

Apportioning non-linearity in conceptual rainfall–runoff models: examples from upland UK catchments

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ABSTRACT

Rainfall–runoff modellers distinguish between flow generation and flow routing processes, and many models treat the two types of process independently. These models commonly assume that the dominant non-linearity in the rainfall–flow response resides in the flow generation process. This paper revisits three upland UK catchments where such an assumption has previously been made and explores the apportioning of non-linearity, its identifiability and how it is affected by catchment type, season, data time-resolution, objective function and model equations. The catchments showed stronger routing non-linearity than expected and comparatively little non-linearity in flow generation both in wet winter periods and in mixed wet-dry summer periods, although in one catchment this result was sensitive to a modification of the model equations. Aggregating data to time resolutions approaching the response times of the catchments makes the flow generation appear more non-linear than it actually is, less so if performance is assessed using log-transformed flows. In cases, using conceptually distinct models achieved similar Nash–Sutcliffe efficiency (NSE) performances; however, using a single non-linear routing function with a linear or near-linear loss model was considered the most efficient overall. Using this model, NSE values of up to 0.99 were obtained.

Key words | Hodder, kinematic, lumped models, Pontbren, top-down modelling, ungauged catchments

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INTRODUCTION

The attraction of rainfall–runoff models of the metric-conceptual type (Wheater *et al.* 1993) is the potential for combining prior knowledge of hydrological response (via the prior model structure and prior values or ranges of parameters) with empirical estimation procedures, with the aim of well-identified models which capture the relevant response modes of the system. Despite the attraction of simplicity and low parameter uncertainty, the metric-conceptual model approach involves the problem that the empirical estimation procedure will be conditional on prior perceptions about model structure, as well as on the dataset used and assumptions about the nature of its errors. This problem is well-recognised and has led to a number of attempts to reduce the reliance on prior perceptions while maintaining conceptually plausible models (e.g. Young 2003; Lee *et al.* 2005; Lin & Beck 2007; Fenicia

et al. 2008) and to quantify the uncertainty in model parameters and predictions associated with model structure and data errors (e.g. Kavetski *et al.* 2006; Bulygina & Gupta 2009; Bulygina *et al.* 2011).

The parameter estimation problem may be of particular concern when conceptual models are applied to regionalisation of hydrological responses (McIntyre *et al.* 2005; Littlewood & Croke 2008). Regionalisation requires the modeller to establish the dependency of the hydrological response – either in the form of model parameters or as response signatures – on catchment characteristics, for the purpose of prediction and/or for understanding the physical controls on response. This generally involves estimating parameters for a set of gauged catchments, and developing empirical relationships between the parameter estimates and catchment characteristics. Uncertainty in the parameter

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values may be introduced from various sources: the calibration data, the choice of objective function, inherent equifinality, dependency of parameters on the pre-conceived model structure or approximations used in the numerical solution. The consequent uncertainty is a major obstacle to prediction in ungauged catchments and hydrological understanding (Wagener *et al.* 2004).

The conceptualisation of a catchment usually explicitly distinguishes between runoff generation (i.e. the effective rainfall estimate, equal to total rainfall minus the losses) and routing (the travel time distribution of effective rainfall as it makes its way to the catchment outlet). Although both are known to be non-linear processes in theory, many (if not most) conceptual models assume that the predominant non-linearity lies in the runoff generation and that a linear approximation to routing is justifiable (Beven 2001). The reasons for this are: (1) as mentioned above, the traditional view that most of the non-linearity is associated with runoff generation; (2) the data are often aggregated to time-steps larger than the average response time of the catchment so that the detail of the routing processes becomes unidentifiable; and (3) very few forms of non-linear routing can be solved accurately without using time-demanding numerical solutions to the governing differential equations (Moore & Bell 2002). There are therefore at least three reasons why a modeller might choose to presume either linear routing or, at least, a numerically convenient form of non-linearity.

Although it is common, the assumption of linear routing does not promote faith that the model is fit for purpose. The theoretical presence of non-linearity is often reflected in performance improvements when it is included (Wittenberg 1994; Romanowicz *et al.* 2006; Segond *et al.* 2007). Even when performances between alternative models are indistinguishable for practical purposes, inferences about processes may be biased by the assumption of routing linearity (McIntyre *et al.* 2011). One approach to avoiding the assumption altogether is physics-based, or bottom-up, modelling where routing non-linearity is specified on the basis of prior theory rather than an arbitrary assumption. Where the physical basis for the model (e.g. surface and subsurface flow pathways and hydraulic properties) is well enough defined and where the numerical solutions to the non-linear equations are efficient enough to make the model

computationally tractable (e.g. Al Qurashi *et al.* 2008), this might work well. Of interest here, however, are the cases where the dominant source of information is the rainfall-runoff time-series data so that a more conceptual approach is applicable.

This paper will explore the benefits and difficulty of including a realistic degree of routing non-linearity in conceptual rainfall-runoff models of upland UK catchments. Before defining the specific objectives of the paper, it is useful to review in more detail why routing non-linearity may be important and why it is often neglected or treated simplistically.

ROUTING IN CONCEPTUAL RAINFALL-RUNOFF MODELS

The theory of runoff routing under idealised conditions has been documented extensively, both for surface and subsurface pathways (Parlange *et al.* 1981; Germann & Beven 1985; Moore & Bell 2002; Dooge & O’Kane 2003). Of most relevance to conceptual rainfall-runoff models are the simplifications of theoretical equations that lead to the power law relationship:

$$q = ky^m \quad (1)$$

where, in the context of surface flow, q is flow per unit area and y is water depth (or volume V per unit surface area). Where friction dominates the energy loss, so that acceleration and pressure gradient terms can be neglected, this is an expression of the non-linear kinematic wave equation (Dooge 2005; Ding 2011). Different values of k and m in Equation (1) (or indeed alternative equations) might be applied to distinguish between different flow routes in a catchment (e.g. hillslope surface, groundwater and channel routing); however, this paper is mainly concerned with the spatially lumped models that do not attempt such a distinction. Parameters k and m depend on the physical properties of the system, with m often assumed equal to 1.67 for fully turbulent surface flow and theoretically equal to 3 for laminar surface flow (Moore & Bell 2002), while k depends on the surface roughness and topography. Theoretical analysis of saturated subsurface flow under idealised conditions

also leads, under certain assumptions, to the form of Equation (1) where y represents the groundwater storage. For example, $m = 2$ for a homogeneous unconfined aquifer outflow under Darcy's law and Dupuit's assumption, and $m = 1$ for an idealised confined aquifer (Moore & Bell 2002). A slowing of flow with increasing depth, for example due to increased friction associated with over-bank flow, is signified by $0 < m < 1$, while $m < 0$ signifies that depth reduces as flow increases, intuitively unrealistic in a natural system.

