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Natural Environment Research Council

RQFS
A RIVER QUALITY FORECASTING SYSTEM

SYSTEMS ANALYSIS

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Executive Summary

This Systems Analysis study investigates the feasibility of extending the River Flow Forecasting System, or RFFS, used currently to forecast flows and levels throughout Yorkshire's rivers, to also forecast water quality variables. The Institute of Hydrology's Quasar water quality model is examined as a possible basis to provide the underlying model structure. A solution based on combining the KW flow routing model equation, used within the RFFS, with the Quasar water quality equations is proposed.

Incorporation of a new model within the RFFS is made straightforward through the adoption of a generic model algorithm interface in the original design of the RFFS's Information Control Algorithm, responsible for coordinating forecast construction in real-time. The task of developing a water quality Model Algorithm is pursued and significant progress made. Problems with the code structure of the pre-existing Quasar model are identified and work undertaken to create a "streamlined" version suitable for real-time use as an RFFS Model Algorithm. Work on the coding is sufficiently advanced to confirm the functional feasibility of extending RFFS to make water quality forecasts.

The success of a water quality forecasting system depends, in addition to the modelling environment, on both the suitability of the model structure and the data available to support calibration and operational implementation. Problems likely to arise are exposed through a case study on the Aire through Leeds. The availability of suitable data to support the calibration of a dynamic model is seen as an important problem. Programmes for additional tracer experiments in the short-term and more extensive continuous monitoring in the longer-term are recommended. The configuration of existing flow routing models on the Aire are examined and this reveals a need for a more consistent approach to support both water quantity and quality forecasting.

The main conclusion of the study is that the RFFS provides an ideal modelling environment for both flow and water quality forecasting in real-time. Recommendations for further work are given, which include the need to proceed with the implementation of RQFS in a case study area supported by further tracer experiments and monitoring. Further work on modelling is proposed including consideration of other model formulations and the use of ensemble forecasting to help delimit the range of uncertainty in forecasts. The latter would be of particular help in a decision support context.

Preface

This report has been prepared for the National Rivers Authority Yorkshire Region, now the Northumbria and Yorkshire Region, by the Institute of Hydrology under sub-contract to Logica Industry Ltd. The work has been undertaken by Mr R.J. Moore, Head, Systems Modelling Group, and by Mr R.J Williams, Head, Pollution Hydrology Section at the Institute of Hydrology.

Thanks are due to Mark Tinnion who served as NRA Project Manager, and to Richard Freestone and Adrian Barraclough (Environmental Modelling) who were the main customers and served on the project steering committee. Their enthusiasm for the project was especially appreciated along with helpful guidance on water quality management in Yorkshire and support in providing data and other information to advance the study.

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1. Introduction

The River Flow Forecasting System, or RFFS, has been developed in a generic way to allow not only reconfiguration to other river systems but extension to make forecasts of variables other than river level and flow. A generic model algorithm interface is provided within the RFFS to accommodate new models: these may be improved models of flow in rivers but may equally be models of other variables. It is natural to consider an extension to accommodate the quality of water in addition to the quantity of water at the selected forecast points. The purpose of this report is to examine the feasibility of extending the RFFS to incorporate water quality variables. It also considers the feasibility of implementing this River Quality Forecasting System, or RQFS, to the rivers in Yorkshire.

Section 2 presents an outline of the differential equations used to represent flow and water quality in IH's Quasar model. Analytical solutions to these equations are included as the Appendix to this report. The flow model is compared with the KW channel routing model used in the RFFS and implications for implementation discussed. Section 3 discusses the task of incorporating the Quasar equations into the RFFS as a water quality model algorithm. Section 4 considers an example implementation of the model algorithm, using the River Aire through Leeds as a case study to investigate the nature of the task and expose any possible difficulties. Finally, Section 5 presents a summary and major conclusions of the study along with a set of recommendations. Included as Annexes are the project proposal for the study, a project meeting report and a document inventory.

2. Water Quality Modelling in the RQFS

2.1 INTRODUCTION

Quasar provides representations for nine water quality variables together with river flow. This Section provides an overview of the representations used. The major processes involved are outlined along with the assumptions underlying the model formulations. When dealing with river flow, the formulation used within the RFFS is introduced along with that used in Quasar, and the implications for RQFS implementation are considered.

2.2 RIVER FLOW

This sub-section begins with an outline of the KW (kinematic wave) channel flow routing model employed within the RFFS. The basic form of the model is introduced focusing on its derivation from both the kinematic wave model and from simple storage principles. This is followed by a review of the channel flow model used within Quasar. The similarities and differences with the KW model are established with reference to the derivation of each model from storage principles and the method used to solve the resulting model equations. Finally, the implications of the two channel flow routing formulations on the RQFS implementation are discussed.

The KW model formulation begins with the 1-D kinematic wave equation in partial differential equation form where channel flow, q, and lateral inflow per unit length of river, u, are related through

$$\frac{\partial q}{\partial t} + c\frac{\partial q}{\partial x} = cu \qquad (2.2.1)$$

where c is the kinematic wave speed. Consider time, t, and space, x, to be divided into discrete intervals Δt and Δx such that k and n denote positions in discrete time and space. Invoking forward difference approximations to the derivatives in (2.1) we have

$$q_k^n = (1-\theta)q_{k-1}^n + \theta\left(q_{k-1}^{n-1} + u_k^n\right) \qquad (2.2.2)$$

where the dimensionless wave speed parameter θ = c Δt/Δx and $0 < \theta < 1$. This is a recursive formulation which expresses flow out of the n'th reach at time t, q^n_k, as a linear weighted combination of the flow out of the reach at the previous time and inflows to the reach from upstream (at the previous time) and as the total lateral inflow along the reach (at the same time). If the stretch of river to be modelled has length L, and is subdivided into N reaches of equal length, so Δx = L/N, then a condition for stability is that c < L/(N Δt).

An alternative derivation of equation (2.2.2) can be sought from a simple hydrological storage approach. The n'th reach can be viewed as acting as a linear reservoir with its outflow related linearly to the storage of water in the reach such that

$$q_k^n = \kappa\ S_k^n, \tag{2.2.3}$$

where κ is a time constant with units of inverse time. If S^n_k is the storage in the reach just before flows are transferred at time k then continuity gives

$$S_k^n = S_{k-1}^n + \Delta t\left(q_{k-1}^{n-1} - q_{k-1}^n + u_k^n\right) \tag{2.2.4}$$

and the equivalence to (2.2.2) follows, given $\theta = \kappa\ \Delta t$.

The channel flow routing model used to represent river flow in Quasar is based on the continuity equation and a simplified momentum equation. Specifically, a reach of river having a storage S, an outflow q and an inflow u can be described by the continuity equation

$$\frac{dS}{dt} = u - q \tag{2.2.5}$$

where dS/dt represents the rate of change of storage and t is time. It is then assumed that discharge, q, varies with storage such that

$$q = kS \tag{2.2.6}$$

where k is a time constant with units of inverse time. The reciprocal quantity, $\tau = k^{-1}$, is commonly referred to as the reach residence time. Immediately the correspondence between κ in the KW model and k in the Quasar model can be recognised. Combining equations (2.2.5) and (2.2.6) gives the linear form of the Horton-Izzard equation (Dooge, 1973, Moore, 1983)

$$\frac{dq}{dt} = k(u - q). \tag{2.2.7}$$

The time constant k is expressed in terms of the reach length, L, and the mean reach velocity, v, such that

$$k = vN/L \tag{2.2.8}$$

where N denotes the number of sub-reaches present over the reach length L. Again note the equivalence of L/N to Δx and of k to c/Δx. It is further assumed that the mean velocity, v, is related to discharge q through a relation of the form

$$v = \alpha + \beta q^{\gamma} \tag{2.2.9}$$

where α, β and γ are parameters. Invariably, α in applications of Quasar is set to zero. In this case substitution in equation (2.2.7) gives the nonlinear Horton-Izzard equation

$$\frac{dq}{dt} = a(u - q)q^{b} \tag{2.2.10}$$

with a = βN/L and b = γ. Note that analogous generalisations are available for the KW model where the dimensionless wave speed θ is allowed to vary as a cubic function of discharge (or other functions provided).

The two models differ most radically in terms of the solution scheme employed. The simple discrete solution used in the KW model has been described above. In contrast the scheme used in Quasar is based on a solution of the linear Horton-Izzard equation using a constant value of k calculated from the discharge at the start of the solution time interval. The value of k is recalculated at the start of each solution time step based on the new initial discharge. Solution is accomplished using either a variable step-size Runge-Kutta numerical scheme for solving the ordinary differential equation or using the analytical solution of the linear Horton-Izzard equation. A feature of the scheme used is that an immediate response results to an input to the reach. In contrast the KW scheme results in a pure time delay for each sub-reach present and is considered more realistic. This advantage is particularly important when the flow model is used to underpin a water quality model. Then it is important that a time delay mechanism operates so that the effects of a pollution pulse is not immediately seen at the downstream end of a reach.

