehead, P.G., Williams, R.J. O'Conne, P.E., Balck, R.J., Templeman, R.F. Gray, R. (1982). Operational management of water quality in river systems. Final Report on Contract ENV 400-80 UK(B).
- Wikramaratna, R.S. and Wood, W.L. (1981). On the Coupled Equations of the Groundwater Quality Problem in Numerical Methods for Coupled Problems - Proceedings of the International Conference held at University College, Swansea. September 1981. Pineridge Press.
- Wikramaratna, R.S. (1981). The Flow of Groundwater in a Coastal Aquifer. MSc Dissertation, University of Reading.
- Wikramaratna, R.S. and Wood, W.L. (in press). Control of Spurious Oscillation in the Saltwater Intrusion Problem. Submitted to the International Journal for Numerical Methods in Engineering (March 1982).
- See also appendix 4, where a list is given of overseas repayment studies containing a water quality/hydrochemistry component.

APPENDIX 6

The role of IH in water quality modelling (a preliminary review)

by P E O'Connell

## CONTENTS

### SUMMARY

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- ON THE ROLE OF IH IN UK WATER QUALITY RESEARCH



## SUMMARY

In recognition of the problems posed by deteriorating water quality, hydrological research has in recent years been concerned with both water quantity and quality within the hydrological cycle. This development is reflected in the current research programme of IH which has over a number of years been developing an in-breadth and in-depth approach to the integrated treatment of quantity and quality.

The main thrust of the IH work is towards the development of integrated models of flow and quality; this is designed to build on an extensive modelling capability acquired over many years, and to bring this expertise to bear on the challenging water quality problems of today. In this context, a distinction is drawn between descriptive models which seek to provide fundamental insight into the behaviour of water quality in time and space, and prescriptive models which are designed to assist in identifying cost-effective water quality management strategies.

The paper, in describing our past experience and current aspirations sets out the role of IH within the full spectrum of water quality-oriented resource studies. There is an area that is very clearly identifiable as a WRC preserve and this concerns chemical and biological studies which aim to be descriptive of processes within sewage treatment, water purification, and natural river systems. Into this area IH would never wish to trespass.

However, such research does not stand in isolation, and it does seem to us that the extension of these primary research results in certain application areas is an entirely valid field for hydrological endeavour. Where the nature of the problem is such that total system modelling is needed, then the hydrologist's experience of operational research techniques, his familiarity with the statistical nature of the variables, and most of all the merging of quality and quantity determinands for the purpose of decision making, renders it more than arguable that the hydrologist must make an important

contribution. It has to be admitted that a grey area exists in descriptive modelling of some natural river processes where traditional hydrological interest in sediment, bed load movement and water temperature brings him very close to water quality matters. For the most part we endeavour to show by example the many areas where hydrology in general and IH in particular can contribute to water industry activities in quality fields that complement, rather than duplicate or compete with WRC expertise.

On the descriptive side, process studies of the movement of nitrates in the unsaturated zone, and of the hydrodynamics of sediment/water interactions are leading to a more fundamental understanding of some basic problems; these studies also underpin the development of deterministic distributed water quality models which offer the main hope for understanding the movement of pollutants at the catchment scale. Here, a solid foundation has been provided by the availability of distributed rainfall-runoff models developed over many years at IH, and water quality has been monitored over several years on IH experimental catchments to support this work.

On the prescriptive modelling side, IH can offer a number of approaches depending on the problem at hand and on the data which are available. Dynamic water quality models are seen as greatly supplementing the use of conventional steady-state models, particularly in solving problems which derive from the transient violation of water quality standards, by modelling the time history of flow and quality at various points in a system; IH at present has an extensive capability in identifying, calibrating and applying these models which seek to draw on the existing knowledge of physical, chemical and biological mechanisms and represent these at the field scale. The uncertainty in model predictions deriving from the imperfect representation of the real world by the model is also explicitly quantified.

In many situations, the more detailed information provided by the dynamic modelling approach may not be necessary, and summarizing statistical information may suffice, particularly when there may

be no measured information on water quality at a point of interest. IH has carried out several studies to provide on a national scale summary statistics of water quantity, the Floods Study and Low Flows Study being good examples. Work is currently in hand to extend this approach to both flow and quality; exploratory studies involving the use of flow descriptors from the Low Flow Study have been carried out in conjunction with the Southern Water Authority and Freshwater Biological Association.