However, it may be expected that the nature of surface and subsurface flow from a real catchment is potentially less predictable than implied by the form of Equation (1) and theoretical values of m . Theoretical development of Equation (1) disregards components of the small-scale physics of water flow (Beven 2001), and both the form of Equation (1) and the values of k and m depend on the micro and macro-scale features of the surface; they are therefore expected to change over time and along the flow path. For example, stronger non-linearity (higher m) may be introduced if surface roughness decreases with increasing water depth due to surface vegetation properties (Holden *et al.* 2008), or reduced (lower m) due to over-bank flow effects (Romanowicz *et al.* 2006). There may be subsurface flow thresholds due to activation of macropores, karstic flow paths and groundwater springs (Grayson *et al.* 1997; Hughes *et al.* 2011), and interactions between flow routing and flow losses may affect the hydrograph shape (Croke 2006).

Although alternative q - y relationships have occasionally been used to address these issues (e.g. Wagener *et al.* 2004; Lee *et al.* 2005; Fenicia *et al.* 2008), it is common to employ a routing model in the form of Equation (1) for each of the routing pathways being considered (e.g. Mein *et al.* 1974; Wittenberg 1994; Mwakalila *et al.* 2001; Segond *et al.* 2007). Most such models employ a pre-specified value of m (e.g. $m = 1, 2$ or 3) which allows an exact or approximate analytical solution to the routing model (e.g. Moore & Bell 2002; Lamb & Kay 2004; Oudin *et al.* 2008). In almost all such cases, no theoretical or empirical evidence is offered to support the assumed value of m ; it seems it is fixed for the purpose of numerical efficiency with the implicit acceptance that it may produce suboptimal fits to observed flow. The number of modelling studies which presume linear routing stores, $m = 1$, is particularly

large. This includes models used for making predictions and inferences in particular catchments (Lees 2000; Young 2003; Wagener & McIntyre 2005; McIntyre & Al Qurashi 2009), large studies aiming to produce methods for generalising parameter values (McIntyre *et al.* 2005; Lee *et al.* 2006), as well as studies which aim to identify the catchment and climate features which control runoff response (Beven *et al.* 2008; McIntyre & Marshall 2010). The implications of assuming a particular value of m have not been well studied in any of these contexts.

Despite the argument that routing non-linearity deserves to be given more attention in conceptual modelling, top-down identification of systematic non-linearity may be difficult. The unobserved spatial patterns of rainfall will activate different parts of the catchment, introducing apparent stochastic variability into routing parameters (Botter 2010). Errors in precipitation and streamflow measurement, and parameter equifinality, may obscure non-linear signals (Kavetski *et al.* 2006). The flow is typically derived from stage-discharge equations, which themselves have uncertainty in their degree of non-linearity (Romanowicz *et al.* 2006). As previously noted, temporal and spatial aggregation of data and models may obscure non-linear signals. Given these issues, an initial exploration of non-linearity in routing, which aims to eliminate errors associated with model inputs and space-time aggregations, would ideally use high-resolution and high-accuracy rainfall-runoff data from relatively small and uniform catchments, an approach that is followed in the case study.

In summary, the assumptions commonly used about routing in conceptual rainfall-runoff models are numerically convenient and avoid the potentially difficult task of data-based optimisation of non-linearity. Although prior assumptions about routing are often considered to be adequate, accuracy is likely to be suboptimal. With little or no theoretical or empirical basis, presumptions about routing are intellectually unsatisfactory.

The hypotheses pursued in this paper, all explored using case studies of upland catchments in the UK, are as follows.

- The performance of optimised non-linear routing models can be considerably better than either assuming linear routing or a numerically convenient degree of non-linearity.

- The identification of routing non-linearity can contribute to process understanding, and can avoid false inferences about runoff generation non-linearity.
- Linearisation by discrete time solutions and hybrid analytical-numerical solutions can ameliorate the numerical burden of a non-linear routing model of the form of Equation (1) without significant loss of accuracy.
- The loss of information when moving to data of lower temporal resolution can make the accurate and precise allocation of non-linearity between runoff generation and routing increasingly problematic.
- The differences in non-linearity between catchments can be partly explained by known differences in catchment properties.

CASE STUDY DESCRIPTION

Catchment descriptions

The Pontbren experimental catchment in Wales was instrumented from autumn 2004 to winter 2009/2010. The experiment is described extensively by Jackson *et al.* (2008), McIntyre & Marshall (2008, 2010) and Marshall *et al.* (2009). Results from two of the catchment's flow gauges (gauges 5 and 9, see McIntyre & Marshall (2010) for locations) are reported in this paper. The results from these two gauges are representative of those from the 12 other Pontbren gauges. The catchment areas are 2.4 and 4.1 km² for gauges 5 and 9, respectively. Both catchments are dominated by slowly permeable clayey loams, with peaty upper soil layer in the higher elevations of the gauge 9 catchment. That catchment also contains two lakes with a combined catchment area of 1.3 km², 32% of the gauge 9 catchment area. Other relevant catchment properties are listed in Table 1. Six tipping-bucket rain gauges in and around the catchment are used to estimate rainfall (see McIntyre & Marshall (2010) for locations). Based on continuity of data and absence of significant snow, two periods were selected for modelling: 1 December 2006–31 January 2007 and 10 May 2007–9 July 2007. Figures 1 and 2 include the observed flow and rainfall at the two gauges for these periods. The former period is wet with only 3 days without rainfall; the latter period has long dry and wet spells.

Table 1 | Properties of the gauged catchments

Gauge	Pontbren 5	Pontbren 9	Hodder Place
Catchment area (km ²)	2.4	4.1	260
Elevation range (mAOD)	282–405	262–438	40–544
Improved grassland coverage (%)	70	13	61
Open water coverage (%)	0.3	2.6	0.6
Woodland coverage (%)	7.7	1.1	7.0
Other land cover (%) ^a	22	83.3	31.4
BFI-HOST	0.27	0.34	0.33
Average response time (hours) ^b	2.4	13	9.4
Annual average rainfall	1,449 ^c	1,449 ^c	1,602

^aPredominantly moorland, arable land and roads.

^bAs reported by McIntyre & Marshall (2010) and Young (2003).

^cMeasured from 1 April 2007 to 31 March 2009.

The third case study gauge is the Hodder Place gauge at the outlet of the Hodder catchment, northwest England. Details of the catchment can be found in O'Donnell *et al.* (2008), Ewen *et al.* (2010) and Bulygina *et al.* (2012). The catchment area is 260 km². Soils are mixed, but much of the catchment is dominated by peat and other slowly permeable soils. There is one reservoir with a catchment area of 37 km², 14% of the Hodder Place catchment area. Other relevant properties of the Hodder Place catchment are listed in Table 1. Four tipping-bucket rain gauges in the catchment are used to estimate rainfall (see Ewen *et al.* (2010) for locations). As in Pontbren, winter and summer periods are selected for analysis: 1 December 1991–31 January 1992 and 1 August 1992–30 September 1992. Figures 1 and 2 include the observed flow and rainfall at Hodder Place for these periods.