In applications of Quasar, the boundaries of the river reaches are defined at the confluence of tributaries, weirs, effluents, abstractions, or at other locations where changes in water quality might occur. Each reach is further divided into cells or sub-reaches. Flow variation in each cell is analogous to the variation in concentration of a conservative pollutant under the assumption of uniform mixing within the cell.

2.3 NITRATE

Two processes affect the rate at which the nitrate concentration changes in the water column. These are nitrification and denitrification. The differential equation describing the rate of change of nitrate concentration with time is given as

$$\begin{aligned} \frac{dx_2}{dt} &= \frac{u_2 - x_2}{\tau} \\ &\quad - k_5 x_2 \qquad \text{denitrification} \qquad\qquad (2.3.1) \\ &\quad + k_{15} x_6 \qquad \text{nitrification} \end{aligned}$$

where u_2 and x_2 are the input and output nitrate concentrations and k_5 and k_{15} are the rate coefficients associated with the processes indicated. x_6 is the ammonia concentration. If the Dissolved Oxygen level goes to zero, then the terms involving k_{15} and k_5 are left out.

Nitrification is the process resulting in the conversion of ammonium to nitrite and then to nitrate. The two biochemical reactions are shown below:

NH_4^+ + 2 O_2 ---(nitrosomas bacteria)---> NO_2^- + 2 H_2O
NO_2^- + 2 H_2O ---(nitrobacter bacteria)--> NO_3^- + H_2O + $2H^+$.

Curtis *et al* (1974) studied nitrification in rivers in the Trent Basin and found growth rates for nitrosomas and nitrobacter were virtually the same. Laboratory work by Alexander (1965) showed nitrobacter was five times as efficient as nitrosomas in transforming nitrite and ammonium, respectively. This indicates that the ammonia (ammonium ion) concentration is the rate controlling process. Knowles and Wakeford (1978) modelled the change in nitrate concentration to be dependant on the temperature, ammonia and nitrosomas concentration. In Quasar the rate of change of nitrate concentration is dependant on the concentration of ammonia, the temperature, T, and the ammonia nitrification rate, K_{15}, which is usually in the range of 0.01 to 0.5 $days^{-1}$ and is calibrated such that

nitrification = K_{15} $10^{(T.0.0293)}$ ($days^{-1}$) .

In denitrification, nitrate is reduced to nitrogen gas and oxygen by denitrifying bacteria. The simplified reaction is

$2\ NO_3 \dashrightarrow 3\ O_2 + N_2\ (g)$.

The oxygen produced is consumed by bacteria as an oxygen source so does not add to the oxygen concentration in the river. The process is first order, proportional to the nitrate concentration, requires the presence of mud and for every 10°C increase in temperature the rate of denitrification increases by a factor of 1.9 (Toms *et al* 1975) which is assimilated into the temperature dependant constant of the denitrification equation such that

$$\frac{dNO_3}{dt} = -K10^{(0.0293T+0.0294)}AC_N \qquad (2.3.2)$$

where A (m^2) is the surface area of mud in contact with water, C_N is the concentration of nitrate in water in mg l^{-1}, T is the temperature in Celsius. K is a constant in the range of 0.29 (clean gravel type bed), to 3.0 (soft muddy bed supporting denitrifying bacteria). In Quasar denitrification is based on this work using the equation

denitrification = k_5 1.0698 10 (T 0.0293)

k_5 is in units of day^{-1} and lies in the range 0.0 to 0.5.

2.4 CONSERVATIVE

A conservative water quality variable, such as chloride, is represented by the equation

$$\frac{dx_3}{dt} = \frac{u_3 - x_3}{\tau} \qquad (2.4.1)$$

where u_3 and x_3 are the input and output concentrations. This representation may also be used to represent variables not explicitly incorporated, so as to provide a worst case scenario.

2.5 DISSOLVED OXYGEN

The change in dissolved oxygen concentration is modelled as a result of photosynthetic O_2 production, benthic oxygen demand, reaeration (natural or due to the presence of a weir), nitrification, and loss due to BOD such that

$$\begin{aligned} \frac{dx_4}{dt} &= \frac{u_4 - x_4 + w}{\tau} && && (2.5.1) \\ & + k_{11} - P - R && \text{net algae } O_2 \text{ contribution} \\ & - k_4 k_6 x_4 && \text{benthic oxygen demand} \\ & + k_2 (CS - x_4) && \text{reaeration} \\ & - 4.43\, 10^{0.0293T} . k_{15} x_6 && \text{nitrification} \\ & - k_1 x_5 && \text{loss due to BOD} \end{aligned}$$

where u_4 and x_4 are the input and output dissolved oxygen concentrations and k_i are the rate coefficients associated with the processes indicated. x_5 and x_6 are the BOD and ammonia concentrations respectively and w is the contribution or loss of oxygen due to the presence of a weir in the reach.

Reaeration at weirs

The contribution or loss of dissolved oxygen due to the presence of a weir in a river is described by the equation

$$x_4 = x_S - \frac{(c_S - u_4)}{R_r} \qquad (2.5.2)$$

where c_S is the oxygen saturation concentration, u_4 is the dissolved oxygen above the weir and R_T is the deficit ratio (DOE, 1973). The DO deficit ratio takes into account the type of weir using a factor B, the pollution of the water (percent saturation), A, the height from the top of the weir to the downstream water level (m), h, and the temperature, T (°C) of the water as shown in the equation below:

$$R_T = 1 + 0.38ABh(1 - 0.11h)(1 + 0.46T). \qquad (2.5.3)$$

Algae contribution to dissolved oxygen

Algae, aquatic plants and phytoplankton utilize water, carbon dioxide, and sunlight to photosynthesize sugar and oxygen which is released to the water column. Respiration, which depletes the dissolved oxygen store in the water, occurs throughout the day. These two processes result in the highest dissolved oxygen concentration at midafternoon and the lowest concentration during the early hours of the morning. The two processes are described below and related in the differential equation by $k_{11} = P - R$ where P represents photosynthetic oxygen production and R represents respiration.

Photosynthetic oxygen production

Photosynthetic oxygen production in river systems has been described by Owens *et al* (1964) in which oxygen production is related to the light intensity and plant biomass or algal levels. They found that once there is sufficient plant biomass to provide adequate and uniform cover of the river bed the plant biomass has apparently no affect on the rate of photosynthesis due to self-shading. Whitehead *et al* (1981) used a modified version of the Owens model and estimated the relevant parameters for the Bedford Ouse. A similar approach was adopted for Quasar and the following relationship is used:

Chlorophyll-a concentrations less than 50 mg/l

$$P = k_8 \left(1.08^{(T-20)}\, I^{0.79}\, 0.317\, Cl_a\right) \text{ (mg/l-day)}$$

Chlorophyll-a concentrations greater than 50 mg/l

$$P = 1.08^{(T-20)}\, I^{0.79} \left(k_8 (0.317 \times 50) + k_9\, 0.317\, Cl_a\right) \text{ (mg/l-day).}$$

The two rates at which photosynthetic oxygen production occurs (k_8 and k_9) must be specified. k_8 is usually in the range of 0.0 to 0.03 day^{-1}, and k_9 is in the range of 0.0 to 0.02 day^{-1}. The two rates take account of the self shading effect at high algae concentrations. Cl_a is the chlorophyll-a concentration g/m^3, I is the solar radiation level at the earth's surface in watt hours per m^2 day. I is only input during sunlight hours determined from longitude and latitude data and also from the time of year assuming no cloud cover.

Respiration

The loss of oxygen due to algae respiration is described by an equation developed from Kowalczewski and Lack (1971) based on observed algae concentration measured as chlorophyll-a and respiration rate for the River Thames. It is

$$R = (0.14 + 0.013\, Cl_a)\, 1.08^{(T-20)} \text{ (mg/l-day).}$$

Benthic oxygen demand

Oxygen is also lost by benthic oxygen demand (river bed or mud respiration). There has been considerable research into this process (Edwards and Rolley, 1965) and the following equation for the benthic oxygen demand, M, has been used:

$$M = \frac{k_4 x_4^{0.45}\, 1.08^{(T-20)}}{d}$$

where x_4 is the river DO concentration ($mg\ l^{-1}$), d is the river depth (m) and k_4 is the rate of oxygen uptake by the sediment. The original work of Edwards and Rolley was conducted on the highly polluted muds of the River Ivel and later studies by Rolley and Owens (1967) showed that the parameter k_4 varied considerably from river to river. In the Thames a value for k_4 of 0.15 day^{-1} was found to provide the best fit to the observed DO data. In Quasar the equation representing benthic oxygen demand is given as

$$M = \frac{k_4 x_4 1.08^{(T-20)}}{d}.$$

k_4 is usually in the range of 0.0 to 0.1 day^{-1}.