All of the above studies can draw on considerable supporting expertise available at IH; in this context, the IH hydrochemistry group set up in 1972 (and recently reinforced by the IGS hydro-geochemistry group), can offer valuable support either through direct chemical guidance or routine laboratory facilities. Other supporting areas in which IH is strong are instrumentation, the design of sampling experiments and data base management.

The relevance of IH expertise to water quality problems has been recognised by a number of Water Authorities and other organizations in the UK; for example, dynamic water quality models for real-time management are currently under development by IH for the AWA, and another study is under negotiation with TWA. This suggests that a role exists for IH in UK water quality research, a role which is seen as complementing rather than duplicating or conflicting with, that of WRC.

## On the role of hydrological modelling in water quality research

The environmental problems associated with deteriorating water quality have in recent years resulted in a gradual worldwide shift in hydrological research from modelling the movement of water quantity in the hydrological cycle to modelling both water quantity and quality. The research effort currently being deployed in this area was represented in a recent symposium organized by the International Association of Hydrological Sciences on 'Modelling the Water Quality of the Hydrological Cycle' held in Baden, Austria in September, 1978. To maintain its position as a leading research institute in its field, IH has therefore in recent years had to undertake studies in which water quality is considered. In particular, the comprehensive range of hydrological models available at IH is being extended to include water quality explicitly; inevitably it has been necessary to acquire the supporting expertise to do this.

The deterioration of water quality in a river system over time is invariably associated with increasing levels of pollutants; in this context two types of question may be posed:

- (i) why are pollutant levels continuing to increase, and will they continue to do so?
- (ii) what are the most cost-effective management strategies that can be adopted to offset the deterioration in water quality and ensure that desired water quality standards can be maintained?

The problem of nitrate levels in surface waters elicits both types of question. While a comprehensive answer to the first question has not as yet been obtained, some water authorities are already having to consider the second question and extensive capital investment will be necessary over the next ten years to maintain the recently stipulated EEC standards if present trends in nitrate levels continue.

In relation to the above questions, two distinct modelling approaches may be identified. In addressing questions of type (i), descriptive models are required in which the physical, chemical and biological processes through which pollutants are transformed, transported and dispersed in their passage over and through the soil, in the groundwater zone and in stream channels are described in full. The degree of detail and complexity associated with descriptive models is not a prerequisite to providing answers to questions of type (ii); here the structure of the model and its level of complexity will reflect the particular objective associated with model use, thus earning it the title of prescriptive model. For example, a relatively simple input-output mass balance model could be used to describe the relationship between upstream and downstream water quality in a river reach and provide adequate short-term forecasts for effective operational management. Extensive use is made of systems analysis techniques in identifying and fitting prescriptive models.

Over the years, IH has developed a wide spectrum of models for describing the behaviour of water quantity in time and space; these models have either been descriptive in providing important insight into the behaviour of hydrological processes and systems, or prescriptive in that they have been used to aid decision-making in the planning and management of water resources.

Current research at IH is involved with the development of both descriptive and prescriptive models in which water quantity and quality are coupled. This note outlines the problems which these models can resolve and demonstrates that IH has the necessary supporting expertise to develop integrated water quantity/quality models. Furthermore, in the context of the national research effort in water quality, IH has unique expertise to offer, to complement rather than duplicate or conflict with, the research efforts of WRC.

## 2. On the IH capability in water quality modelling

### 2.1 Fundamental process studies

Studies are currently being undertaken at IH in which the behaviour of water quality within individual component processes of the hydrological cycle is being explored; these studies are directed towards answering questions of type (i) and underpin water quality modelling studies on the catchment scale.

#### (a) Nitrate movement in the unsaturated zone.

The Institute is involved in several studies of the processes of nitrate movement, both in the soil surface zones in situations where lateral runoff is important (lysimeters at Plynlimon) and in the unsaturated zone of the all-important chalk aquifers. Nitrate movement and distribution is being studied and modelled in conjunction with unsaturated water flux measurements in the upper chalk at Bridgets Experimental Husbandry Farm (MAFF funded) and at Fleam Dyke (DOE funded, in conjunction with IGS, terminating in April 1980).