These case studies were chosen due to the availability of good-quality 15-minute rainfall and flow data, and because between them they provide some variation in hydrological responses in the context of upland UK. Additionally, all three catchments have been modelled before (Young 2002, 2003; Bulygina *et al.* 2009; McIntyre & Marshall 2010), which provides benchmark performances and parameter estimates. Relatively short (2-month) periods were used for the analysis to facilitate extensive Monte Carlo analysis. Winter and summer periods were analysed separately to

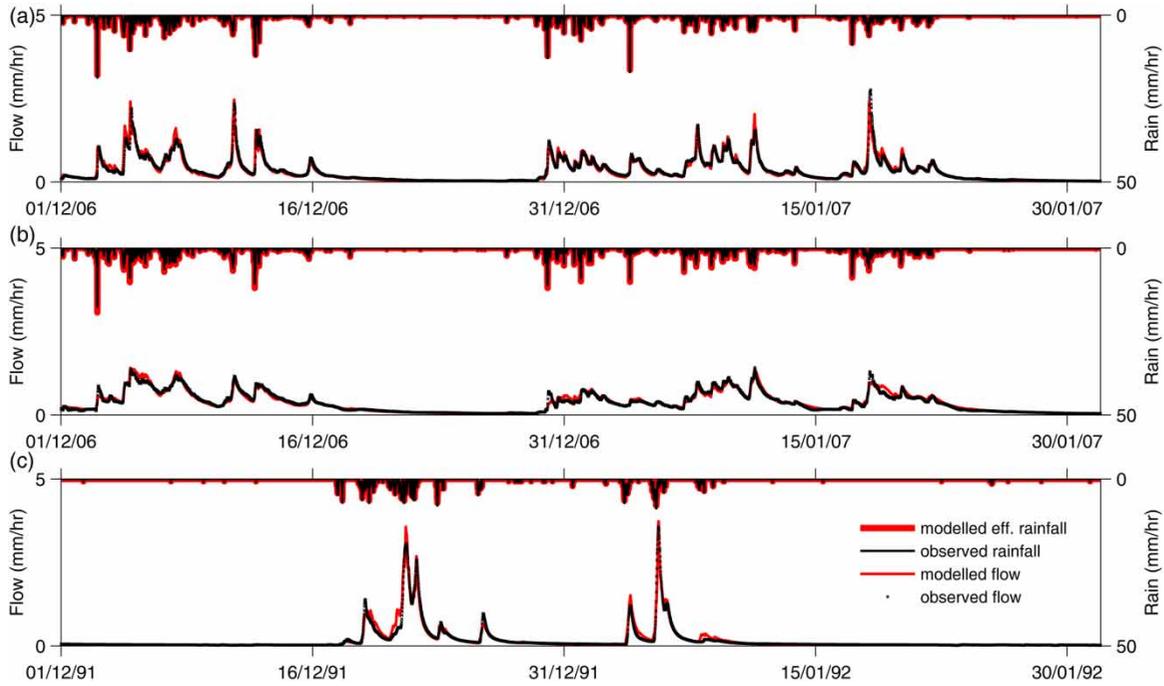


Figure 1 | Winter period time-series and example model result using one non-linear store. (a) Pontbren G5, (b) Pontbren G9, (c) Hodder Place.

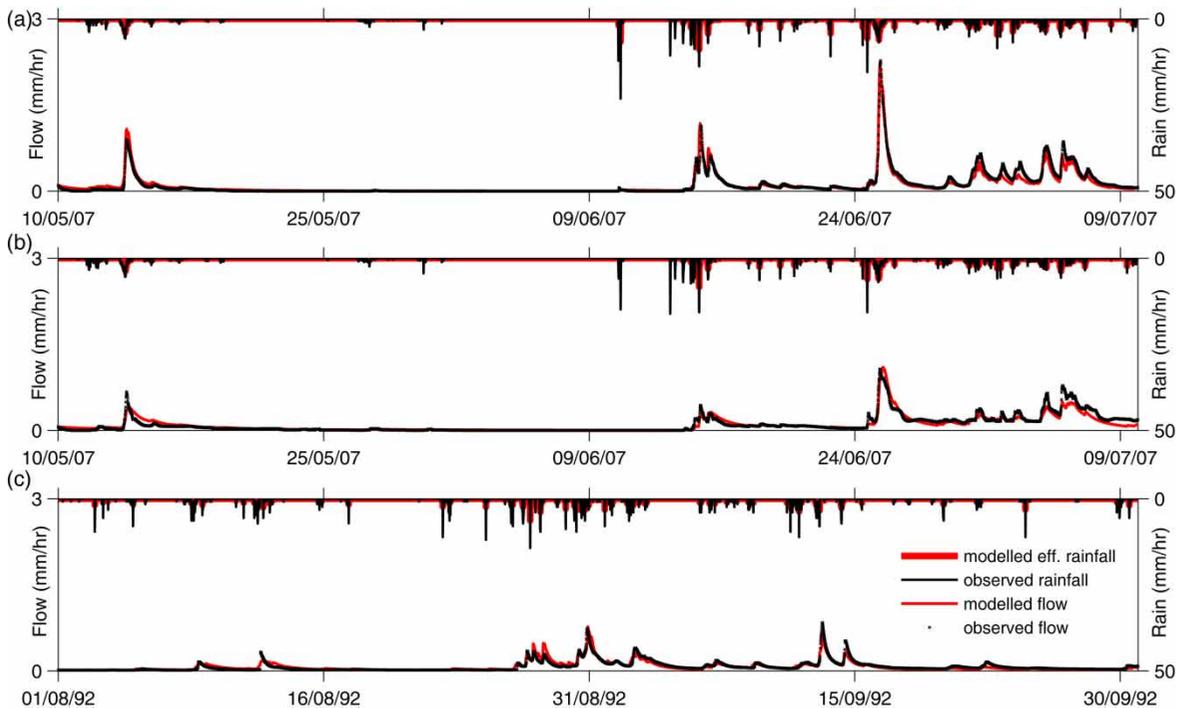


Figure 2 | Summer period time-series and example model result using one non-linear store. (a) Pontbren G5, (b) Pontbren G9, (c) Hodder Place.

look for seasonal effects on the nature of the non-linearity. The rainfall and flow data are available as averaged values over 15-minute time intervals. As well as using 15-minute input and output resolution ($\Delta t = 15$ minutes), the data are aggregated to time intervals of $\Delta t = 1, 4$ and 24 hours to explore how time resolution influences the apparent nature of response non-linearity. The spatial rainfall used as inputs to the model were calculated from the gauged values based on Thiessen polygons. The use of Thiessen polygons (and any alternative rainfall estimation technique) will introduce a mixture of random and systematic errors to the rainfall estimates and hence into modelled flow; this is assumed not to significantly affect the evaluation of non-linearity in rainfall-runoff response here.

Rainfall-runoff model

The models used are spatially lumped conceptual models, which are used in a 'top-down' manner in the sense that parameters are empirically identified. The model is divided into a runoff generation module, which conceptually represents the vertical movement of water and evaporation losses, followed by a flow routing model representing the horizontal transfer of water to the catchment outlet. The routing models tested all use either a single store or two parallel stores, with the continuous relationships between volume of stored water and outflow defined by Equation (1). Equation (1) can be used to derive a model that can be directly solved for flow:

$$\frac{dq}{dt} = \frac{dq}{dy} \frac{dy}{dt} = mky^{m-1} \frac{dy}{dt} \quad (2)$$

Hence,

$$\frac{dq}{dt} = mk^{1/m} q^{1-1/m} \frac{dy}{dt} \quad (3)$$

where dy/dt is the rate of change of volume (per unit area) in the store, equal to the balance of effective rainfall and outflow, so that:

$$\frac{dq}{dt} = \alpha q^\beta (u_{t-\delta} - q) \quad (4)$$

where $u_{t-\delta}$ is effective rainfall at δ time units before t to allow for a lag in response, $\beta = 1 - 1/m$ and $\alpha = mk^{1/m}$. If a two-parallel store model is being used, then α and β need to be estimated for each store (in this case, subscripts f and s are used in this paper to distinguish between the parameters of the faster-responding and slower-responding stores, respectively) and there is an additional parameter γ that defines the proportion of effective rainfall going to the faster-responding of the two stores.

