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Ecological Modelling 86 (1996) 183-188

ECOLOGICAL MODELLING

Overview of a simple model describing variation of dissolved organic carbon in an upland catchment

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Abstract

Hydrological mechanisms controlling the variation of dissolved organic carbon (DOC) were investigated in the Deer Creek catchment located near Montezuma, CO. Patterns of DOC in streamflow suggested that increased flows through the upper soil horizon during snowmelt are responsible for flushing this DOC-enriched interstitial water to the streams. We examined possible hydrological mechanisms to explain the observed variability of DOC in Deer Creek by first simulating the hydrological response of the catchment using TOPMODEL and then routing the predicted flows through a simple model that accounted for temporal changes in DOC. Conceptually the DOC model can be taken to represent a terrestrial (soil) reservoir in which DOC builds up during low flow periods and is flushed out when infiltrating meltwaters cause the water table to rise into this "reservoir". Concentrations of DOC measured in the upper soil and in streamflow were compared to model simulations. The simulated DOC response provides a reasonable reproduction of the observed dynamics of DOC in the stream at Deer Creek.

Keywords: Carbon; Hydrology; River ecosystems; TOPMODEL

1. Introduction

A quantitative understanding of the factors controlling the variation of dissolved organic carbon (DOC) in headwater streams is needed for a number of reasons, not the least of which is because DOC interacts strongly with other dissolved substances (heavy metals in particular) and plays an important role in the transport of contaminants.

In Deer Creek near Montezuma, Colorado, measurements of dissolved organic carbon (DOC) from July 1991 to August 1992 show rapid decreases in concentration from a peak very early in the snowmelt period (on the ascending limb of the hydrograph); the peak concentration of DOC in the stream occurs well before the peak discharge. Among the main factors controlling DOC variation in such headwater streams are the hydrological catchment responses, including flow paths through and residence times of water in the catchment. Models of the relationships between hydrological flows and DOC transport are important for quantifying the hypothesized mechanisms and thereby indicating whether observations are consistent with hypotheses.

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SSDI 0304-3800(95)00049-6

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To evaluate the model, DOC concentrations were measured in the upper soil and the stream at several locations. Water sampled from lysimeters in the upper soil showed an accumulation of DOC during periods of low flow and a pronounced decline in DOC concentrations during snowmelt. These results, along with the general fidelity with which variations in stream DOC are captured using the model, support the hypothesized flushing mechanism.

2. Site description

The site of the study is the Deer Creek catchment, located in Summit County, Colorado near Montezuma. The catchment is mountainous, ranging in elevation from about 3350 m to 4120 m, and drains an area of 10.6 km^2. Approximately half of the catchment is above the tree line.

3. Methods

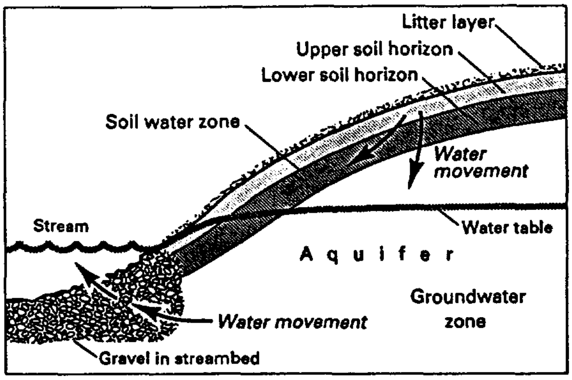
3.1. Field instrumentation

Details of the field measurement procedures are given by Boyer (1993). Briefly, a stream gage was installed at the mouth of the catchment that provided a stage record from which the daily discharge was computed. Tension lysimeters, which provide water samples from the upper soil, were installed at several locations on hillslope transects. Water samples from the stream and soil lysimeters were collected, at a frequency ranging from daily near the beginning of snowmelt to weekly later in the summer, for determination of DOC concentration.

3.2. Hydrological modeling

We applied the hydrological model TOPMODEL (Beven and Kirkby, 1979) to simulate the catchment hydrology. The features of the UVA-USGS version of the model that we use have been described by Wolock (1993). The topographic index which is at the core of TOPMODEL, $\log_e(a/\tan\beta)$, was calculated from

a) Low flow conditions



b) High flow conditions

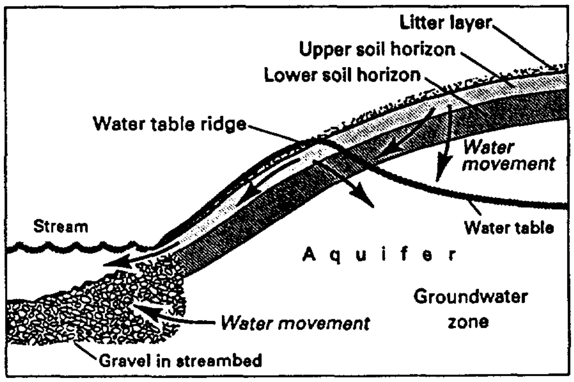


Fig. 1. Hydrological flushing of soil water. (a) During periods of low flow, subsurface flow is through lower soil horizons. (b) During high-flow conditions (spring snowmelt), the water table rises and flow to the stream is through the upper soil horizons as well. (Taken from Hornberger et al., 1994.)