IH is probably the only body in the UK performing nitrate studies in which chemical and physical measurements are made simultaneously and intensively at specific sites over long periods and with controlled fertilizer regimes. A proposal to expand this work further in conjunction with IGS by including a microbiologist is under consideration. In the meantime IH is collaborating with Oxford University Agricultural Sciences Department in their two CASE studentships, in which water movement and the biological process of nitrification and denitrification are being studied at their Wytham, Oxford, clay site.

#### (b) The hydrodynamics of fluvial sediment/water interactions

This work has arisen as a natural extension of the Institute's past work on the theoretical and practical aspects of chemical dilution gauging. In some gauging exercises, significant losses of tracer to the suspended material have been observed. This has led to the setting up of a study to investigate the role of

hydrodynamic dispersion in sediment/water interactions; this work is particularly relevant to heavy metals, and complements geochemical work on sediments carried out at Imperial College for DOE in which hydrodynamic aspects have not been considered.

## 2.2 Catchment experiments involving water quality

Since 1976, IH has been monitoring a number of water quality determinands on some of its experimental catchments. For the headwater catchments of the Wye and Severn, nutrient concentrations are being monitored on a daily, and at high flows, hourly basis; the objective is to quantify any significant difference in the concentrations from forest and grassland.

Nutrient concentrations are also being monitored for a 172 hectare catchment at Shenley Brook End in Milton Keynes, Bucks. Here the main objective is to relate nutrient levels in streamflow to agricultural practices including fertilizer application in an intensively farmed area.

All of the above catchment experiments are being funded by MAFF.

## 2.3 Deterministic distributed water quality modelling

IH has over many years been developing deterministic distributed rainfall-runoff models of catchment behaviour; here the term 'deterministic' implies that the behaviour of the real world can be represented exactly by known physical relationships. Such models are a pre-requisite to studying the movement of pollutants on a catchment scale; classical lumped catchment models cannot cope with distributed sources of pollutants. In the case of nitrates, individual process studies are currently in progress which relate to the movement of nitrates over the soil, and in the saturated and unsaturated zones. However, it is unlikely that a complete answer to type (i) questions can be obtained on a catchment scale without employing deterministic distributed models in which the equations describing flow and quality are solved on a three-dimensional finite difference grid representation of the catch-

ment. The structuring of these models will utilize the results from the process studies described above; the data collected from the catchment experiments will allow nitrate questions to be investigated initially.

#### 2.4 Dynamic-stochastic water quality models

All of the above studies are oriented towards the development of descriptive models which can be used to address questions of type (i). In this and the following section, the modelling approaches to be described can be regarded as specific to type (ii) questions; they are discussed in the context of specific water quality management problems which they could be used to solve.

In the UK, there has been considerable emphasis in the past on the use of steady-state water quality models for use in long-term planning. However, many problems in water quality management today derive from transient violations of water quality standards which are governed as much by the hydrological behaviour of a system as the discharge of pollutants at various points within it. As water quality standards are now often considered in terms of the percentage of time for which the standards must be maintained, it follows that dynamic water quality simulation models must in the future occupy an important role in the management of water quality.

In applying a model to a management problem, it is important to recognise that the model is at best an imperfect representation of 'real-world' behaviour, that model simulations and forecasts are subject to error, and that decisions based on the model will be subject to uncertainty. A model which explicitly recognises the presence of this error is termed a stochastic model; models which also represent the dynamic interaction between flow and quality are termed dynamic-stochastic water quality models.

There are two situations in which dynamic-stochastic water quality models could be employed:



- (i) to supplement the use of steady-state models at the planning/design stage in carrying out more detailed investigations of alternative system designs. Specifically, dynamic models would be used to evaluate the efficacy (ultimately measured in terms of cost-effectiveness) of a design in maintaining standards at various points in a system and of exploring some of the subtle effects which can occur over time (eg the build-up of a pollutant in a pumped-storage reservoir through continued recycling of water). A typical time unit for such models would be one day; water quantity simulation models on this time-scale have been used for several years in evaluating the reliability of systems for water supply.
- (ii) to assist in the short-term operational control of river systems. The increasing use of automatic water quality monitors and telemetry now means that there is considerable scope for using short-term forecasts of water quality for decision-making. An obvious application is the forecasting of water quality at a water supply off-take due to the accidental discharge of a pollutant upstream.