In this paper, there is therefore a maximum of six calibrated routing parameters: α_f , β_f , α_s , β_s , δ and γ . The β parameter, as well as being calibrated, will be fixed to a numerically convenient value of 0, 0.5, 0.67 or 1.0 (corresponding to $m = 1$, $m = 2$ and $m = 3$ in Equation (1), respectively, and to an exponential type storage) depending on which is closest to the optimised values.

The integration of Equation (4) is performed using exact or approximate analytical solutions when $\beta = 0, 0.5, 0.67$ or 1.0 (Moore & Bell 2002). Otherwise, Equation (4) can be solved with a specified maximum truncation error using the high-order numerical integrator function ode45 of MatLab, integrating over each individual input time-step in turn to avoid integrating over function discontinuities. Alternatively, it can be solved using the approximation that dq/dt is constant within each time-step but varies between time-steps, which may be considered as a linearisation of the model, so that an explicit Euler solution scheme can be accurately applied. This provides scope to reduce computation time but with unknown linearisation error and may lead to unsatisfactory results (Kavetski *et al.* 2011). As a second alternative solution scheme, in the time-steps when $u_{t-\delta} = 0$ and $\beta \neq 0$ (irrespective of the value of β) Equation (4) may be analytically integrated to give:

$$q_n = \frac{1}{(\beta\alpha\Delta t + q_{n-1}^{-\beta})} \quad (5)$$

where Δt is the model input-output time interval. This can significantly reduce the computational burden. For example, in the Pontbren case study, even in the wet winter period, $u_{t-\delta} = 0$ for approximately 65% of the 15-minute time-steps. In all cases, the initial conditions are estimated from the observed flow values.

To provide the time-series of u , the runoff generation model is a power-law relationship between catchment wetness and runoff ratio:

$$u = \mu r y^\lambda \quad (6)$$

where y is a measure of catchment wetness, r is rainfall rate aggregated to the specified time resolution, μ is a volume balance parameter and λ is a non-linearity parameter.

This 'wetness index' model is commonly used and has been widely found to give good performance (Lees 2000; Young 2002, 2003; McIntyre *et al.* 2011). Observed flow (q') is often used as the wetness index where the immediate purpose is model identification rather than scenario analysis (Young 2003; Beven *et al.* 2008; McIntyre & Marshall 2010). The use of an observed wetness index avoids the speculation involved in developing a soil moisture model to estimate y . The good performance achieved with this wetness index allows the investigation to focus on identifying the routing component. In this study, comparison of the calibrated values of coefficients λ and β provides a direct comparison of the importance of the two conceptually distinct types of non-linearity.

Parameter estimation

For parameter estimation, the Nash-Sutcliffe efficiency (NSE) criterion is used. Although in many cases the information it provides is limited to that of model performance (Schaeffli & Gupta 2007), it has been found to be a reasonable indicator of performance for the case study catchments (Young 2003; McIntyre & Marshall 2010; McIntyre *et al.* 2011) (note that in these three papers, NSE is referred to as R_T^2). The NSE applied to the base 10 logarithms of the flows ($\text{NSE}_{10\log}$) is used for comparison. To explore parameter response surfaces and ensure that good estimates of the global optima have been found, a uniform random search procedure was used with constraints $0 \leq \lambda \leq 2$ and $0 \leq \beta \leq 2$ (although $\beta > 1$ is physically unrealistic, it is of interest to see how well the model performs in that part of the parameter space). During optimisation, the lower and upper constraints on δ were [0, 60] minutes for the Pontbren gauges and [120, 240] minutes for the Hodder; the corresponding constraints on α were [0.01,

0.4] and [0.0001, 0.2] $\text{minutes}^{-1/m}$. These constraints were based on time lags and response times estimated in earlier studies (Young 2003; McIntyre & Marshall 2010). Iteration of these constraints was used in estimating the conditional λ - β response surfaces. Using a non-linear optimisation algorithm in conjunction with the random search did not improve upon the NSE values (within a tolerance of two decimal places) from the random search alone. The only parameter which is not calibrated by optimising the NSE is the water balance parameter μ : it is fixed so that the volume of effective rainfall equals the observed volume of flow.

Summary of procedure

The above method description may be summarised as follows.

1. With 15-minute resolution data from one catchment, use the NSE criterion to optimise a five-parameter (α , β , δ , λ and μ) non-linear model defined by Equations (4) and (6) in the winter period, solving using a high-order numerical integrator.
2. Repeat (1) using the linearised solution, then using the hybrid analytical-numerical solution, then with analytical solutions by fixing β to numerically convenient values including $\beta = 0$ (linear store).
3. Repeat (1-2) using a two-parallel store model with eight parameters (α_f , β_f , α_s , β_s , δ , γ , λ and μ).
4. Repeat (1-3) using 60-minute, 4-hour and 1-day resolution data.
5. Repeat (1-4) using the summer period.
6. Repeat (1-5) using the two other case study gauges.
7. Repeat (1-6) using the $\text{NSE}_{10\log}$ criterion.
8. Assess performances, parameter values and parameter uncertainty, and discuss results in the context of the aforementioned hypotheses.

RESULTS AND DISCUSSION

Following the hypotheses raised, the results of primary interest are: (1) performances across alternative routing structures and inferences about catchment conceptualisation; (2) the relative magnitudes of β and λ , their uncertainty and

what, if anything, this can tell us about processes; (3) how to maintain accuracy while minimising numerical burden; (4) the effects of time resolution of model inputs on ability to accurately identify non-linearity; (5) the variability of β and λ between catchments and how this might be explained; and (6) the potential influence of model equation error on results.

Model performance and conceptualisation

Using the highest-possible data resolution (15 minutes), the performances of various routing models over the three gauges for the winter and summer periods are listed in Table 2 and example time series results are depicted in Figures 1 and 2. It is clear from Table 2 that there is a significant increase in performance when including a non-linear routing parameter in a single-store model. The difference in winter period performance between a single non-linear store and a two-parallel linear store model is small, with the former model having NSE values of 0.96, 0.96 and 0.96 for the three gauges and the latter model 0.96, 0.97 and 0.95.