Reaeration

Oxygen is added to the system by the natural reaeration of the river at the surface. Several workers have developed empirically and physically based equations. Owens *et al* (1964) derived the equation;

$$\text{reaeration} = k_2 (c_S - x_4)$$

where k_2 (days^{-1}) is the reaeration constant given by

$$k_2 = \frac{9.4^{V^{0.67}}}{d^{1.85}}.$$

V is the stream velocity in ft s^{-1} , d is the river depth in ft. This equation is valid within the experimentally observed ranges (velocity 0.1-5.0 ft s^{-1}; depth 0.4-11.0 ft). The temperature coefficient for the reaeration constant is defined as

$$k_{(T^\circ C)} = k_{(20^\circ C)} 1.024^{(T-20)}$$

c_S is the saturation concentration for DO defined as;

$$c_S = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3 .$$

In Quasar this equation has been used with the temperature correction applied such that

$$k_2 = \frac{5.316\ V^{0.67}\ 1.024^{(T-20)}}{d^{1.85}}.$$

As these variables (river velocity, temperature and depth) are all either input at the beginning of the model or generated during the model run the user does not have direct control of the reaeration coefficient and therefore the amount of oxygen added due to natural reaeration.

If there is ammonia in the water column this will be converted to nitrate. During this reaction oxygen is consumed. Thus there is a term for oxygen depletion as a result of nitrification.

BOD

The biochemical oxygen demand is caused by the decay of organic material in the stream. As the material decays it consumes oxygen, a process which is included in the model as

$$\text{BOD} = k_1\ x_5\ (\text{mg/l-day})$$

where k_1 is the rate coefficient for the loss of BOD and x_5 is the concentration of BOD in the stream.

2.6 BIOCHEMICAL OXYGEN DEMAND

The change in the biochemical oxygen demand is due to decay, sedimentation and addition due to dead algae. The differential equation describing the rate of change of BOD concentration with time is given as

$$\begin{aligned} \frac{dx_5}{dt} = {} & \frac{u_5 - x_5}{\tau} && \\ & -k_1 x_5 && \text{BOD decay} \\ & -k_{18} x_5 && \text{sedimentation} \\ & +k_{10} && \text{BOD contribution by algae} \end{aligned} \tag{2.6.1}$$

where u_5 and x_5 are the input and output BOD concentrations and k_1 and k_{18} are the rate coefficients associated with the processes indicated. If the Dissolved Oxygen level goes to zero, then the term involving k_1 is left out.

BOD decay

The biochemical demand is caused by the decay of organic material in the stream. As the material decays it consumes oxygen. Knowles and Wakeford (1978) found the rate of change due to oxidation to be dependant on the temperature such that

$$\text{BOD} = 1.047^{(T-20)}\, k_1\, x_5 \text{ (mg/l-day)}$$

where k_1 is the rate coefficient for the loss of BOD and is usually in the range of 0.0 to 2.0 day^{-1} and x_5 is the concentration of BOD in the stream in mg/l.

Loss by sedimentation

Loss of BOD can also occur by sedimentation. This occurs at a rate proportional to the amount of BOD present. The sedimentation rate is currently set at 0.1 day^{-1}.

BOD contribution by algae

As algae die they contribute to the BOD. The rate of contribution is proportional to the product of the concentration of algae and the rate of BOD addition by dead algae, usually in the range of 0.0 to 0.1 day^{-1}.

Ammonium Ion

The nitrification of ammonia is an oxygen consuming (oxidation) process which adds to the BOD load of the river. The differential equation describing the rate of change of ammonia concentration is

$$\frac{dx_6}{dt} = \frac{u_6 - x_6}{\tau} \tag{2.6.2}$$

$-k_{15}x_6$ loss by nitrification

where u_6 and x_6 are the input and output ammonia concentrations and k_{15} is the nitrification rate. The ammonia nitrification rate is dependant on the temperature and described by the equation

Ammonia nitrification rate = $k_{15}\ 10^{0.0293T}$.

2.7 AMMONIA

The concentration of ammonia, NH_3, is not actually produced as an output by the model, but it is computed from the ammonia concentration, pH and temperature data. This is determined by considering the following equilibrium

$NH_4^+ = NH_3(aq) + H^+(aq)$

The concentration of the ammonia is then given by the equation

$$NH_3 = \frac{NH_4^+}{10^{pKA-pH}} \tag{2.7.1}$$

where pKA is the dissociation constant, KA adjusted for temperature. The value of pKA is assumed to vary inversely with absolute temperature (this assumption being derived from the equation for Gibbs Free Energy) such that

$$pKA = \frac{2754.9}{273.15T}$$

where T is the temperature in degrees Celsius.

2.8 TEMPERATURE

The differential equation for temperature is

$$\frac{dx_7}{dt} = \frac{u_7 - x_7}{\tau} \tag{2.8.1}$$

where u_7 and x_7 are the input and output temperatures.

2.9 E. COLI

Changes in E. Coli are due to decay and can be represented as

$$\begin{aligned} \frac{dx_8}{dt} &= \frac{u_8 - x_8}{\tau} \\ &\quad -k_{16}\tau_8 \qquad \text{E. Coli decay} \end{aligned} \tag{2.9.1}$$

where u_8 and x_8 are the input and output E. Coli concentrations and k_{16} is the rate of E. Coli decay (usually in the range 0.0 to 2.0 days^{-1}).

2.10 pH

The model representation of pH assumes that H^+ ions are conservative, so

$$\frac{dx_9}{dt} = \frac{u_9 - x_9}{\tau} \tag{2.10.1}$$

where u_9 and x_9 are the input and output H^+ ion concentration calculated from pH values.

3. Water quality model algorithm

3.1 INTRODUCTION

The River Flow Forecasting System, or RFFS, has been implemented throughout the rivers of Yorkshire and makes forecasts of flow and/or level at some 150 locations. The design of the system is such that the specific models used to construct the forecasts are essentially separate from the generic code used to configure models together and to control the flow of information through a model network. This is achieved through the specification of a generic model interface which allows any model structure to be accessed by the Information Control Algorithm, or ICA, in the construction of forecasts. Up to now this generic model structure has been used to accommodate models which define the flow of water, and associated water levels, through a model network of a river basin or set of river basins. Model algorithms exist to merge different sources of rainfall data (radar and raingauge measurements and rainfall forecasts), to transform snowpacks to snowmelt, to represent the catchment response to rainfall and to route flows through non-tidal and tidal rivers. However, the design of the interface is sufficiently generic to accommodate other variables, in addition to water flow and level, and extension to accommodate water quality variables is functionally straightforward. The model algorithm interface is discussed in more detail in the next sub-section. Discussion then proceeds to an examination of the specific task of implementing the Quasar water quality equations, previously outlined in Section 2, within the RFFS as a model algorithm.

3.2 THE RFFS-ICA MODEL ALGORITHM INTERFACE

The model algorithm interface to the ICA essentially comprises a highly general Fortran subroutine argument list. Included in the argument list are such variables as inputs, outputs, model state variables, model parameters, control and transient variables and the start and end of the period to be forecast. A single execution of a model algorithm for a specific forecast requirement involves making a forecast for a defined period, starting at the time when the model state variables were last stored and passing through the current time to a user-defined time in the future, the "forecast lead time". It is often the case that models coded for offline use, including model calibration and planning tools, are not structured for use in this real-time mode. In particular, for repeated application using the same, often long, data set it is common to hold all the data as arrays in memory. This is the case for model calibration or multiple simulations of a Monte Carlo planning application. In contrast, the real-time application makes repeated forecasts over a specified duration, often short, incrementing the time-origin of the forecast each time to make use of the last state set stored, usually corresponding to the time of the last model run or a short time before. The coding design adopted within any pre-existing model can impact on the magnitude of the task of creating an RFFS-ICA model algorithm from it, or indeed any form of model to be used in real-time. This is discussed further in the next sub-section in the context of the pre-existing Quasar code.

3.3 THE RQFS MODEL ALGORITHM

This RQFS Systems Analysis study chose to investigate the Quasar code as a possible basis of developing the RQFS model algorithm. Here, the problems associated with this task are reviewed and conclusions drawn.

The Quasar code at the inception of this study existed as a program developed on DEC PDP and VAX computers over the last 15 years or so. The code had evolved to meet new requirements, such as Monte Carlo runs to support planning applications, and "what if?" runs to investigate pollutant spills. It's early development had been influenced by the restrictions imposed by limited computing power, including the need for overlays and the use of pointers to quicken access to data in memory. Changes in the standards and style of coding in Fortran also occurred over the development period of Quasar. The previous sub-section has also highlighted the difference in structure of a model used for calibration, design or planning and the "streamlined" form required for real-time application. Most of these problems were present in the case of the Quasar code and effort has been expended in restructuring the code prior to implementing it as a model algorithm.

