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M. Bruen

E. Mockler

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A variable-structure catchment model as the engine for a water quality decision support tool facilitating scientific debate and collaboration.

M. Bruen[a], E. Mockler[b]
[a,b]*Centre for Water Resources Research, University College Dublin, Ireland*
([a]michael.bruen@ucd.ie, [b]eva.mockler@ucd.ie)

Abstract: Distributed or semi-distributed models are usually cascades of lumped models, each with an identical structure. This, classical, approach has a number of drawbacks; (i) each lumped model must be sufficiently general and thus complex to cope with the range of hydrological situations possible and (ii) it precludes debate and discussion between scientists about the most appropriate model conceptualisation and in particular it precludes using different conceptualisations in different areas to adapt the model to different hydrologic regimes, perhaps even in the same catchment. Both of these lead to distributed models that are unnecessarily complex and over-parameterised with consequent implications for parameter estimation. The rigid, fixed, structure also adds to the difficulty in modelling specific pollution mitigation measures at scales smaller than the catchment model. A hydrological model that has a flexible and variable structure has been developed to address these issues. Based on a network structure, the model allows scientists to discuss and alter the catchment hydraulic connectivity, incorporating personal knowledge as well as field experience and to change the degree of complexity used to model individual processes. In particular, knowledge of subsurface materials and hydraulic connections can be incorporated into the model structure. As the water quality component is still in development, the case study here focuses on investigating the hydrology in a karst catchment in the West of Ireland.

***Keywords**:* Flexible hydrological model; collaboration; flexible network; pathways; Ireland.

1 INTRODUCTION

1.1 Motivation to Facilitate Collaboration

Water as an essential requirement for human life, agriculture and nature, is affected by generating and transporting pollutants and is also the medium for the chemical reactions that transform or degrade them. Hence hydrological modellers interact with a wide variety of other disciplines. While much attention has been focussed on making hydro-environmental models and model output accessible to stakeholders and other end-users e.g. McIntosh et al. (2011), there are considerable differences in requirements for modelling interaction with these end-users compared with interaction between disciplines. Here we take a look at how model structures can be produced that facilitate interaction between the modeller and experts in other disciplines so as to facilitate productive collaboration in the modelling process, allowing these experts from other disciplines to suggest structural changes and see the result of those changes and so promote confidence in the resulting completed model.

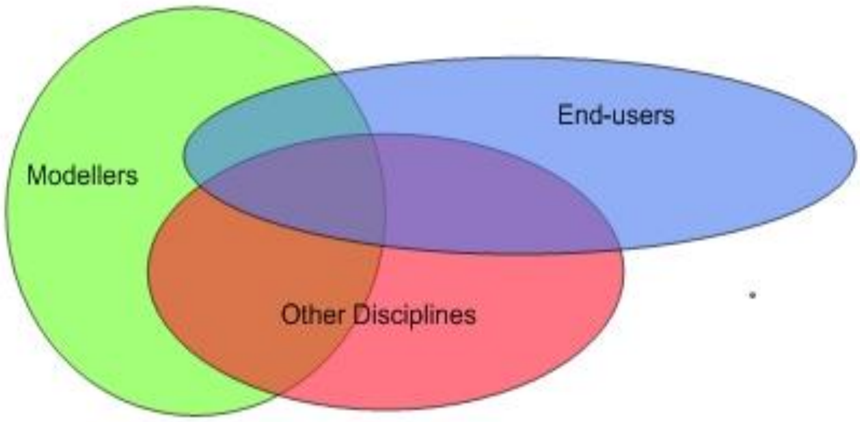

Figure 1. Modellers, other expertise and stakeholders/end-users

For fruitful collaboration with experts from other disciplines, the modeller must, ideally,

i. communicate information on the internal model structure and how it works.

ii. be able to easily incorporate suggestions from other domain experts about the important variables, processes, parameters and structural linkages that should be incorporate into the model.

iii. be able to show these collaborators the effects on model performance of including their suggestions.