DEM data as described by Wolock (1993). Average soil depth was assumed to be 1 m; an "upper horizon", the presumed reservoir for high DOC levels, was assumed to be 0.5 m thick. TOPMODEL was calibrated for Deer Creek using the Rosenbrock optimization algorithm. (See Hornberger et al., 1985, for a description of the use of the Rosenbrock method in conjunction with TOPMODEL.) The parameters optimized were two soil parameters, one intended to represent the rate of decrease of hydraulic conductivity with depth divided by porosity and the other the hydraulic conductivity of the surface soil (see Beven and Wood, 1983), and two snowmelt parameters, one the threshold temperature for melting and the other the coefficient relating the maximum rate of melting to the average daily temperature (see Bras, 1990).

3.3. Chemical modeling

The conceptual model is that DOC in riparian and hillslope soils is "flushed out" by the formation of a ground-water ridge during periods of snowmelt (Fig. 1). This would suggest that DOC in the vadose zone might build up during periods of low flow (through leaching from overlying organic-rich litter and through microbial activity) and that this DOC would be pushed out into the stream during periods of high flow. Such a conceptual model would indicate that concentrations of water flowing from the soil to the stream should be high in the initial part of a rainstorm or snowmelt event and then decrease as meltwaters continue to flush the zone formerly above the water table but now exposed to significant streamward flow of water. The simplest mathematical representation of flushing such as envisioned in the conceptual model is from a continuously stirred tank reactor (CSTR). In response to the influx of a flushing solution, such a simple device produces an exponential decline in concentration in the outflow solution with time.

We constructed a simple mixing model, based on a CSTR, to explain temporal variation of DOC concentrations in the Snake River. We envision two subsurface reservoirs: one representing the "upper soil" and one representing the "lower

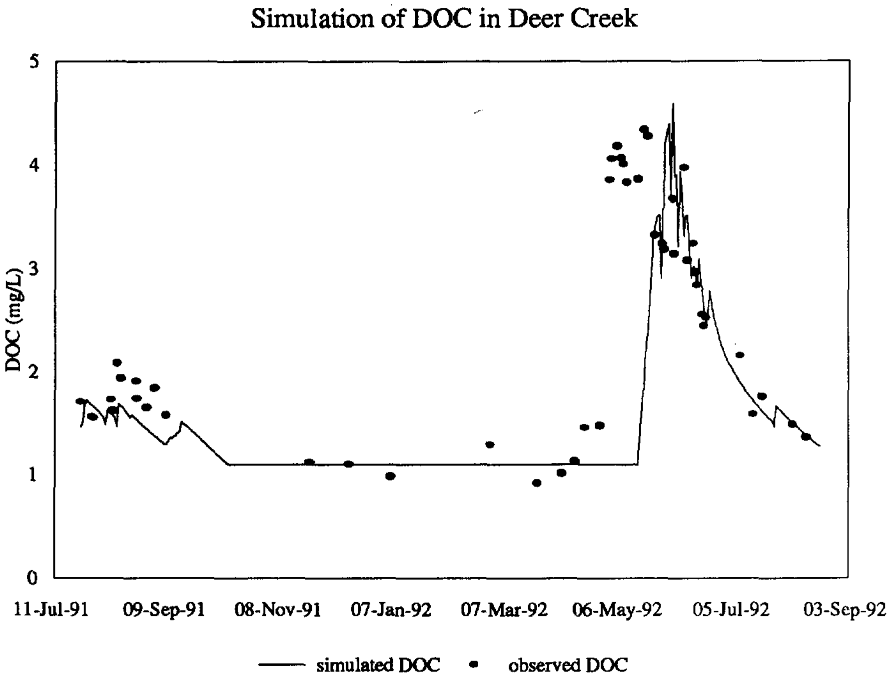


Fig. 2. Simulated and observed values of DOC for Deer Creek.

soil". Flows through the two subsurface reservoirs are apportioned on the basis of results from TOPMODEL. We use a simple proration to apportion flow to the upper reservoir.