Greater structure has been imposed on the code, where necessary, and pointers removed to clarify and simplify the code. Embedded options within the code have been removed where these are best controlled as external rather than internal tasks. An example of this is the "what if?" on pollutant spills which is best invoked as an external task through the shell of the RFFS, involving the setting of input data used by the model algorithm. Isolation of the model to function for a single reach, rather than a multi-reach cascade, was found to require considerable care and understanding. Decomposing the structure to this level then allowed insertion within a single reach of the multi-reach KW flow model.

The code has now been stripped down to a form amenable to call from a model algorithm. Because the water quality equations are driven by flow, consideration has been given to the option of structuring the code to first use the KW flow routing model algorithm to forecast the multi-reach flows of a routing section. These would then form inputs to a second model algorithm restricted to forecast the water quality variables, given the flows as input. Largely on account of the need to transfer all sub-reach flows from one model algorithm to another, a design based on integrating the quality model as an extension of the existing KW model algorithm has been preferred. Coding of this extended KW model algorithm, called FA_RQFS, is ongoing. Suffice it to say that this subroutine incorporates calls to the RQFS_REACH subroutine which encompasses the routines to implement the Quasar equations over the prescribed forecast period.

Further work is also required on the associated Model Algorithm Description File which allows the ICA to understand the model structure, including its parameters, state variables, transients, inputs and outputs, etc. However, this task is well defined by the ICA Data Structure Definitions and straightforward. Application of the new Model Algorithm is then simply invoked by setting up Model Component Description Files and Forecast Requirement Description Files for a specific network configuration requiring water quality forecasts. These files define the inputs and outputs and model algorithms to use to meet given forecast requirements, and of course require model parameter values for specific stretches of river to be given. Again this may involve work in model calibration.

Definition of new water quality variable data for locations in Yorkshire will require the designation of URNS (Unique Reference NumberS) in addition to those already defined in the RFFS database. Data conversions, such as unit conversions, may also be required to be coded in the database shell. In principle, once these database tasks have been completed the generic nature of the RFFS shell's display software will provide immediate access to plots of observed and forecast water quality values, as is the case presently with flow, level, rainfall intensity, gate setting etc.

3.4 CONCLUSION

The design and coding of the RQFS model algorithm has progressed sufficiently to highlight not only the problems of implementation, but has also gone a substantial way in overcoming them. The feasibility of implementing quality forecasting within RFFS, at least at a functional level, is now beyond doubt. The performance will not really depend on the RFFS as a modelling environment but more on the appropriateness of the chosen model, and the availability of water quality data for the purposes of initialisation and updating in real-time and for model calibration off-line.

4. River Aire Case Study

4.1 INTRODUCTION

The feasibility of implementing RQFS for the rivers of Yorkshire will be investigated in this section through a case study on the River Aire through Leeds. This location was chosen as a consequence of the project inception meeting on 27 January at Park Square, Leeds, reported in Annex B. The main reasons for this selection were the availability of data to support the case study along with a practical need for a water quality model to manage pollution incidents and effluent discharges along the stretch of Aire between Esholt STW and Fleet Weir, above the confluence with the Calder.

The case study is used in this section to first identify forecast points where there is a specific requirement to forecast water quality. This is guided in part by a review of the sites already designated as forecast points for flow and level forecasting along the Aire and by locations with supporting water quality data. The hydrometry, in the form of river flow and level stations on the main river and principle tributaries, along with available water quality data sources are reviewed to assess the feasibility of model calibration and guide model configuration. A simple simulation using the pre-existing Quasar system, supported by tracer data for the Aire, is used to reveal any potential problems in the use of a Quasar-type modelling approach. The section concludes by summarising the main problems associated with implementing the case study and recommendations on how a case study implementation might proceed.

4.2 RFFS FLOW/LEVEL FORECAST POINTS ON THE RIVER AIRE

By way of background Figure 4.2.1 presents the RFFS river network schematic for that part of Yorkshire which incorporates the main River Aire from the gauging station at Kildwick to its confluence with the Calder at Castleford. Small circles are used to designate the forecast points for which flow and/or level are to be constructed operationally within the RFFS. The forecast points for Kildwick to Fleet Weir, upstream of Castleford, are presented in Table 4.2.1 along with the river gauging and level stations along this stretch of river; note that the river gauging sites automatically qualify as forecast points. It is seen that there are only three gauging stations, with stage-discharge relations, on the main river: at Kildwick Bridge, at Armley Road and at Fleet Weir. There are also river gauging stations at three tributary stations: Cross Hills, Keighley and Shipley. Seven of the designated flow/level forecast points have no form of river measurement and at 6 sites where levels are measured there is no corresponding stage-discharge curve to infer flows from levels. However, in calibrating channel flow routing models for the Aire, model-inferred ratings have been derived for two of these: Stockbridge and Cottingley. At the other four level-only sites it is likely that there was no suitable data available to support model calibration, or available in real-time, anyway.

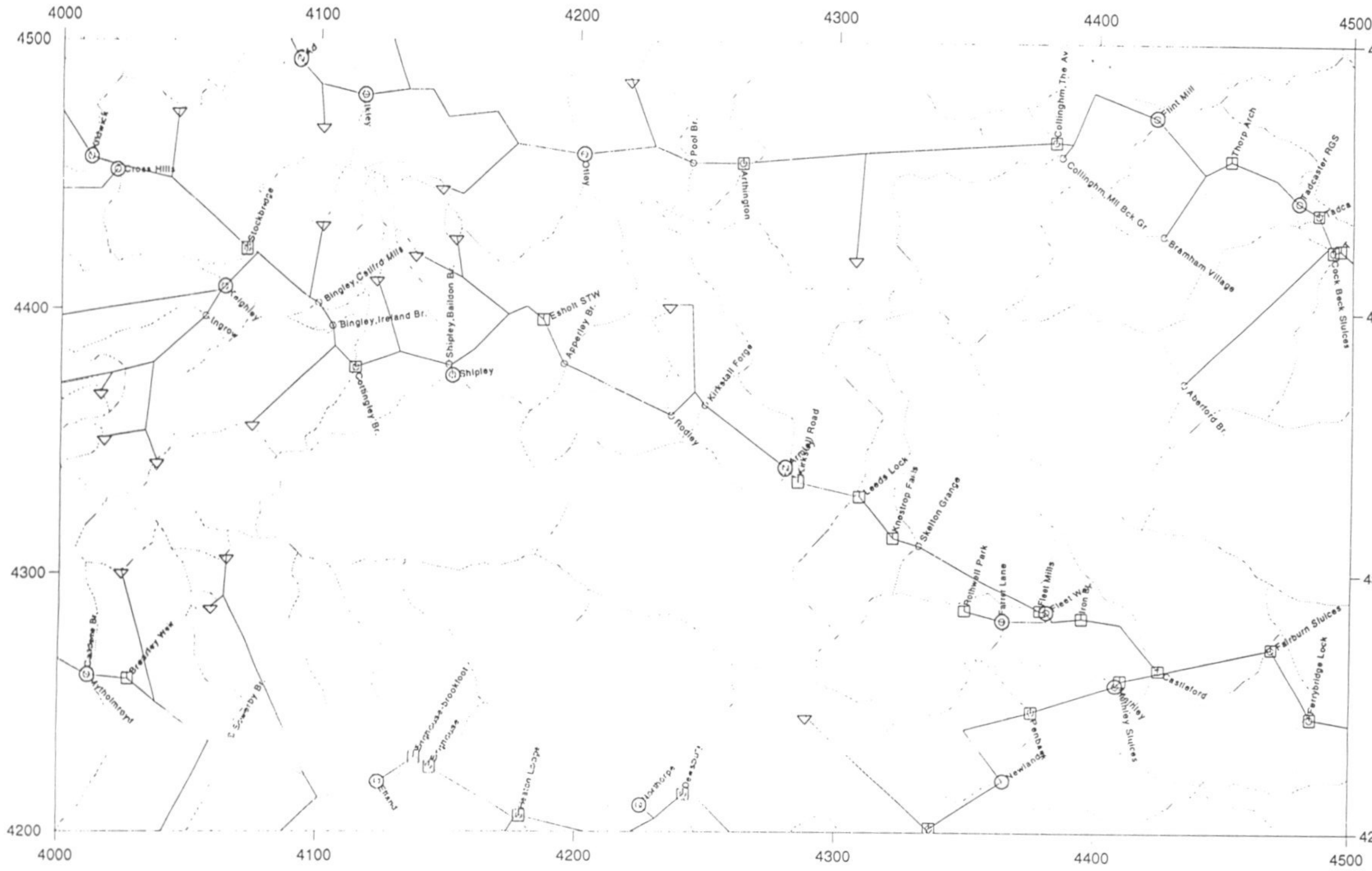

Figure 4.2.1 RFFS river network schematic for the River Aire (large circle: river gauging station; small circle: forecast point; square: river level station; triangle: reservoir; dashed line: subcatchment boundary)