For effective collaboration a model structure should be able to achieve all three functions and our variable structure hydrological model was developed to do this.

1.2 Examples of Domain Experts Queries

In hydro-environmental modelling, the suggestions from other disciplines may include;

From meteorologists:
Effects of different degrees of spatial and temporal disaggregation of meteorological data and of additional meteorological variables, e.g. wind speed and direction in relation to aerial deposition of pollutants, or temperature.

From agricultural experts:
Effects of additional information on land-use practices, land-spreading of potential contaminants, stocking densities etc.

From hydrologists:
Effects of complexity of infiltration (simple runoff coefficient, soil moisture balance, or Richardson equation), runoff or routing processes, e.g. linear channel, Muskingum, kinematic or full dynamic routing. Effects of catchment averaging.

From hydrogeologists:
Effects of sub-surface water exchanges, e.g. gain or loss of water from catchment (since catchment is defined by surface topography), or information from independent sources about water fluxes and pathways.

From biologists:
Effects of predicted flows and contaminant concentrations and/or fluxes on river ecology, e.g. the acute vs. chronic nature of impact.

2 FIXED vs. FLEXIBLE MODEL STRUCTURE

2.1 Examples from Water Quality Modelling

There are many existing models for investigating fluxes of nutrients and other contaminants in catchments, including SWAT (Arnold & Fohrer 2005), HSPF (Bicknell et al, 1997), HYPE (Lindstrom et al, 2010), INCA-N/P (Wade et al. 2002; Dean et al. 2009) and MONERIS (Behrendt et al. 2002). These models, similarly to most traditional models, regardless of their complexity have been developed with a fixed internal structure so that all that can be done to fit them to particular catchments is to change the numerical values of their parameters. Also, the structure has to be, ab initio, as complex as the authors think necessary to accommodate a wide range of catchment types and sizes. One way to address this issue is to use a flexible modelling framework to link the modeller's choice of components from a menu of existing fixed structure models. Several such flexible modelling frameworks have been used in order to evaluate model structure to gain insight to which model structures are best suited to specific hydrological conditions, including the USGS Modular Modelling System (Leavesley et al. 2002), Rainfall-Runoff Modelling Toolkit (Wagener 2002) and Framework for understanding Structural Errors (Clarke 2008).

An alternative approach is to incorporate the desired flexibility at a more fundamental level, i.e. in the internal structure and connectivity of the individual modelling components. The resulting flexible structure environmental model offers many benefits, in particular the ability to simplify the model structure by only including components to model the relevant processes in the specific catchment in question and , importantly, to omit components that model processes not active in that particular catchment. This ability to include and exclude components and to change the connectivity between them facilitates debate and discussion about the most appropriate model conceptualisation for different hydrologic regimes. This approach is not completely new, for example, Kavetski and Fenicia (2011) discuss how the dialogue between modeller and experimentalist in hydrological science can benefit from a common language to exchange qualitative and quantitative information. Their SUPERFLEX model framework (Fenicia et al., 2011) facilitates the development of conceptual hydrological models that represent dominant catchment dynamics in a physically meaningful way while remaining parametrically parsimonious and computationally efficient. This is achieved by modelling hydrological systems with combinations of generic components, or building blocks, enabling modellers to hypothesis and experiment to gain further understanding. Another example is the Watershed Bounded Network Model (WBNM, Boyd 1996), a flood hydrograph model that uses a surface network structure.

Our PAthways Computational Engine (PACE) model aims to bring these benefits to a broader audience, interested in water quality modelling and environmental consequences, by using a network model structure to allows scientists to discuss and alter the catchment hydraulic connectivity, incorporating personal knowledge as well as field experience and to change the degree of complexity used to model individual processes, including source mobilisation and fate of water-borne contaminants. In particular, knowledge of subsurface sources, materials and hydraulic connections can be incorporated into the model structure.