We assume that DOC in the lower reservoir is constant. From data we estimate that the DOC in the lower reservoir is 1.2 mg l^{-1}. To account for build-up of DOC in the soil, we use the model of Grieve (1991). DOC in the upper reservoir varies according to:

$$\begin{aligned}\mathrm{DOC}_{\mathrm{upper}}(t+1) &= \mathrm{DOC}_{\mathrm{upper}}(t) + a * 10^{0.04T} \\ &\quad - (1 - \mathrm{e}^{-kT}) * \mathrm{DOC}_{\mathrm{upper}}(t) \\ &\quad - \left(1 - q_{\mathrm{upper}}(t)/V_{\mathrm{upper}}(t)\right) * \mathrm{DOC}_{\mathrm{upper}}(t)\end{aligned}$$

where t indicates time, T is temperature, a and k are rate constants for evolution and decay of DOC (see Grieve, 1991), q_{upper} and V_{upper} are, respectively, the flow through and wetted volume of the upper soil reservoir, and the time step is one day. Although the appropriate temperature is a soil temperature, we used air temperature as a surrogate. We used $a = 0.11$ and $k = 0.002$.

The DOC in the stream is calculated as a simple mixture of waters from direct snowmelt and from the upper and lower soil reservoirs:

$$\begin{aligned}\mathrm{DOC}_{\mathrm{stream}} = (&\mathrm{Flow}_{\mathrm{overland}} * \mathrm{DOC}_{\mathrm{snow}} \\ &+ \mathrm{Flow}_{\mathrm{upper}} * \mathrm{DOC}_{\mathrm{upper}} \\ &+ \mathrm{Flow}_{\mathrm{lower}} * \mathrm{DOC}_{\mathrm{lower}})/\mathrm{Flow}_{\mathrm{total}}\end{aligned}$$

4. Results

The simulated hydrological response for 1991–1992 was used as input to our simple DOC model. The simulated DOC response provides a reasonable reproduction of the observed dynamics of DOC in the stream at Deer Creek (Fig. 2). This was expected from the results presented by Hornberger et al. (1994) who successfully applied this model to describe DOC dynamics in the Snake River, a stream that is confluent with Deer Creek immediately downstream of our study reach. We attribute the apparent "delay" in the simulated DOC response to the fact that the initial time of rise is late in the simulated discharge hydrograph;

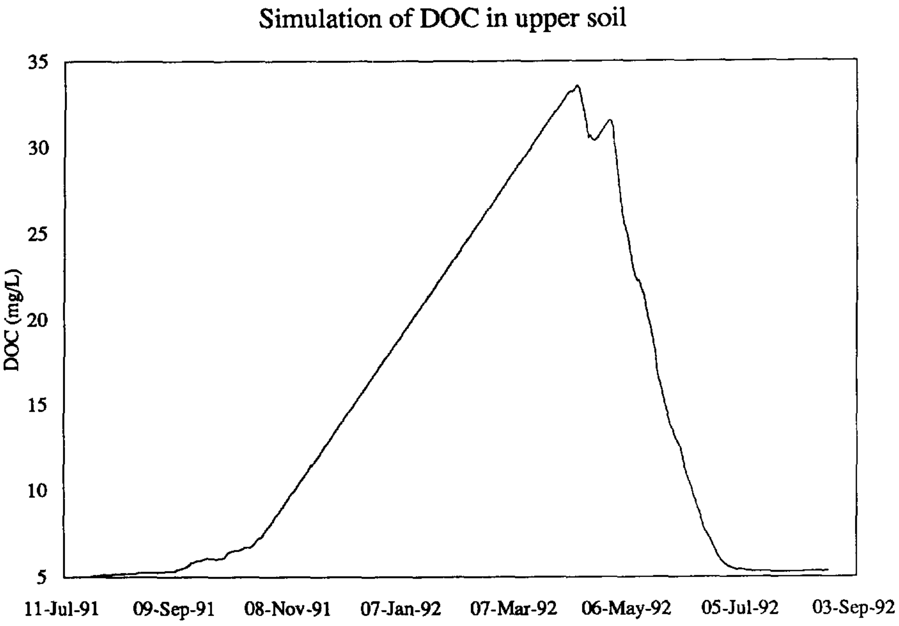


Fig. 3. Simulated values of DOC in the upper soil reservoir.

presumably, the temperature index model calculates the initiation of significant snowmelt to be later than when the melt is actually initiated. The model captures the essence of the sharp decline in DOC concentrations in the stream after a peak early in the melt hydrograph. The real test of the modeling approach is whether the simulated DOC in the hypothetical soil reservoir was in any sense "close to" that measured in soil solution.

Simulated DOC in the upper soil reservoir ranged from about 5 mg l^{-1} to about 35 mg l^{-1} with peak concentrations preceding the initiation of the snowmelt runoff (Fig. 3). Peak measured concentrations of DOC in soil lysimeters ranged up to more than 80 mg l^{-1} but most showed peak concentrations in the 20 to 50 mg l^{-1} range (Boyer, 1993). Results from a riparian lysimeter, which may be most appropriate for conditions that we are simulating, show DOC concentrations that are very similar to those simulated (Fig. 4).