Table 4.2.1 River gauging stations (RGS), river level stations (RLS) and forecast points on the Aire from Kildwick to Fleet Weir

Main river station	Tributary station	Station type
Kildwick		RGS
	Cross Hills	RGS
Stockbridge		RLS
	Keighley	RGS
Bingley (Castleford Mills)		FP
Bingley (Ireland Br.)		FP
Cottingley Bridge		RLS
Shipley (Baildon Bridge)		FP
	Shipley	RGS
Esholt STW		RLS
Appleby Bridge		FP
Rodley		FP
Kirkstall Forge		FP
Armley Road		RGS
Kirkstall Road		RLS
Leeds Lock		RLS
Knostrop Falls		RLS
Skelton Grange		FP
Fleet Mills		RLS
Fleet Weir		RGS

4.3 RQFS WATER QUALITY FORECAST POINTS ALONG THE AIRE

Consideration of the requirements for water quality forecasts along the Aire highlighted the need for forecast points at the six locations shown in Table 4.3.1. Three of these are on the main Aire at the outfalls from three sewage treatment works: at Esholt, Keighley (Marley) and Bingley (Dowley Gap). A fourth is where a poor quality tributary, Bradford Beck, joins the Aire. The other two sites are downstream of Leeds, at Knostrop to the power station offtake at Skelton Grange and at the Canal Cut Offtake and at its point of return. There is also a less site specific requirement to forecast longitudinally along the river, at any point, for point source pollution forecasting. Such a forecast requirement stems from the need to support the management of the river during pollutant spills which might occur anywhere along the river and affect non-specific points.

Table 4.3.1 Water quality forecast points for the Aire case study

Site	Grid Reference
Esholt STW	SE 187 396
Keighley STW (Marley)	
Bingley STW (Dowley Gap)	
Bradford Beck (poor quality tributary)	
Knostrop and downstream	SE 322 313
Canal Cut Offtake (downstream of Leeds) and Return	

4.4 DATA SOURCES TO SUPPORT THE AIRE CASE STUDY

The sources of data of relevance to the RQFS water quality Forecast Points are summarised in Table 4.4.1. Only one continuous water quality monitoring site has existed on the Aire, at Sandoz in the vicinity of Esholt STW. This ceased operation after collecting about a year's worth of data. At Esholt STW itself only flows are recorded and at Rodley STW records exist on flow and concentration of the effluent.

Table 4.4.1 Data sources for the Aire case study

Site	Grid reference	Data description
Esholt at Sandoz	4217 4373	continuous monitor: DO, temp., cond., amm., turb. (15 min. frequency). Now ceased operation. ~ 1 year record.
Esholt STW		flows only
Rodley STW		flows and concentration

This Systems Analysis study has progressed work on the assembly of data records to support a future case study implementation on the Aire. These records are summarised below:

(a) Water quality data on sampled effluents, for the period January to September 1992, from Yorkshire Water. These data are primarily for Esholt and Knostrop with a little data for Runda and Rodley.

(b) Effluent flow data, in Ml/d, for Esholt STW as daily totals and 7-day averages for the period January to December 1992.

(c) 15 minute river level data for Esholt and Leeds Lock, transferred from the NRA's Hydrolog archive.

(d) Ad hoc river level data, at least daily, for Esholt and Kirkstall Road, obtained from NRA's Telmaster system.

(e) 15 minute flow data, in l/s, for Esholt STW for February, April and August 1992, held as daily summary files.

This take-on of data has highlighted the difficulty of accessing data from different systems within the NRA and Yorkshire Water, in a variety of formats (computer printouts, Hydrolog comma separated variable format, Lotus Symphony spreadsheet format, and Telmaster format). Often the data are not sampled at the frequency required for dynamic real-time modelling of water quality, being often daily.

Table 4.4.2 summarises the river level and flow records available to support the case study, including information on the records held at IH. Fifteen minute level records exist at the three gauging sites at Kildwick, Armley and Fleet Weir. The Table serves to highlight that only daily level records exist for Esholt STW and Kirkstall Road from Telmaster.

Table 4.4.2 Aire case study river level data (RGS: River Gauging Station; RLS: River Level Station)

Station name	**Station no.**	**Grid reference**	**Station type**	**Type of record**	**Record at IH**
Kildwick			RGS		Full, 15 min
Stockbridge			RLS		
Cottingley Bridge			RLS		
Esholt STW		SE 187 396	RLS	Daily level: Telmaster	15 min, Hydrolog
Armley			RGS		Full, 15 min
Kirkstall Road		SE 2595 3557	RLS	Daily level: Telmaster	
Leeds Lock		SE 303 332	RLS	Logging (Hydrolog)	
Knostrop Falls		SE 322 313	RLS	Logging (Hydrolog)	15 min, March-Sept 1992
Skelton Grange Power Station			RLS	Weekly chart	14.00 daily: April-Sept 1992
Fleet Weir		SE 381 285	RGS	Weekly chart	15 min

4.5 INTEGRATION OF RQFS INTO RFFS FLOW ROUTING MODELS FOR THE AIRE

Table 4.5.1 summarises the reach sub-division employed within the RFFS for modelling the River Aire from Kildwick to Fleet Weir using the KW flow routing model algorithm. Figure 4.5.1 presents the model network schematic for the Aire showing how the model components (empty squares), and the forecast requirements (square within a square) they meet, link together. Four model components are used with their boundaries chosen to coincide with sites for which level records existed to support model calibration. The number of sub-reaches used within each varies from 2 to 10, and this does not necessarily reflect the length of river represented by each model. When calibrating the flow routing model it is often possible to reduce the number of sub-reaches used, for example by adjusting the parameters affecting the wave speed, whilst still obtaining as good a forecast performance. Additional storages at node points between sub-reaches can also be introduced in the model to provide additional attenuation without adding to the number of sub-reaches. Advantages of using fewer sub-reaches include a simpler model form and faster model execution. In the case of the Aire this has led to different forms of model structure being developed for different model components. It is likely that, whilst justified for modelling flow, a more consistent approach may have to be taken when the aim is to model both flow and quality along a stretch of river. The need to assign new forecast points to meet water quality requirements, and the inclusion of quality for some polluted lateral inflows, is likely to necessitate a reconfiguration of some of the existing flow routing models. This is a relatively straightforward task for the Aire case study, given that there are only four models involved.

The next two sections report work undertaken with the pre-existing Quasar model, aimed at using tracer data for the Aire to establish the velocity-flow relation to be used within Quasar and to perform an initial simulation to expose any problems that might be encountered in applying a Quasar-type model to the River Aire.