2.2 Background to Model Development

Detailed water quality catchment models quantify the flows along hydrological flow paths and determine the fluxes of sediment, nutrients, pathogens or other contaminants along each pathway. This can inform users about potential sources of pollution within a catchment and enable them to (i) evaluate the impacts of future activities or (ii) to forensically examine serious pollution incidents to determine their cause. With the increasing need for more detailed hydrological and hydro-chemical information to satisfy the demands of the EU Water Framework Directive (WFD), the Irish Environmental Protection Agency (EPA) promoted the development of the Pathways Catchment Management Tool (CMT). This tool is to aid environmental managers to identify critical source areas for selected contaminants and evaluate alternative strategies for land use and their impacts on aquatic ecosystems and target areas for enforcement of regulations. In Ireland, this is complicated by extreme heterogeneity in geology and soils and land-use (Archbold et al., 2010).

A review of existing catchment models showed that none fulfilled all of the requirements of the stakeholders or had the flexibility to incorporate new research findings specific to Irish conditions (Bedri and Bruen, 2012). It was therefore decided to develop a new GIS based application linked with a new flexible hydrological model for investigating the movement of pollution through our river basins and identifying the potential sources of contaminants. The new PAthways Computational Engine (PACE) is a semi-distributed flexible conceptual model suitable for catchment scale modelling. This model is currently in development and this paper will focus on hydrological modelling without the associated water quality modelling. Its structure facilitates the use of AI techniques to fine-tune model structure based on GIS mapping of relevant information on topography soil, geology etc. As with most conceptual models, it can be applied at a broad range of temporal and spatial scales in any region once populated with the required data. The Pathways CMT will assist users in modelling Irish catchments with the PACE model by defining appropriate model conceptualisation and parameter values with the assistance of national GIS datasets.

3 VARIABLE MODEL STRUCTURE

3.1 Pathways Computational Engine

The Pathways Computational Engine is a network based model with a variable structure. The model's governing equations are formulated in the state-space form which has many advantages including data assimilation and importantly, the simplification of the design of flexible modular software (Clark and Kavetski, 2010). The nodes of the model represent the flow paths and sum the outputs of the model links, which contain the transformation equations. In this manner, the aim is to achieve a new flexible structure the builds on existing science and has the capacity to incorporate new knowledge either in a change of the network structure or the transform equations.

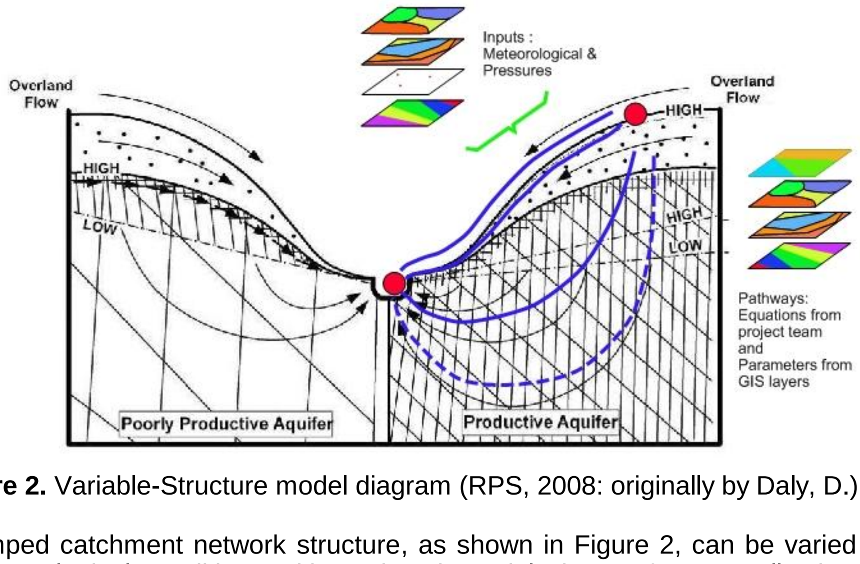

Figure 2. Variable-Structure model diagram (RPS, 2008: originally by Daly, D.)