The Institute of Hydrology has over the years built up an extensive capability in modelling the dynamic-stochastic behaviour of hydrological systems. Depending on the problem at hand, such models can incorporate as much of the physics of system behaviour as is considered necessary, or can employ simple input-output relationships which require a minimum of modelling effort. Sophisticated statistical tools, programmed into computer packages, have been applied in the identification and calibration of these models from field data; these tools allow uncertainties in model predictions and forecasts to be quantified, thus accounting for the term 'stochastic'. Recently, the increasing use of telemetry has led to the development of models and forecasting techniques which can be run on mini/micro-computers and which utilize new information efficiently as it becomes available in real-time.

Dynamic-stochastic water quality models require descriptions of the interactions between chemical variables, biological components and hydrological aspects. It is not the intention of IH to carry out research into the detailed chemical/biological interactions that obtain; in fact much work has been done at the laboratory scale at WRC to establish these mechanisms. Rather, the intention is to identify, from field data, these mechanisms which dominate at the catchment/river-basin scale and to estimate the values of the various model coefficients. Most of the water quality modelling work carried out in the past in the UK has tended to incorporate mechanisms and coefficients determined at the laboratory scale directly into models at the field scale. In employing the IH approach, extensive use would be made of tracer experiments to determine travel times (an existing capability already referred to above) as well as the existing expertise in modelling and in implementing models on small mini/micro-computers when this is relevant.

The field of dynamic water quality modelling is one which has been gaining increasing popularity internationally in addressing water quality management problems. In fact, one of the first comprehensive studies of its viability was carried out on the Bedford Ouse during the period 1971-75 as part of a study funded by DOE. There the prime intention was to explore the effect on water quality at the water supply abstraction point at Bedford of the development of the new city at Milton Keynes upstream. Since then, several similar studies have been carried out in Australia. The principal investigator on the Bedford Ouse Study joined IH in 1978, and further development work has ensued to broaden the scope of the approach.

## 2.5 Studies concerned with the statistical description of river water quality characteristics

The dynamic-stochastic water quality modelling approach described in the previous section is aimed at providing the complete time history of flow and water quality at various points in a system.

However, there are situations where summarizing information is all that is required to solve specific problems; further, there may be no measured information on water quality at a point of interest. The statistical studies summarized below are designed to have modest computational requirements for ultimate application.

(a) The probability distribution of water quality measures downstream of a point source of pollutant

The objective of the study would be to ascertain what set of inputs, ie percentiles of upstream river water and effluent quality and quantity, to use in order to give a downstream distribution for which a desired water quality standard is maintained for 95% of the time. This is the percentile point which is employed in granting consents for effluent discharge and river quality objectives. The application of the technique in its full form has modest data requirements and moreover by relating the primary variable such as a percentile of river flow distribution to catchment characteristics, the method's use can be extended to the ungauged or partially gauged site.

(b) Relating water quality parameters to catchment characteristics

A pilot study has been proposed to appraise the potential of existing and new small catchment experiments for providing the necessary data to establish prediction equations relating water quality parameters, particularly the mean and variability of the level of nitrates or other agricultural nutrients, to land use and other characteristics of the catchment and stream network. The study is geared to estimate the practicality and costs of running such experiments for 5-10 years at sufficient sites to sample meaningfully from the range of climate, land use, slopes and other variables. This project has been the subject of discussions with WRC and D of E officers and has received a high priority and favourable report from Triad D.

(c) Application of hydrograph analysis to water quality

Liaising with water quality staff in the water industry has shown that much greater use can be made of river flow data in solving

their problems; techniques developed for analysing aspects of hydrograph behaviour, e.g. the number of consecutive days when flow remains below a threshold, can be applied directly to water quality work.

Ideas have been mooted to combine hydrograph analysis with water quality determinands to yield a descriptor of the quantity/quality regime which is potentially very powerful. A good example is the base flow index which was developed in a study at IH for estimating, inter alia, statistics of low river flows at ungauged sites. The most frequent application of this work has been in estimating dilution rates for sewage effluent. River Purification Boards and several Regional Water Authorities are using the results of this research in water quality work including sewage works review and design. IH has been closely involved in applying the techniques in the Southern Water Authority area.

The Freshwater Biological Association are studying the relationship between the physical and chemical factors which control river communities in the United Kingdom and a second project is studying the relationship between trout populations and water quality and quantity regimes in Teesdale. In both these areas of research the Institute of Hydrology has been involved and in the former project preliminary results have shown the success of an index of base flow in predicting the variety and type of invertebrate communities.