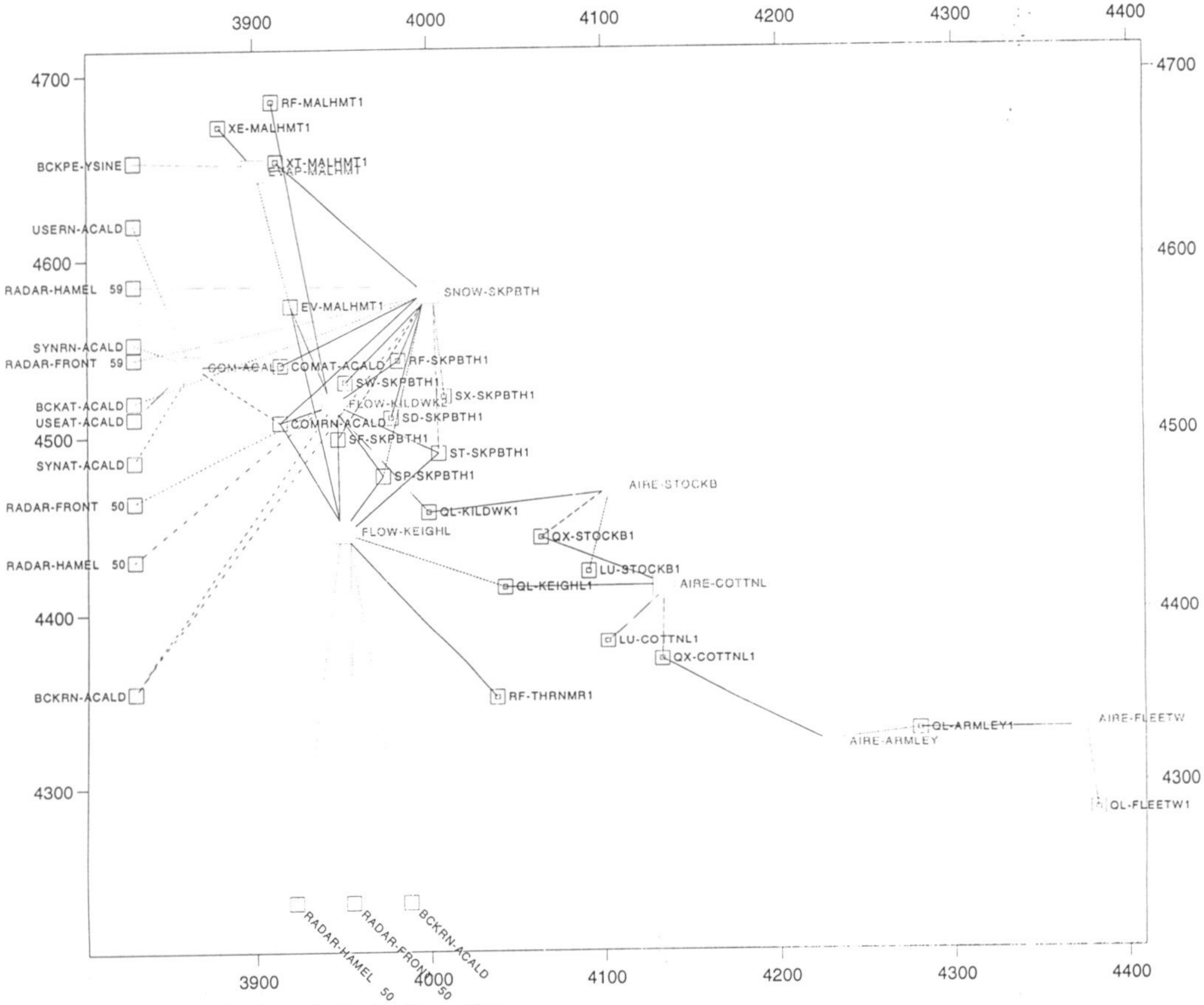

Figure 4.5.1 RFFS model network schematic for the River Aire

Table 4.5.1 Model components used on the River Aire between Kildwick and Fleet Weir

Model Components	**Input(s)**	**Output**	**No. of reaches**
Kildwick to Stockbridge	Kildwick	Stockbridge (L,Q)	4
Stockbridge to Cottingley	Stockbridge, Keighley	Cottingley (L,Q)	2
Cottingley to Armley	Cottingley	Armley (Q)	10
Armley to Fleet Weir	Armley	Fleet Weir (Q)	2

4.6 VELOCITY-FLOW RELATIONSHIPS FOR THE RIVER AIRE

A Rhodamine B tracer experiment on the River Aire during February 1992 was carried out by the University of Sheffield, Department of Civil and Structural Engineering. A single shot of Rhodamine B was injected into the outfall from Esholt STW and concentrations were determined at three downstream sites: Rodley STW (6.5 km), Kirkstall Power Station (13 km), and Skelton Grange Power Station (20.5 km). Values of reach mean velocity and flow rate were calculated at each of the three stretches of river and reported in the project report provided by the University of Sheffield.

These data were used to calculate the parameters of the velocity flow relationship in Quasar, for each of the reaches. In Quasar the relationship:

$$v = \beta q^{\gamma} \qquad (4.6.1)$$

is used, where v is the velocity (m/s) and q is the flow rate (m^3/s). Since velocity data are available only at one flow rate a value for either β or γ must be estimated. Experience has shown that a sensible value for the exponent γ in lowland rivers is around 0.67. Thus rearranging equation (4.6.1), β can be estimated for a flow rate of 7 m^3/s as

$$\beta = v/3.68 \; . \qquad (4.6.2)$$

The values obtained for β, given γ is set to 0.67, are given in the table below:

Reach	β
Eshalt - Rodley	0.114
Rodley - Kirkstall	0.063
Kirkstall - Skelton Grange	0.043

4.7 SIMULATION OF TRACER WITH QUASAR

A simple reach structure for the River Aire has been set up and a map file created for use with Quasar. The map file has been set up with a constant flow rate of 7 cumecs in order to model the Rhodamine tracer experiment. Using the impulse options in Quasar a G30 discharge has been set up to give a similar mass load of a conservative tracer into the river at the appropriate reach. The model has been run using a range of numbers of lags in the reaches. Although it has been possible to reproduce the dispersion, the time delay observed in reality has not been simulated successfully. A large number of lags are needed to achieve a tight enough curve and this results in slow run times.

It is concluded that a pure time delay feature should be included in the model equations if they are to be used for predicting movement of pollutant pulses downstream at the time resolution required by the RQFS. As it is intended to use the RFFS flow equations to drive the quality model, and since these incorporate a time delay, the problem should be resolved by the RQFS approach.

4.8 CONCLUSIONS

This case study review has highlighted the shortage of data for model calibration of water quality on the Aire, and for the data that exist the variety of systems and formats used in its archiving. There is clearly a need for a well designed sampling programme to support model calibration and this might most effectively be accomplished in the short-term by a set of tracer experiments over a range of discharges. This would at least support the calibration of the RQFS for forecasting the effects of conservative pollution spills down the river. In the longer term a programme based on continuous water quality monitoring of a range of water quality determinands along the Aire should be given serious consideration.

There is no intrinsic difficulty in configuring the RQFS as a model algorithm along the Aire from Kildwick to Fleet Weir, thereby capitalising on the substantial infrastructure that the RFFS already supports for real-time forecasting. Some recalibration of the existing flow routing models, using more consistent reach sub-division configurations, is likely to be required to ensure that both flow and quality variations are adequately represented.

5. Summary, Conclusions and Recommendations

5.1 SUMMARY

This Systems Analysis study has considered the feasibility of extending the River Flow Forecasting System, or RFFS, to incorporate forecasting of water quality in addition to flow and level. The approach taken has been to first consider the choice of water quality model and an extensive review of IH's Quasar water quality model has been made alongside the KW flow routing model used for forecasting flow in non-tidal channels in the Yorkshire RFFS. This led to the conclusion that the water quality equations used in Quasar should be integrated with the flow equation used by the KW model to form a RQFS water quality model algorithm for use in the RFFS.

Section 3 addressed the problem of coding the RQFS model algorithm and highlighted the advantage of the RFFS's generic model algorithm interface in accomplishing this task. This interface is such that the task of forecast construction, performed by the Information Control Algorithm or ICA within the RFFS, is essentially independent of the specific models configured into the system. No internal code changes to the ICA itself are required, only coding outwards from the interface to specify a new model to a well-defined generic structure. Work has progressed on coding this algorithm and this has exposed shortcomings in the structural coding of Quasar for use as a basis for a model algorithm to be applied in real-time. As a result, significant work has been undertaken in re-structuring the Quasar model code prior to incorporating it as a model algorithm. This work has been completed but awaits testing in a model algorithm environment. The task of incorporating the code into a new RQFS model algorithm, which combines the KW flow routing and Quasar water quality equations, remains to be completed.

The feasibility of applying the RQFS software to Yorkshire's rivers has been examined through the use of a case study, based on the Aire through Leeds, in Section 4. Requirements for quality forecasts were reviewed alongside the requirements for flow/level forecasts already identified as part of the RFFS implementation. Problems with insufficient data to support model calibration were revealed along with a lack of water quality data in real-time to support model updating. Data that do exist derive from a variety of systems, each using different formats This made the task of data take-on not straightforward; often the data time interval was too coarse (typically daily) to support dynamic modelling under a changing flow regime. A lack of consistency in the sub-reach configuration of the channel flow routing models used in the RFFS along the Aire, whilst not significant for flow forecasting, was recognised as a potential problem when water quality forecasts are also required. However, the recalibration required was not seen as a significant issue. Initial simulation of the Aire, supported by tracer data, using the pre-existing Quasar system highlighted the need for a time delay in the model which the RQFS is now able to accommodate through its use of the KW flow routing equations.

5.2 CONCLUSIONS

The main conclusion of this Systems Analysis study is that the RFFS provides an ideal forecast construction environment for water quality modelling in real-time. Its generic design readily allows extension from forecasting flow to forecasting water quality. The generic model algorithm interface allows a new model algorithm to be developed independent of the complexities of the information control code within the RFFS. The coding task is also helped by a well defined interface structure. Once a model algorithm has been coded it can immediately enjoy the benefits of the RFFS user environment, including the display of forecasts. Significant progress has already been made in coding the water quality model algorithm.

The success of the RQFS will depend primarily on the suitability of the coded model and the data used to support its calibration, as well as its updating in real time. The work has not progressed sufficiently to comment on model performance on Yorkshire rivers but an important conclusion is the need for more data at a suitable time resolution to support any future implementation of RQFS.

5.3 RECOMMENDATIONS

RQFS implementation in Yorkshire

(1) The RFFS provides an ideal forecast construction environment within which to implement a real-time water quality forecasting model. It is recommended that it be adopted for real-time water quality forecasting for Yorkshire rivers.

(2) The RQFS Model Algorithm, based on a combination of the KW flow routing equation and the Quasar water quality equations, should be coded to completion and tested for use on Yorkshire rivers.