The lumped catchment network structure, as shown in Figure 2, can be varied to suit the geological conditions with each sub-model chosen from a collection of modules. Sub-catchments can then be connected with river reach links, as in Figure 3, and the network can be further altered with by-passes or links between sub-catchments.

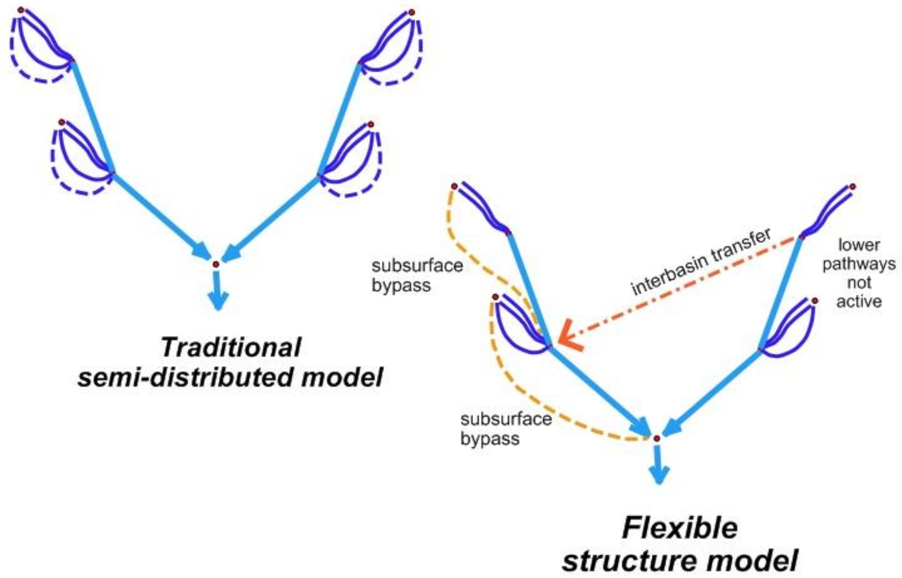

Figure 3. Example of node-link flexible possibilities.

3.2 Spatial and Temporal Data

The Pathways CMT is being developed to assist users in modelling Irish catchments with the PACE model by generating the required input files from national datasets. Semi-distributed models can be defined based on Irish EPA defined sub-catchments, with a mean area of 10km^2, and the specific structure of the sub-catchment is initially determined from GIS data including aquifer and soil type. An advanced user will be able to further adjust connections within the model network to test hypotheses on hydraulic connectivity. GIS data for soils, geology, aquifers and pressures etc. is incorporated into the model parameters to determine the distribution of flows and contaminant fluxes along surface and groundwater pathways. The hydrological component requires time series of rainfall and PE as direct inputs, typically in the range of sub-hourly to daily as availability allows. The water quality version of the model has greater data requirements depending on the contaminants investigated. These include land use practices, point sources of pollution and initial conditions. Actual evaporation and flows are produced as outputs from the model at the same time step as the temporal input data. The flows at the outlet of the catchment and at each node can be viewed along with total fluxes of any modelled contaminant such as sediment, nutrients and pathogens.

4 CASE STUDY

4.1 Case study of transfer between sub-catchments

Ireland has extensive karst features and glacial deposits providing subsurface flow paths not apparent from surface topography and so not be included in traditional semi-distributed models. In particular these channels may allow a catchment to gain or lose water from/to other catchments. This results in an imbalance in the water-balance for each catchment. In PACE, these can be modelled by altering the network model to include additional subsurface flow links.