Re-fitting the model on the summer period data, these two alternative models also gave more or less the same NSE performance. The single non-linear store model, however, has one less parameter and inspection of the time series also shows that it gives a generally more satisfactory fit to hydrograph recessions. This is supported by a recession analysis, which shows a non-linear relationship between observed dq/dt and q . If the parameter sets optimised in

the winter period are applied to the summer period, this also suggests that a single non-linear store is preferable (with NSEs of 0.93, 0.88 and 0.65 for the single non-linear store and 0.93, 0.90 and 0.50 for the two linear stores). The addition of non-linearity to either store of the two-store model did not improve upon the simpler models. (For example, the final column in Table 2 shows the optimal performance for a non-linear fast store.)

McIntyre *et al.* (2011) illustrated that examining the realism of the simulated effective rainfall could help distinguish between models. They found that if the linear routing models are used, then in order to fit the largest peak flows the model needed to generate much more effective rainfall during these events than there was rainfall. This is mathematically possible here too because the constraint $u < r$ is not imposed when fixing μ or when optimising λ in Equation (6). In the present study, this type of result is seen at gauge 9 when using two linear stores, providing some additional (although inconclusive) evidence to support the use of the more parsimonious non-linear single-store routing model for that gauge.

It is concluded that, although it is difficult to distinguish between performances of alternative models, the distribution of response times in this set of catchments is simple enough to be represented by a single store (i.e. the unit hydrograph is defined by an exponential distribution, where the parameter of the distribution is a function of flow rather than being constant). This contrasts with the more usual, alternative assumption that simulating the distribution of response times requires two parallel stores (the

Table 2 | NSE performances for alternative routing structures

Gauge no.	Calibration period	Performance evaluation period	One linear store (3) ^a	Two linear stores (5) ^a	One non-linear store (4) ^a	Two non-linear stores (6) ^a
Pontbren 5	Winter	Winter	0.89	0.96	0.96	0.97
Pontbren 9	Winter	Winter	0.93	0.97	0.96	0.96
Hodder Place	Winter	Winter	0.87	0.95	0.96	0.96
Pontbren 5	Winter	Summer	0.84	0.90	0.93	0.93
Pontbren 9	Winter	Summer	0.83	0.89	0.88	0.90
Hodder Place	Winter	Summer	0.39	0.48	0.65	0.50
Pontbren 5	Summer	Summer	0.90	0.94	0.94	0.94
Pontbren 9	Summer	Summer	0.84	0.93	0.89	0.93
Hodder Place	Summer	Summer	0.75	0.84	0.86	0.86

^a Number of calibrated parameters.

unit hydrograph is defined by two superimposed exponential distributions), neither of which vary in time (e.g. Young 2003; McIntyre & Marshall 2010). The redundancy of a slow store is consistent with the view that the Pontbren streams have little connection with groundwater, and the simple kinematic-type response of Equation (1) is consistent with the steepness of the catchments and absence of over-bank flow due to the incised channels (Marshall *et al.* 2009).

Parameter values, parameter uncertainty and further inference about processes

To evaluate the relative non-linearity in the flow generation and flow routing components, the values of parameters λ and β estimated for the single non-linear store models are examined. Table 3 shows the estimates for the winter and summer periods. Although there is random sampling error in the estimates, the same values (to two decimal places) were found after repeating the search procedure for Pontbren gauge 5 (and this convergence was assumed to hold for the other gauges). Parameter λ is zero or near-zero in all winter cases. The runoff generation is therefore implied to be linear or near-linear in this period. Although these were generally wet periods, they included dry spells (Figure 1) and, where observed in Pontbren, the ground was not continually saturated (Marshall *et al.* 2009). The linearity of runoff generation is therefore somewhat unexpected. For two of the three gauges, the assumption of linear routing leads to higher values of λ (Table 3) and thus potentially misguided inferences about dominant processes. The values of λ found for these two gauges under

linear routing are similar to those found by Lees (2000), Young (2002), Ratto *et al.* (2007) and McIntyre & Marshall (2010), who assumed linear routing stores for comparable case studies.

The optimal value of β in the winter period varies from 0.76 to 0.87. These relatively high values of β illustrate greater non-linearity than can be explained by idealised sub-surface or surface flow equations, and they are greater than calibrated values typically found in the literature (e.g. Wittenberg 1994; Mwakalila *et al.* 2001; Segond *et al.* 2007; Ding 2011; although Moore & Bell (2002) note that $\beta = 1.0$ was found applicable to the River Dee in Wales). There may be some influence from the two lakes, however the Stocks reservoir only influences 14% of the Hodder area and the data in McIntyre & Marshall (2008) imply that the Pontbren lake outlet has a relatively linear stage-discharge. The unexpectedly high values of β imply activation of faster flow pathways at higher flows, for example activation of overland flow observed in the Pontbren catchment (Marshall *et al.* 2009) and reduced friction as flow depths increase (Holden *et al.* 2008; Ballard *et al.* 2011). In the summer period, the optimal values of β are similar to those in winter while the optimal values of λ are much higher, presumably because of the increased importance of non-linearity associated with wetting and drying cycles.

Figures 3(a), (e), (i) and 4(a), (e), (i) show the response surfaces for the three gauges in the winter and summer periods using $\Delta t = 15$ minutes (the other time-steps are discussed later). These response surfaces are two-dimensional in the λ - β space (constructed by taking 10,000 samples of λ and β with other parameters fixed at previously optimised values, calculating the NSE for each sample, and fitting a surface through the results and plotting using the MatLab 'mesh' function). The surfaces illustrate the NSE-optimal combinations of λ - β and their uncertainty. These results show that, in both the winter and summer periods using $\Delta t = 15$ minutes, the NSE-optimal values of both parameters are well identified with little observable interaction between them. From this it may be concluded (conditional on this model structure, the optimised values of α and the NSE performance measure) that in this winter period the system is linear or near-linear in flow generation and non-linear in routing, with the source of non-linearity migrating slightly to

Table 3 | Optimised values of non-linearity parameters (β_f fixed at zero)

Gauge no.	Calibration period	One non-linear store		Two linear stores	
		λ	β	λ	β_s and β_f
Pontbren 5	Winter	0.01	0.87	0.02	0
Pontbren 9	Winter	0.04	0.78	0.31	0
Hodder Place	Winter	0.00	0.76	0.33	0
Pontbren 5	Summer	0.20	0.79	0.51	0
Pontbren 9	Summer	0.35	0.60	0.65	0
Hodder Place	Summer	0.30	0.81	0.56	0