(3) An operational implementation requires some further work in the RFFS shell environment, principally for the database to identify a new set of variables on water quality. Whilst not significant in terms of time, it is essential that this work be undertaken. Functionality to plot longitudinal profiles featured in the design of the RFFS but there may be further development required in the GUI of RFFS, and if necessary this should be done.

(3) Further work should be undertaken on the Aire case study through Leeds, to extend the take-on of data to permit model development, calibration, testing and operational implementation of the RQFS. New data on tributary flows may be required and re-configuration of the reach models to accommodate them.

(4) Additional case studies should be considered along with appropriate sampling and tracer programmes. For example, water supply intakes at Moor Monkton and Acombe Landing have recently been threatened by pollutant spills upstream and may be deserving of special attention. In this case the shortcomings of a steady-state approach to water quality forecasting were exposed under conditions of variable, higher flows.

Monitoring and data requirements

(1) There is an urgent need to implement a data collection programme to support the application of RQFS for real-time water quality forecasting for the rivers of Yorkshire.

(2) In the short-term, modelling of conservative pollutants should be supported by a programme of tracer experiments for a range of flows along critical stretches of the rivers of Yorkshire.

(3) In the longer-term implementation of continuous water quality monitors should be seriously considered, choosing locations that are critical from the water management point of view and also useful for model development. In particular, the latter requirement implies the deployment of sensors at both upstream and downstream locations of a critical stretch of river, to support modelling of the self-purification processes operating in rivers.

Modelling

(1) Further consideration of alternative model equations should be given, in addition to forms based on Quasar. In particular, the Aggregated Dead Zone, or ADZ, model employed by the NRA within Yorkshire needs to be reviewed as a potential candidate for use as a Model Algorithm within the RFFS. Any new model formulation would need to be considered, particularly, in terms of its representation of dispersion of pollutants and its ability to make use of tracer-inferred dispersion coefficients.

(2) At present the RFFS does not provide uncertainty estimates on its forecasts. An approach based on ensemble forecasting, drawing on ideas from Monte Carlo simulation, should be investigated to provide an indication of the range of possible outcomes in addition to the expected values of water quality variables in the future.

(3) Extension of the determinands presently handled by the Quasar equations needs to be considered against the specific needs in Yorkshire and their feasibility of implementation. Known problems are metal contaminants from industrial discharges and foaming due to detergents. The existing equations are designed to represent thermal discharges and algal blooms that exist as problems within Yorkshire. However, there may be a need to re-examine these equations in the specific Yorkshire context.

(4) This report has assumed that simple error prediction, based on an ARMA dependence model, be used for updating the water quality model in the event that water quality data are available in real-time. This updating method is independent of the model structure and therefore no special development of it is required for application to the RQFS model errors. However, consideration should be given to alternative updating schemes based on state correction where model errors are used to adjust model state variables to achieve better agreement between model forecasts and observed water quality concentrations.

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Appendix Analytical solutions to the water quality differential equations used in Quasar

Flow

$$x_1(t) = \exp(-1/\tau)x_1(t-1) + \left(1 - \exp(-1/\tau)\right)u_1$$

Nitrate

If the dissolved oxygen concentration is zero the solution is:

$$x_2(t) = \frac{(1-\exp(-D))u_2\tau^{-1}}{D} + x_2(t-1)\exp(-D)$$

If the dissolved oxygen concentration is greater than zero the solution is:

$$\begin{aligned} x_2(t) = {} & \frac{(1-\exp(-D))u_2\tau^{-1}}{D} \\ & + \frac{k_{15}x_6(\exp(-F)-\exp(-D))}{k_5-k_{15}} \\ & + \frac{k_{15}u_6\tau^{-1}(1-\exp(-D))}{DF} \\ & - \frac{k_{15}u_6\tau^{-1}(\exp(-F)-\exp(-D))}{F(k_5-k_{15})} \\ & + x_2\exp(-D) \end{aligned}$$

where

Time constant	τ (hr)
denitrification rate	$k_5 = 1.0698 \, . \, 10^{0.0293T}$ (day^{-1})
ammonia nitrification rate	$k_{15} = 1.0698 \, . \, 10^{0.0293T}$ (day^{-1})
ammonia nitrification rate	$k_{14} = 1.0698 \, . \, 10^{0.0293T}$ (day^{-1})
upstream ammonia concentration	u_6 (mg/l)
downstream ammonia concentration	x_6 (mg/l)
upstream nitrate concentration	u_2 (mg/l)
downstream nitrate concentration	(mg/l)
	$D = k_5 + \tau^{-1}$
	$F = k_{15} + \tau^{-1}$

Conservative

$$x_3(t) = \exp(-1/\tau)x_3(t-1) + \big(1-\exp(-1/\tau)\big)u_3$$

where τ is a time constant, and u_3 and x_3 are the upstream and downstream conservative concentration in mg/l.

Dissolved Oxygen

The dissolved oxygen concentration is affected by algae photosynthesis and respiration, reaeration, denitrification, and benthic and biochemical oxygen demand. The analytical solution in this case is:

$$\begin{aligned}
x_4(t) = {} & \frac{(u_4 + w)\tau^{-1}(1 - \exp(-A))}{A} \\
& + \frac{k_{11}(1 - \exp(-A))}{A} \\
& + \frac{k_2 c_s (1 - \exp(-A))}{A} \\
& - \frac{k_4 k_6 x_4 (1 - \exp(-A))}{A} \\
& - \frac{k_1 x_s (\exp(-B) - \exp(-A))}{G} \\
& + \frac{k_1 u_5 \tau^{-1} (1 - \exp(-A))}{AB} \\
& + \frac{k_1 u_5 (\exp(-B) - \exp(-A))}{GB} \\
& - \frac{k_{14} x_6 (\exp(-J) - \exp(-A))}{k_2 - k_{14}} \\
& - \frac{k_{14} u_6 \tau^{-1} (\exp(-J) - \exp(-A))}{J(k_2 - k_{14})} \\
& - \frac{k_{14} u_6 \tau^{-1} (1 - \exp(-A))}{JA} \\
& + x_4(t-1)\exp(-A)
\end{aligned}$$

where

$$A = \frac{5.316 V^{0.67} 1.024^{(T-20)}}{h^{1.85}(1440/\Delta t)} ,$$

h is the depth and Δt the model time step, and

$B = k_1 1.047^{(T-20)} + \tau^{-1}$
$J = 4.57\ k_{15}\ 10^{0.0293T} + \tau^{-1}$
$G = A - B$
$k_1 = 1.047^{(T-20)}$ (BOD decay rate)
k_4 = rate of sediment oxygen uptake
$k_6 = (\exp(0.0693(T-15)))/h$
k_{11} = contribution of O_2 due to photosynthesis and algae respiration
$k_{14} = 4.57\ 10\ \exp(0.0293T)$ (day^{-1}) (4.57 is the ammonia nitrification rate)
u_4 = upstream DO (dissolved oxygen) (mg/l)
x_4 = downstream DO (mg/l)
u_5 = upstream BOD (Biochemical Oxygen Demand) (mg/l)
x_5 = downstream BOD (mg/l)

Biochemical Oxygen Demand

If the dissolved oxygen concentration goes to zero

$$x_5(t) = \exp(-C)x_5(t-1) + \frac{(u_5\tau^{-1} + k_{10})(1 - \exp(-C))}{\tau^{-1}} .$$

If the dissolved oxygen concentration is greater than zero

$$x_5(t) = \exp(-N)x_5(t-1) + \frac{(u_5\tau^{-1} + k_{10})(1 - \exp(-N))}{N}$$

where

$C = k_{18} + \tau^{-1}$
$N = k_{13} + \tau^{-1}$
k_{10} = (rate of BOD addition by dead algae). (Algae Concentration) (day^{-1})
$k_{13} = k_1 + k_{18}$
k_{18} = 0.1 day^{-1} (Sedimentation rate of BOD)
u_5 = upstream BOD concentration (mg/l)
x_5 = downstream BOD concentration (mg/l).

Nitrification

The corresponding analytical solution demonstrates the fact that loss of ammonia is due to nitrification which is dependent on the concentration of dissolved oxygen. Nitrification ceases if the dissolved oxygen becomes zero. The equation is

$$x_6(t) = \exp(-1/\tau)x_6(t-1) + (1 - \exp(-1/\tau))u_6 .$$

If the dissolved oxygen concentration is greater than zero then

$$x_6(t) = \exp(-F)x_6(t-1) + \frac{u_6\tau^{-1}(1-\exp(-F))}{F}$$

where

F = $k_{15} + \tau^{-1}$
k_{15} = (Ammonia nitrification rate) $10^{(0.0293T)}$
u_6 = Upstream ammonia concentration (mg/l)
x_6 = Downstream ammonia concentration (mg/l)

Temperature

$$x_7(t) = \exp(1/\tau)x_7(t-1) + (1-\exp(-1/\tau))u_7$$

where u_7 and x_7 are the upstream and downstream temperature.