Upon finding that the water balances are not closed in sub-catchments a hydrologist may hypothesis that there is a flow path along a transecting aquifer between the sub-catchments. A traditional model would have a generic lumped catchment model for each of the sub catchments, which may be adequate if the total outflow is the only quantity of interest. But if this particular aquifer flow path is affecting the internal flows and possibly associated water quality, then including it in the model structure may prove beneficial.

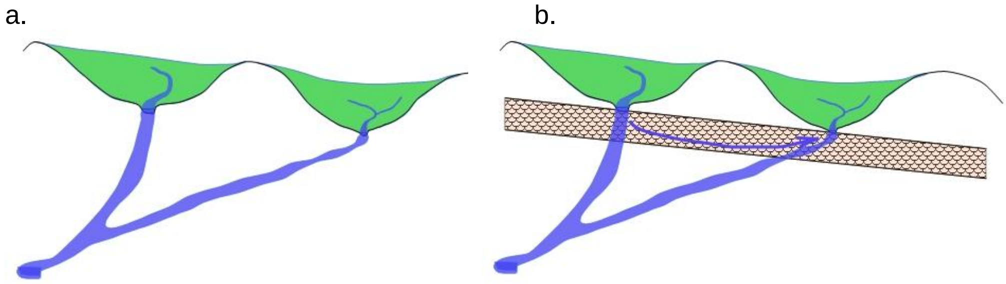

Figure 4. Connected catchments (a) and catchments showing aquifer flow path (b)

4.2 Deel Catchment

The Deel sub-catchment is a tributary of the Moy catchment in the West of Ireland, with an area of 156km^2. Hydrometric statistics from the catchment are derived from data from the Office of Public Works from 1972 – 2006. The average annual rainfall from this period is 1587mm/year, the mean flow at the Ballycarroon flow station is 6.6m^3/s and the estimated evapotranspiration losses are 443mm/year. This suggests estimated gains to the catchment of 185mm/year, which is over 10% of the total yield. The catchment bedrock is mostly limestone and sandstone formations and with some karst features.

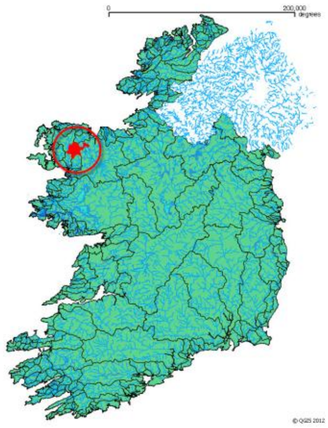

Figure 5. Deel Catchment

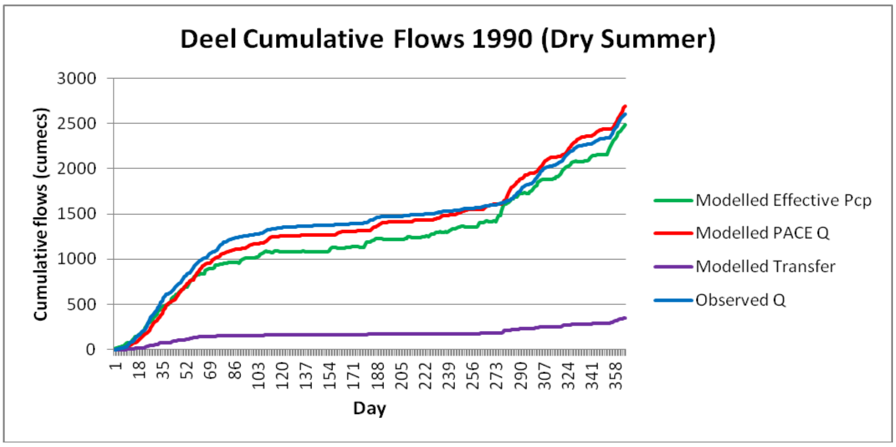

Figure 6. Deel modelled and observed cumulative flows 1990

The flexible network model of the PACE model is used to investigate the possible hydrological connections that may be present in this complex catchment. It is hypothised that the unaccounted for flows in the catchment are rain-fed and so an adjacent catchment model used to simulate the transfer of flows. The Deel and adjacent catchment were modelled independently, with the addition of an external transfer into the Deel from the adjacent catchment, implemented by an additional network link.