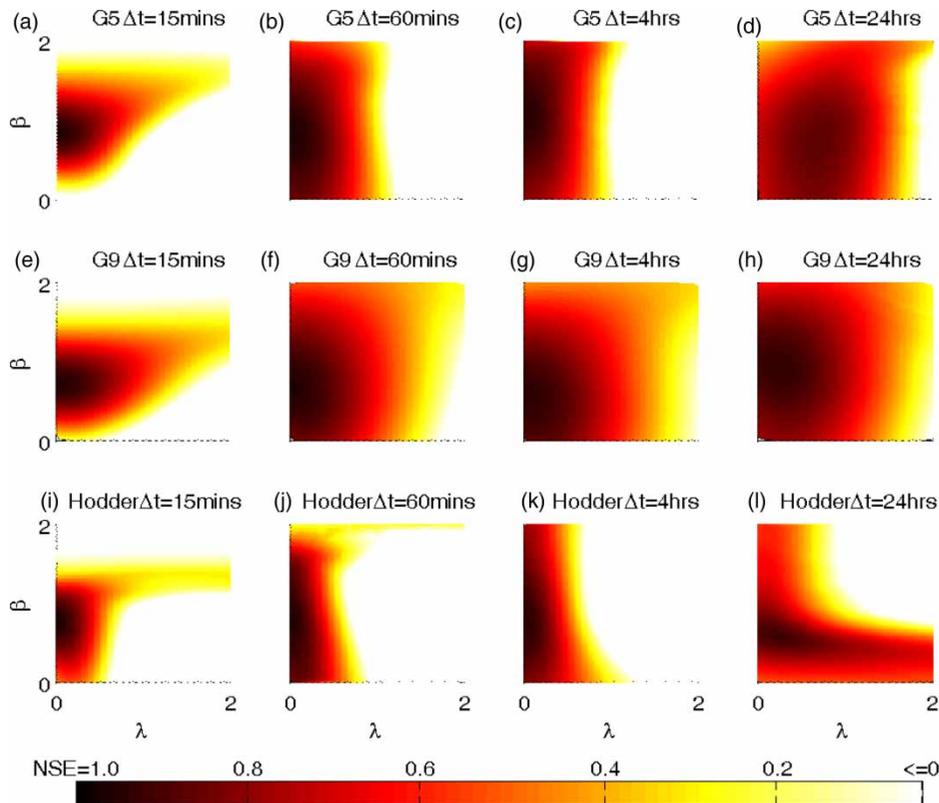


Figure 3 | NSE response surfaces over the λ - β plane in winter period for four different input-output time resolutions using the model defined by Equations (4) and (6).

the runoff generation during the more mixed wet-dry summer conditions.

The response surface plots in Figures 3 and 4 are conditional on the optimised value of α . If α is optimised for each sampled λ - β pair then a reasonable performance is achieved across a wider range of values, although the focus of good performance, at high values of β , remains clear. This is illustrated for the three gauges in Figure 5, where the response surfaces for the winter periods using $\Delta t = 15$ minutes are shown for three alternative values of α : the original value as previously used in Figure 3 and the lowest and highest values that can give an NSE value equal to 95% of the original optimal value. Figure 5 shows that lower or higher values of β are obtained by altering α , while λ remains zero or near-zero. Figures 5(c), (f) and (i) and, to some extent, Figures 3 and 4, illustrate that good flow performance can be achieved with values of β greater than 1.0, which are unphysical, requiring complex values of storage volume. This acts as a reminder that good performance from a model does not necessarily permit

inferences about processes, a caveat that is explored later in the paper.

Influence of input data resolution on inference

Previous investigations have found that input data resolution influences parameter estimates once the resolution decreases towards that of the catchment response time (e.g. Croke 2006; Littlewood & Croke 2008; Kavetski *et al.* 2011; Littlewood & Croke, in press). For the case study gauges, the sensitivity to time resolution of the non-linearity parameters (single-store model) is illustrated by the NSE response surfaces in Figures 3 and 4. These figures show the way in which optimal values and uncertainty change depending on the data time resolution used. In all cases, the ode45 solver was used for the numerical integration, so the variability between plots is associated only with the time-aggregation of rainfall and flow data.

Figures 3(a), (e) and (i) show that there is very little dependency between λ and β and the NSE-optimal values

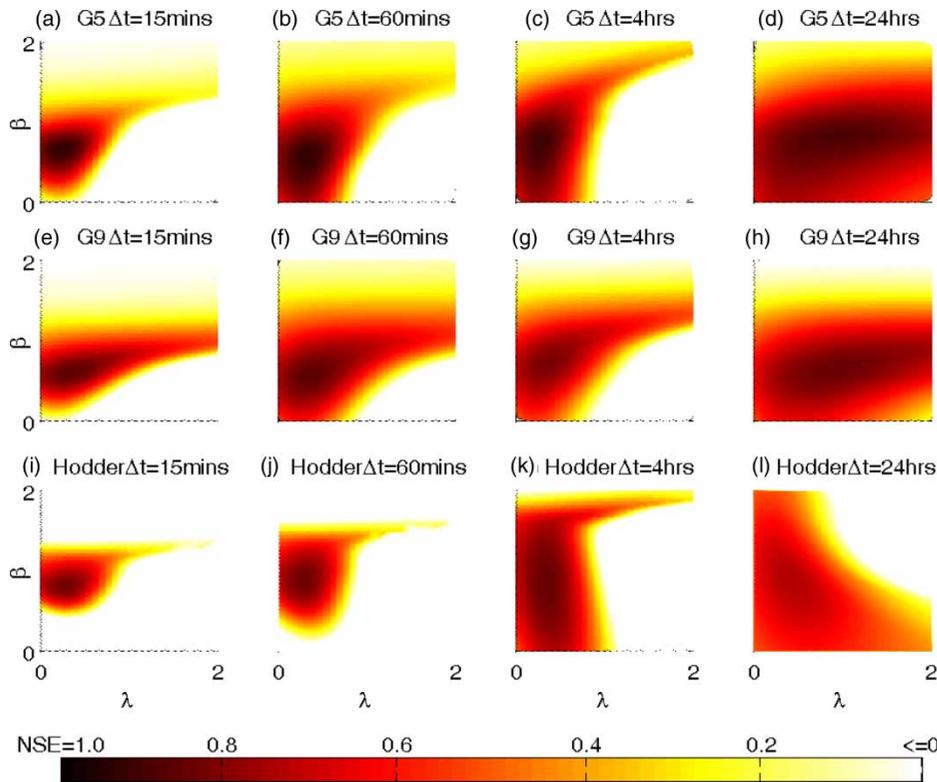


Figure 4 | NSE response surfaces over the λ - β plane in summer period for four different input-output time resolutions using the model defined by Equations (4) and (6).

are well identified given a value of α at $\Delta t = 15$ minutes. Moving to $\Delta t = 1$ hour or $\Delta t = 4$ hours in Figure 3, the uncertainty increases but the conclusions about the optimal parameters do not discernibly change. Moving to $\Delta t = 1$ day in Figures 3(d), (h) and (l), the optimal value of λ moves from its original value, e.g. in Figure 3(a) from 0.01 to 0.75, and the optimal β has reduced from its original value of 0.87–0.74.

The same trend in λ may be observed for the summer period in Figure 4. In other words, at resolutions of 4–24 hours, the inferences about non-linearity in runoff generation are artefacts of smoothing of inputs. Results at Pontbren gauge 9 and Hodder Place are less sensitive to the time-step than Pontbren gauge 5. This may be expected, as the former have much higher response times (Table 1). If α is perturbed from its optimal values (e.g. Figure 5), then although this changes the shape of the response surface the conclusions about the influence of time-step are unchanged.