(d) Description of river water temperature in the United Kingdom

The temperature of river water is an important background variable against which many operational decisions are made, several of which concern water quality. The temperature regime impinges on such problems as suitability of the river for fisheries, for abstractions, for sources and sinks for industrial and energy applications, and for biological studies. Despite a considerable network and history of temperature measurements there is surprisingly no national map showing averages and variability, nor

seasonal fluctuations. Apart from its use in decision-making river water temperature provides a useful 'tracer' helping to identify the source of the water. The proposed study would combine deterministic modelling based upon the energy budget with statistical analysis.

The above four studies draw on the expertise that has been acquired in the Applied Hydrology Division at IH from the Floods and Low Flows Studies. The latter study will provide the basic description of flow for (a) and (c) while the problem of deriving an output distribution from input distributions in (a) has previously been solved in another context. Extensive experience already exists in handling large data sets and in relating flow parameters to catchment characteristics.

## 2.6 Supporting expertise

### (a) Hydrochemistry studies

The preceding sub-sections have drawn attention to the water quality modelling capability at IH. This, reinforced by the presence, at IH, of a strong hydrochemistry research section established in 1972 to study the chemistry of natural waters has recently been enhanced by the transfer to Wallingford of the IGS hydro-geochemistry research unit. This combined expertise, which must make the NERC Wallingford site a major centre for hydrochemistry in the UK, is available to underpin the various modelling studies described above, by providing either direct chemical guidance or routine laboratory facilities.

To date the IH hydrochemistry studies have focussed upon both the speciation of elements in natural waters and the problems of water/sediment interactions. Of course, the speciation work has required an overall appreciation of biological systems and their relevant interactions (assimilation/regeneration) with nutrient material. Indeed, this is particularly evident in the latest work which has involved modelling iodine (as iodate and iodide species) in marine systems as a quasi-nutrient. While admittedly the

hydrochemical nature of this work demands that it be outside the area of direct concern. here, the general experience gained is, nevertheless, of direct relevance.

(b) Instrumentation

The capability of IH in developing instrumentation is evidenced by its automatic weather station and soil moisture neutron probe which are arguably the most successful of their kind developed anywhere. This experience in developing instrumentation to operate effectively under the difficulties and extremes associated with environmental monitoring, could contribute significantly to the development of more reliable automatic water quality monitors. Attention is currently being paid to exploiting the potential of microprocessors in environmental monitoring and control in the future.

(c) Design of sampling programmes and data base management

Water quality studies invariably involve the collection and processing of large bodies of data; it is of paramount importance that the data are sampled at the appropriate points in time and space to enable the objectives of a particular modelling study to be achieved. IH have considerable expertise in experimental design as well as dilution gauging; both are relevant to establishing appropriate sampling points in river systems. IH have been involved in several studies involving the management of country-wide data sets; the quality control, data base management and computing expertise which have been acquired are particularly relevant to the large data sets associated with water quality studies.

On the role of IH in UK water quality research

Hopefully the above will have provided an appreciation of the scope of the water quality modelling expertise available at IH.

The relevance of this expertise has been recognised by a number of Water Authorities and other organizations in the UK. Recently, the AWA have approved a collaborative project with IH to apply dynamic-stochastic water quality models to an existing monitoring and telemetry scheme on the Bedford Ouse. The models will provide on-line forecasts of flow and water quality for pollution inspectors in the Great Ouse River Division and will aid the control of water quality at the Bedford Waterboard Abstraction Plant.

Thames Water Authority are also involved in negotiations with IH to develop dynamic-stochastic water quality models which can be used in exploring alternative strategies for the management of nitrate levels in surface water within the Thames system. WRC have expressed interest in funding the IH work on the movement of nitrates in the unsaturated zone, as have the CEGB in the deterministic distributed modelling of the movement of  $SO_2$  within snowpacks in Norway in relation to game fish-kills.

Some of the current water quality problems in the UK are so challenging that no single organization could be said to possess the full range of expertise relevant to solving these problems. This is recognised by IH who, in defining problem areas for study, have considered only those problems for which they have the relevant expertise at hand. A much more comprehensive approach to other problems could be achieved by capitalising on the strength of IH in water resource modelling by feeding into them the most recent WRC water quality research. IH has no intention of moving into the descriptive modelling of chemical and biological processes below sources of effluents; it is perhaps unfortunate that the use of the term 'water quality' in project proposals is sometimes taken to imply that it is.