E. Coli

$$x_8(t) = \exp(-k_{16})x_6(t-1) + \frac{(1-\exp(-k_{16}))u_8(\tau-1)}{k_{16}}$$

where k_{16} is the rate of E. Coli decay (day^{-1}) and u_8 and x_8 are the upstream and downstream E. Coli (N/100 ml) respectively.

pH

$$x_9(t) = \exp(-1/\tau)x_9(t-1) + (1-\exp(-1/\tau))u_9$$

where u_9 and x_9 are the upstream and downstream pH respectively.

Annex A RQFS: River Quality Forecasting System - A Project Proposal

A.1 BACKGROUND

The River Flow Forecasting System, or RFFS, has been developed in a generic way to allow not only reconfiguration to other river systems but extension to make forecasts of variables other than river level and flow. A generic model algorithm interface is provided within the RFFS to accommodate new models: these may be improved models of flow in rivers but may equally be models of other variables. It is natural to consider an extension to accommodate the quality of water in addition to the quantity of water at the selected forecast points. The purpose of this document is to propose an extension to the RFFS to incorporate water quality and to outline a strategy for examining the feasibility of implementing this River Quality Forecasting System, or RQFS, in the Yorkshire Region of the National Rivers Authority.

A.2 FEASIBILITY STUDY

The feasibility study would include the following:

(i) Consideration of the choice of water quality model algorithm and updating methods to be used within the RQFS. It is currently envisaged that the algorithm would be based on differential equations contained within IH's QUASAR (Quality Simulation Along Rivers) water quality model. However, it might use flow derived from the KW channel flow routing model, already calibrated to Yorkshire's major rivers as part of the RFFS implementation, rather than use the flow model within QUASAR.

(ii) Consideration of the choice of water quality variables to be modelled. Currently QUASAR incorporates representations of the following: nitrate, dissolved oxygen, biochemical oxygen demand, ammonia, ammonium ion, temperature, E. Coli, pH and a "conservative" water quality parameter.

(iii) A review of the requirements for water quality modelling in the Yorkshire Region, through discussion with appropriate NRA staff.

(iv) A review of water quality monitoring and data archives in the Yorkshire Region to support both real-time implementation and model calibration. This would consider both hand sampled data sources and automatic water quality sampling, and the implications on (ii) above.

(v) Consideration of the implications on the Information Control Algorithm within the RFFS. This would include the need for additional URNs (Unique Reference Numbers), the details of implementation probably as a Network separate from the RFFS and how requirements for additional functionality are to be met (eg. longitudinal profiles of water quality variables).

(vi) If time permits, and if the feasibility is demonstrated, a prototype RQFS implementation probably using a simple dummy network and data.

(vii) A strategy for implementation in the Yorkshire Region of the NRA including the identification of any needs for further model development and data collection.

Annex B Notes of RQFS meeting on 27 January 1993

Location: NRA Yorkshire Region, Park Square, Leeds

Present: NRA - Richard Freestone, Adrian Barraclough, Mark Tinnion
Logica - Peter Bird
IH - Bob Moore, Richard Williams

B.1 BACKGROUND

A Quality Survey Map for the Yorkshire Region was produced as part of the National River Quality Survey, which reviewed the NWC classification, and included consideration of DO, NH_3 and BOD. Yorkshire rivers are classified as of good quality along 80% of their length and 20% of unsatisfactory quality. As a general statement rivers in the north of the region are good but those in the south, for example the Aire, Calder and Don are of poor quality. Sewage effluent from the industrial cities of south and west Yorkshire is the main pollutant source. The Aire deteriorates below Bradford receiving effluents from Bradford STW at Esholt and from Leeds STW at Knostrop. The Calder receives effluent from Huddersfield STW, the Don from Sheffield STW at Blackburn Meadows and the Rother from Chesterfield STW and many industrial effluent sources.

The NRA's Environment Programme includes improvement to sewage treatment works with the Don improving in quality from summer 1992 with the refurbishment of Sheffield STW. Improvements to the Rother are planned in 1993/94 with the Don-Rother System achieving Class 2 status in 1995. The works at Huddersfield, Esholt and Knostrop are to be improved but not until after 1996. Major improvements should be soon on the Don within the next 6 years.

B.2 WATER QUALITY MONITORING

The DO spot sampling programme is not effective because this fails to record the worst conditions which occur at night. In response to this problem permanent monitors have been installed at Sandalls, Huddersfield and Michell Cotts (operational from January 1992); a monitor on the Don at Doncaster is expected to become operational in January 1993.

Additional data are collected as part of investigational works. Several months data exist for the Calder at Horbury, 2 months data for a site upstream of Huddersfield STW and several months data for the Aire at Bingley, upstream of Esholt STW.

Dissolved oxygen is of especial concern, especially in the centre of Leeds where significant fish kill can occur at times of limited dilution in summer coinciding with heavy sewage effluent loads. High biochemical activity in summer aggravates the problem; however, storm overflows are not thought to contribute significantly to the problem. A clear benefit is seen for modelling the Aire through Leeds, and to extend upstream to Esholt where spot water quality sampling is undertaken. Travel time data are available for a 24 km reach for discharges of 9 to 10 cumecs: the dye tracer experiment used Rhidamine-WT. More tracer experiments are needed for the Aire over a wider range of flows. Weirs between Esholt and Knostrop provide re-oxygenation. Algal blooms can be a problem but only infrequent algae measurements are taken. However, weeds are the main consumer and a contribution from algae only occurs at the beginning and end of summer.

B.3 MODELLING

There are statistical mass balance (TOMCAT) models of all the dirty rivers - the Aire, Calder, Don and Rother - and these include details of effluent inputs. Also Aggregated Dead Zone (ADZ) models for BOD and NH_3 have been developed using data for 1986-80 (?).

The MIKE-11 model is used for the tidal Hull, where there is a significant problem associated with Beverley STW and the Hull industrial area. There is a continuous monitor at Wansford on the West Beck Driffield Canal.

There is interest in modelling the clean rivers to obtain travel times and dispersion characteristics in support of pollution incidents. Potable abstraction points need to be protected. Work has involved use of Lancaster's ADZ model. The contract began in early April 1992 and involved setting up models and running using 5 tracer surveys. BOD-DO models are not required for these cleaner rivers. The ADZ models are seen as a minimum data method and are most appropriate for modelling conservative pollutants. However, there is a need to model non-conservative ones: for example, a road accident spill affecting the Derwent involved oil, whilst a red diesel (conservative) spill was modelled satisfactorily.

B.4 REPORTS

A report detailing future requirements for continuous chemical monitors in the Yorkshire Region has been prepared.

Regional quality reports for the Don, Calder and Aire are available.

B.5 WATER QUALITY MONITORING PROPOSALS

The following automatic water quality monitors are proposed:

(a) Aire:

downstream of Keighley STW (Marley)
downstream of Knostrop STW
tidal limit at Beale

(b) Calder:

upstream of Huddersfield STW
Methley (upstream of Aire confluence)

Monitors at the following STWs are proposed: Esholt STW, Knostrop STW, Keighley STW.

Huddersfield STW, Halifax STW and Mitchell Laithes (Dewsbury) STW.

A Joint Working Group of Yorkshire Water/NRA have set up a pilot project to install 5 sewage works chemical monitors, which are likely to include Knostrop and Esholt: this project will probably start in 1993. Measurements will include NH_3, UV absorbence, turbidity and TOC.

Manual sampling at weekly intervals is carried out downstream of the major sewage works, and the effluents are sampled more frequently (daily at best).

B.6 AIRE CASE STUDY

The following sites are involved:

Esholt STW, Keighley STW (Marley), Bingley (Dowley Gap) STW, Bradford Beck (a poor quality tributary suffering from sewerage system problems), Knostrop and downstream, Canal Cut offtake downstream of Leeds and its return.

A possible secure site near Leeds for a new monitor, to support a possible Main Phase to the Study, is Skelton power station.

The following historical data sources are available to support the modelling study:

(i) Esholt continuous monitoring data (at Sandoz).

(ii) Esholt STW flows only

(iii) Rodley STW flows and concentration.

(iv) Diurnal/seasonal profile data for STWs.

(v) Minor discharges.

(vi) Flow duration curves for Oulton Beck.

(vii) Spot samples (time, date) of NH3, DO, BOD, N (NO_3, NO_2, and TON), temperature, chlorophyll, pH and phosphate for reach from Sandoz to downstream of Knostrop.

(viii) Canal Cut data (tertiary treatment).

(ix) Fleet Weir weekly spot samples.

There are also weirs at: Armley, Kirkstall PS, Dark Arches, New Mill and Kirkstall Abbey. Surveys of these weirs could be made available.

(x) Travel time data (to be provided on disk plus report).

Annex C Document Inventory

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University of Lancaster (1990) The ADZ Network Manual. IBM-PC Version Edition 0.1. Centre for Research on Environmental Systems.

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