Of course, it is expected that aggregation of data will result in greater uncertainty as is clear from Figures 3 and 4. It is more interesting that for all gauges except gauge 9

moving to $\Delta t = 1$ day introduces sufficient bias in λ to lead to potentially wrong inferences about runoff generation processes. This is not due to the aggregation of the flow data; for example, running the model using 15-minute rainfall data and calculating the NSE using daily flow data gives the same result as depicted in Figures 3(a), (e) and (i), but with higher uncertainty. Rather, the bias in λ is introduced because of the aggregation of the rainfall data. It may be concluded that the parameter optimisation strives to increase the higher flow peaks to compensate for the over-smoothing of the rainfall inputs by increasing non-linearity in runoff generation. The result is an over-estimation of runoff volume during the largest peaks for the sake of optimising NSE. Using the NSE_{\log} objective function leads to less bias in λ when using $\Delta t = 1$ day but does not remove it, consistent with the findings of Kavetski *et al.* (2011).

It is worth remarking that the optimised NSE_{\log} values using the single non-linear store model were better than those in Table 2, for example $NSE_{\log} = 0.99$ for Pontbren gauge 5 in the winter period using $\Delta t = 15$ minutes. Because $\lambda = 0$ in this case, there are only three optimised parameters

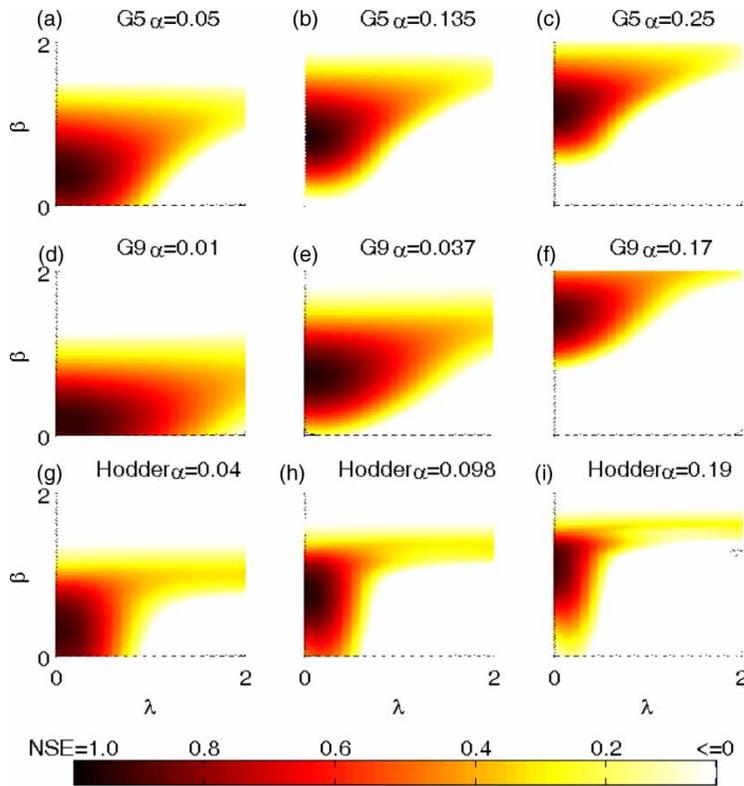


Figure 5 | NSE response surfaces over the λ - β plane in winter period for $\Delta t = 15$ minutes using the model defined by Equations (4) and (6). Within each subplot, α is set to a different good-performing value to illustrate sensitivity of response to α .

(α , β and δ , with μ fixed by mass balance). This is perhaps unprecedented efficiency for such a simple rainfall-runoff model, reflecting at least four aspects of the Pontbren case study: (1) the use of NSE_{\log} reduces the influence of the relatively high errors in the flow peaks (e.g. Figure 1); (2) the catchment-scale response in Pontbren in wet periods is simple: a proportional loss model and a routing response almost perfectly represented by Equation (1); (3) the quality of the experimental data has meant that there is very little noise in the input or output data; and (4) bias in the observed flow potentially introduced by the gauge calibration (McIntyre & Marshall 2008) may be compensated for by optimising α , β and μ .

The high values of NSE_{\log} achieved meant that a deeper analysis of model errors could be performed than is usually achievable. This included the observation of small diurnal signals in the errors, illustrating that improved performance may be achieved by more explicitly considering evaporation. In some events, there was evidence of hysteresis in the response time, indicating that response time is a function

of the rate of change of flow as well as the flow and so there may be scope for another term in Equation (1) (e.g. Ding 2011). However, the identifiability and degree of hysteresis were variable over events and adding it to the model seems unlikely to be fruitful.

Improving numerical efficiency

For the single non-linear store in the winter period using $\Delta t = 15$ minutes, the β parameter ranges from 0.76 to 0.87, leading to the proposition that this parameter may be assumed equal to either 0.67 or 1.0, motivated by the considerable numerical efficiency benefits due to the availability of an analytical solution for these latter two values. Using either of these values led to significant loss of performance, however. A better option for saving computing time when solving the general non-linear store (Equation (4)) is to implement a hybrid numerical-analytical solution, using the numerical integration only when $u \neq 0$ and otherwise the analytical solution (Equation (5)). A third option

for saving computer time is to linearise the non-linear routing by assuming that αq^β in Equation (4) is constant within each time-step but varies between time-steps. For $\Delta t = 15$ minutes, this did not noticeably alter either the model performance or the parameter response surface plots illustrating the suitability of the linearisation in this case, although this is not a general recommendation (Kavetski & Clark 2010). Applying the linearisation when $\Delta t = 1$ hour or $\Delta t = 4$ hours, anomalies were present in the response surface at higher values of β and λ , but not near the optimum values; for $\Delta t = 1$ day most of the response surface was distorted.

Explaining variability between gauges

No relationship was seen between β and λ and available catchment properties describing topography, soil hydrology, land cover, land use or catchment area (Table 1), even when the 12 other Pontbren flow gauges were included. The variation in both β and λ (Table 3) was rather small to expect to identify effects given their uncertainty (e.g. Figure 3), and it is likely that unmeasured catchment properties, e.g. properties of the drainage and stream network, had significant effects. However, consistent with previous work that assumed linear routing (McIntyre & Marshall 2010), a strong relationship was found between catchment properties and the time-averaged routing response time (i.e. $1/\alpha q^\beta$ from Equation (4) integrated over the simulation time period). These results are consistent with regionalisation studies which have found it difficult to explain (or do not attempt to explain) variability in parameters describing rainfall-runoff non-linearity (Lee *et al.* 2006; Beven *et al.* 2008; Pechlivanidis *et al.* 2010).

Sensitivity of results to model equation error

The results reported above show that, in the case study catchments and periods, there is a high level of non-linearity in the rainfall-runoff response that cannot be explained by Equation (6), but can be explained by Equation (4). With the caveats that the first of these equations accurately quantifies the flow generation processes, the second accurately quantifies the flow routing processes and these two processes are independent, this leads to the suggestion that

flow routing non-linearity may be more dominant than often assumed. The caveats about the model equations should not be ignored, despite the good performance of the models in this and previous studies. On the other hand, the caveats are difficult to address because using alternative model structures leads in this case to worse performance and/or increased parameter uncertainty and/or a less clear parameterisation of non-linearity and/or a less clear demarcation between flow generation and routing non-linearity; Equations (4) and (6) were chosen to avoid all these problems.