5. Conclusions

Neither the simulated discharges from TOPMODEL nor the simulated DOC values from the CSTR model can be considered to be even nearly perfect representations of the data. Nevertheless, we conclude that the model results are broadly consistent with the available data collected in the stream and in the upper soil of the Deer Creek catchment. Given the available data, we cannot reject the simple model as a valid description of processes occurring in the Deer Creek system. The measurements of soil DOC from the field sampling program in 1991 and 1992 lend credence to the model over and above that conferred from the simulation of the stream dynamics.

As is often the case, examination of existing data in light of the modeling results suggests additional work that is necessary to more rigor-

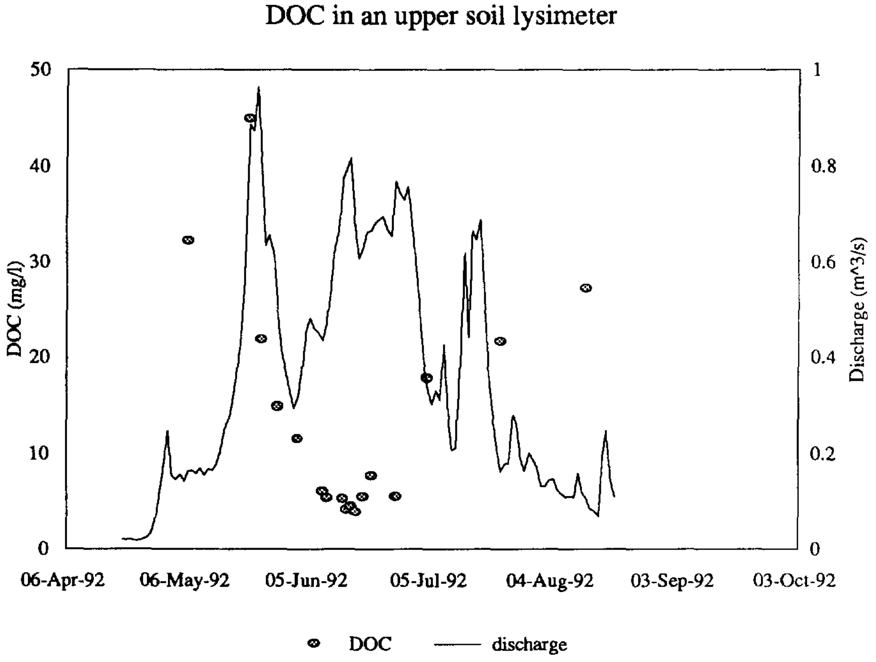


Fig. 4. Observed concentrations of DOC in a shallow riparian soil. Stream discharge is shown to indicate the timing of the snowmelt event.

ously test the hypotheses embedded in the model and to refine the model itself so that comparisons between model results and observations are rendered less ambiguous. In particular, the spatial and temporal variations of snowmelt and soil properties, in addition to topography, should be considered in the refinement of the conceptual model.

Acknowledgements

This work was supported in part by the National Science Foundation through Grant EAR-9304794.

References

Beven, K.J. and Kirkby, M.J., 1979. A physically based, variable contributing area model of basin hydrology. Hydrol. Sci. Bull., 24: 43–69.

Beven, K.J. and Wood, E.F., 1983. Catchment geomorphology and the dynamics of runoff contributing areas. J. Hydrol., 65: 139–158.

Boyer, E.W., 1993. Hydrology and the variation of dissolved organic carbon in soil and stream waters of two headwater catchments; Summit County, Colorado. M.S. Thesis, Department of Environmental Sciences, University of Virginia.

Bras, R.L., 1990. Hydrology: an Introduction to Hydrologic Science. Addison-Wesley, Reading, MA, 643 pp.

Grieve, I.C., 1991. A model of dissolved organic carbon concentrations in soil and stream waters. Hydrol. Processes, 5: 301–307.

Hornberger, G.M., Beven, K.J., Cosby, B.J. and Sappington, D.E., 1985. Shenandoah watershed study: calibration of a topography-based, variable contributing area hydrological model to a small forested catchment. Water Resour. Res., 21: 1841–1850.

Hornberger, G.M., Bencala, K.E. and McKnight, D.M., 1994. Hydrological controls on dissolved organic carbon during snowmelt in the Snake River near Montezuma, Colorado. Biogeochemistry, 25: 147–165.

Wolock, D.M., 1993. Simulating the variable-source-area concept of streamflow generation with the watershed model TOPMODEL. U.S. Geological Survey Water-Resources Investigations Report 93-4124.