Figure 6 shows the cummulative modelled and observed flows for 1990, a year with a relatively dry summer period. This graph suggests that transfer into the catchment is relatively inactive during the dry summer and that additional inflow is linked to rainfall. Figure 7 illustrates a year with a wet summer, 1997, showing the the transfer into the catchment remained active throughout the seasons.

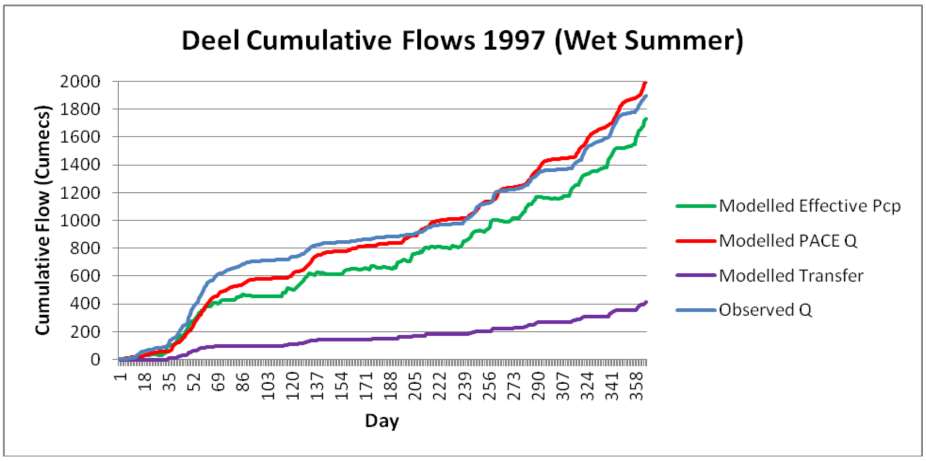

Figure 7. Deel modelled and observed cumulative flows 1997

5 DISCUSSION

The PACE model was used to investigate catchment connectivity in the Deel by including an adjacent catchment in the network structure which delivered a transfer of flows. The flexible network was structured to simulate a rain-fed input by linking the output of a sub-model of the adjacent catchment to the input of a sub-model of the Deel. Figures 6 and 7 show that this transfer of flows is a plausible mechanism to account for the additional flows in the catchement. Although not caried out here, this investigation of the hydrological regime can facilitate the modelling of water quality, especially if the catchment providing the transfer into the Deel also contains active pressures e.g. diffuse inputs of nutrients from agricultural sources. This method of investigating processes through modifying a flexible model structure can be insightful in a broad range of situations. Each river catchment has characteristic dominant hydrological pathways varying with multiple factors including geology, soil type, landuse, season and so on. By determining the important processes for the specific conditions, we can focus our attention on the dominant contaminant transport and attenuation mechanisms.

Domain experts may have issues with aspects of fixed structure models that deter use of the model, or at a minimum reduce their confidence in the model outputs. By enabling/ empowering the non-programming expert with the tools to interact with the structure of a hydrological model, we can enhance their willingness and ability to communicate and collaborate. The model described in the paper is one example of this approach and produces a model be used as the core of environmental and water quality simulation software and related decision support systems.

6 CONCLUSIONS

The EU Water Framework Directive (WFD) has increased the need for detailed hydrological and hydrochemical information. Modelling of water flow paths within a catchment, rather than overall response, is needed to investigate the physical and chemical transport of matter through the hydrological cycle. Furthermore, the WFD has been a catalyst for interaction, understanding and communication between the many disciplines involved in implementing the directive (Bruen, 2009). The Pathways Computational Engine was developed to facilitate collaboration and easily incorporate new science and knowledge from all collaborators.

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