Nevertheless, a limited exploration of sensitivity to model equation error was performed by two modifications to the flow generation model. The first modification is to maintain Equation (6) but to use a simulated catchment wetness index based on a soil water volume balance instead of using the observed flow (Post 2009). This introduces only one extra parameter: a first-order soil water loss rate, assumed constant over time. This model was applied only for the winter period with $\Delta t = 15$ minutes for all three case studies. Optimal NSE values were identical to the original model for the Pontbren gauges (NSE = 0.96 for both gauges) and lower for the Hodder (NSE = 0.94 compared to the original 0.96). The λ - β response surfaces for the two Pontbren gauges (Figures 6(c) and (f)) are similar to those obtained using the original model (Figures 3(a) and (e)), with near-zero optimal values for λ and relatively high optimal values for β . For the Hodder gauge, however, a notably larger optimal value of λ and lower optimal value for β are obtained compared to the original result. The Hodder result is difficult to interpret, but illustrates the potential sensitivity of the allocation of non-linearity to the details of the model equations.

The second modification to the flow generation model recognises the potential for infiltration excess in addition to wetness-driven flow generation:

$$u = \begin{cases} \mu r y^\lambda & \text{when } r < \text{thr} \\ r & \text{when } r \geq \text{thr} \end{cases} \quad (7)$$

where thr is a specified rainfall rate threshold and the other variables were defined for Equation (6). Again, μ is fixed so that the volume of effective rainfall equals the volume of observed flow. Using this revised model, the conclusion

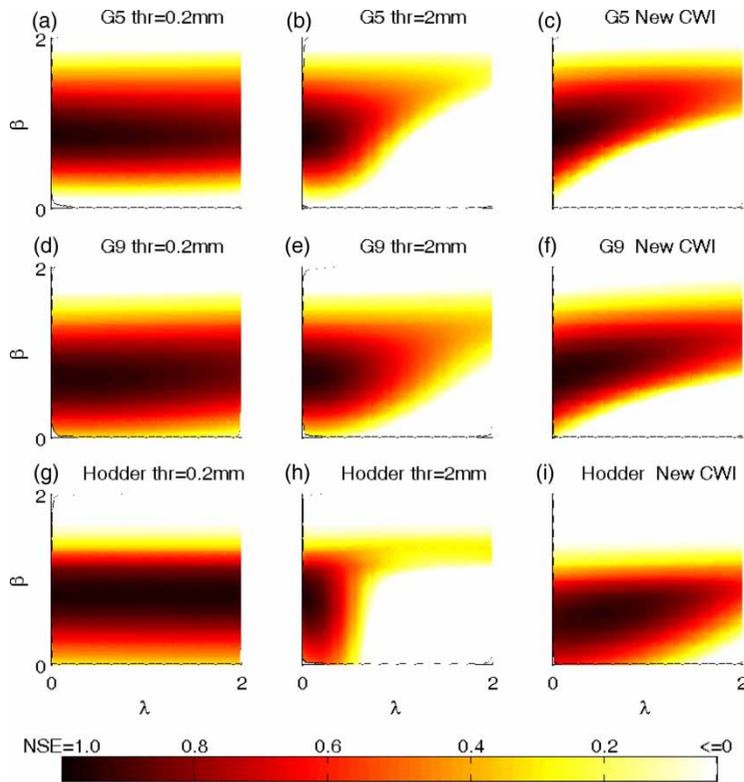


Figure 6 | NSE response surfaces over the λ - β plane in winter period for $\Delta t = 15$ minutes using the model defined: (a, b, d, e, g, h) by Equation (7) with two different thresholds and (c, f, i) by Equation (6) where y is a simulated wetness index.

about the relative importance of β and λ does not change for any of the case studies, except that as thr becomes near to zero the identifiability of λ decreases (with low values of thr , little of the rainfall is influenced by catchment wetness). To examine more carefully whether infiltration excess can explain some of the non-linearity would require more complex models, for example along the lines of Szilagyi (2007).

CONCLUSIONS

The paper has critically evaluated typical routing components used in conceptual rainfall-runoff models in the context of upland UK catchments. In particular, the paper attempted to expose the loss of performance and process insight that may arise from the common assumption of linear routing, and to illustrate some benefits of and difficulties with non-linear routing analysis. Three flow gauges and associated rain gauges provided relatively high-quality 15-minute rainfall-runoff data over relatively wet winter

periods and mixed wet-dry summer periods. The data were aggregated to larger time-steps to explore how information about non-linearity is lost or distorted as the time resolution reduces. To analyse the data, parsimonious models were chosen that had well-identified parameters, and included parameters that directly and distinctly represented the flow generation and flow routing non-linearities, with values of zero representing a linear response and values of 1 representing a strongly non-linear response.

Optimised model performances were considered good. For example, with a four-parameter single non-linear store model and 15-minute time-step, the average NSE value in the winter and summer periods over the three gauges were 0.96 and 0.90. It was difficult to distinguish the performance of a conventional two-parallel linear-store routing model from that of the single non-linear store, both giving similar NSE and visual performance over both test periods. The latter has one less parameter and, on close inspection, provides better fits to hydrograph recessions and in one gauge more satisfactory estimates of effective rainfall. Despite the

performance similarities, the conceptual distinction is large with two-parallel linear stores implying a spatially organised routing of flow and the single non-linear store implying temporally organised (flow-dependent) routing.

Given the single-store model, the routing non-linearity is consistently unambiguous and larger than explained by idealised surface or subsurface routing theory. It is speculated this is mainly linked to the activation of fast-routing pathways and reduction in friction losses as surface flows increase. The assumption of linear routing led to notable bias in the estimate of runoff generation non-linearity. It is concluded from this that comparable previous studies that have made inferences about runoff generation processes under the assumption of linear routing could be usefully revisited. Furthermore, smoothing the 15-minute input data to greater than 4-hour resolution led to a biased estimate of runoff generation and hence potentially wrong inferences about the nature of the non-linearity. This was ameliorated by applying the NSE objective function to the log-transformed flows to avoid over-fitting to the highest observed peak flows.

Approximating the optimised values of the routing non-linearity parameter to values for which convenient analytical solutions exist led to significant performance reductions. However, the numerical burden of solving the optimal non-linear models in continuous time can be avoided by using a linearised approximation that did not introduce noticeable bias to parameters or affect performance when using a 15-minute time-step. Further aggregation of the input signal generally led to numerical stability problems when a linearised solution was used, however.

The modelling experiments were initially limited to the flow generation and flow routing models that gave good performance with good parameter identifiability (up to NSE = 0.99). A further limitation of the initial results was that, in order to explore the response surface of the two non-linearity parameters, other parameters were fixed at their optimised values. Subsequent sensitivity tests showed that conclusions were generally robust to perturbations in the fixed model parameters and also in the model equations. In one of the three catchments however, the flow generation non-linearity become more important under an alternative definition of the soil wetness index and therefore some degree of caution must be attached to conclusions. More

extensive tests, using a greater range of process hypotheses, are recommended.

Overall, this paper has illustrated the potential problems that may arise from insufficient attention to the routing component of a conceptual rainfall-runoff model. The common practices of assuming a linear routing model and prescribing a numerically convenient degree of non-linearity and unsuitable time-aggregations of input data may lead to suboptimal performance and/or wrong inferences about hydrological processes.

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