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Hillslope and stream connectivity: simulation of concentration-discharge patterns using the HYDRUS model

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Abstract: Nutrient concentrations and loads in streamflow are sensitive to rapidly changing stream chemistry and discharge during storms. Mechanistic models that can simulate water and solute movement at hillslope scales could be useful for predicting concentration-discharge (C-Q) patterns and thereby improve our quantitative understanding of terrestrial-aquatic linkages for targeted catchment management. Our objective was to use the HYDRUS model to represent hydro-biogeochemical processes in soils that drive seepage of water and solutes from soil profiles into streams. Specifically we compared measurements in the literature with HYDRUS outputs using two methods for simulating runoff. This model predicts runoff (R) as rainfall that is instantaneously in excess of infiltration, but it is not designed to route runoff as overland flow. Post-HYDRUS addition of seepage to runoff was used to simulate the delivery of dissolved or particulate constituents to a stream (method A). Alternatively, we demonstrated how simulations using HYDRUS could include a hypothetical layer at the top of the soil profile with extremely high porosity and hydraulic conductivity that enabled overland flow and down-slope infiltration, but in this case only dissolved constituents could be considered (method B). These methods were evaluated by comparing the simulated temporal patterns of discharge and concentration with observed patterns. The catchments considered were in Slovenia (4210 ha) and in Australia (11.9 ha).

Methods A and B were shown to adequately simulate some aspects of published discharge-concentration patterns, e.g. runoff dilution or concentration effects, but the temporal patterns of discharge for both methods did not precisely match those measured at small time-steps (e.g. 15 minutes). This limitation was due mainly to inadequate simulation of the down-slope movement of runoff and down-slope infiltration of a portion of this runoff. Method A was generally more useful than method B. Despite this limitation, both methods, if used carefully, should be adequate for many purposes, especially when simulating longer time-steps. Additional hypothetical simulations illustrated the significance of soil hydraulic conductivity, soil water content, and vertical gradients in solute concentrations in soil. Two temporal types of discharge-concentration patterns were observed; short-term hysteresis caused by runoff during and shortly after a rainfall event, and longer-term trends associated with infiltration and seepage. Clockwise and anti-clockwise hysteresis was demonstrated to be potentially due to the temporal asynchrony of peak discharge and peak concentration in runoff. Simulations also demonstrated advantages over using the more common approach of a 2- or 3-component mixing model.

Our results suggest that the HYDRUS model will be useful for the mechanistic simulation of within-soil processes that are needed to predict discharge-concentration patterns at hillslope scales.

Keywords: *Water quality, nitrate, soil, runoff, overland flow, seepage, drainage*

1. INTRODUCTION

Discharge-concentration patterns (C(Q); hysteresis) at a weir can be explained using 2- or 3-component mixing models that rely on signatures of water chemistry from the various sources e.g. rainfall, soil water and ground water, to indicate their proportional contribution to flow (Petrone et al., 2007). Evans and Davies (1998) used this approach to develop nine hypothetical hysteresis patterns from a particular pattern of soil water, ground water (aquifer) and event water (rain) that each had constant but contrasting concentrations. These patterns matched some event data from their own sites and others, but the patterns did not encompass the complete range of hydrologic conditions. Weiler and McDonnell (2006) used hillslope modeling to reproduce hysteresis patterns of nitrate (NO_3) flushing associated with event water that completely infiltrated highly conductive soil surface horizons. These authors also encouraged the use of mechanistic models in virtual experiments for simulating hillslope water and solute transport and transformations, including nitrogen mineralization and nitrification. Such models are needed to fully capture the potential effects of soil and other characteristics that differ between sites.

Several models attempt to mechanistically represent water and solute transport processes in two or three dimensions. The HYDRUS model (Šimůnek et al., 2008) is attractive because it incorporates conservative and non-conservative solutes by using the Richards equation for saturated-unsaturated water flow and the Fickian-based advective-dispersion equations for solute transport. It also includes options for dual permeability, 3-dimensional transport, and ground water. HYDRUS also has an attractive and useful graphical user interface, and a high degree of spatial and temporal flexibility. We also had an interest in the mechanistic simulation of nitrogen dynamics in the soil-plant system, and HYDRUS includes a module with that potential. These attributes offered the potential that HYDRUS might be useful for mechanistic simulations of water and solute transport at hillslope and headwater catchment scales, but its simulation of runoff requires evaluation. Our objective here was to examine how HYDRUS N transport and hydrologic processes in order to simulate observed discharge-concentration patterns. We compared simulated HYDRUS patterns of discharge and concentration with those presented in the literature for contrasting rainfall events and sites,. We also ran hypothetical simulations to illustrate the importance of some within-soil processes for producing various short- and long-term patterns.

2. METHODS

HYDRUS (Šimůnek et al. 2008, version 1.05) was used in a 2-dimensional, sloped, rectangular or trapezoidal configuration. Units used were cm for length and mg/L for concentration. An atmospheric (precipitation) boundary condition was usually specified for the surface, with a vertical seepage face, and no-transfer boundaries for other faces, unless constant flux and constant concentration groundwater input was simulated for part of the lower surface. Seepage refers to water movement out of a soil profile at a seepage face with an atmospheric boundary condition (saturation excess), and can include components of interflow soon after rainfall, stored soil water, and ground water entering the soil profile from an aquifer. We use the term runoff to specifically mean overland flow in excess of infiltration. Some authors use the term deep seepage to imply movement of water deep into a soil profile or into an unconfined aquifer. Such a process was not needed in our simulations, but could potentially be simulated in HYDRUS as a drainage boundary condition; we used a no-flux lower boundary condition except where ground water was included.

Because we wanted to simulate hillslope processes in two dimensions, an average hillslope length was calculated as catchment area divided by stream length. Total and horizon soil depths, hydraulic conductivities, and rainfall were taken from the literature (Table 1). At least 1,200 spatial nodes were used, and time-steps started at very low values (10^{-7} s; to ensure adequate conservation of mass) and increased during stable periods of a simulation to a maximum of 1-10 days. Simulations were built up by specifying firstly water only, then by adding transpiration (root water uptake), and followed by solute transport. A low evaporation rate was included. Before rainfall events were simulated, setting up of a simulation included pre-runs (up to 200 d), average rainfall and solute inputs that enabled a quasi steady-state to be achieved for seepage rate and concentration. Simulated seepage and runoff fluxes were in two-dimensional units (cm^2/d) and converted to three-dimensional output (m^3/d) by multiplying by the length of the third dimension (catchment length = catchment area/length of hillslope) and the cm to m conversion factor.

Two methods of simulating runoff were tested as follows. HYDRUS simulates runoff as rainfall that is instantaneously in excess of infiltration (method A), but it is not designed to route runoff as overland flow. This method required post-processing of HYDRUS runoff and seepage output using a spreadsheet to add these fluxes (without runoff delay delay) for each printed time-step, and thereby estimate stream flow. During post processing, concentrations in runoff needed to be specified in order to be added to seepage and thereby calculate concentrations in stream flow. As an alternative with potentially different outcomes, we also tested the use in HYDRUS of a hypothetical layer at the top of the soil profile with extremely high porosity (0.98) and hydraulic conductivity (K_{sat} = 2E7 cm/d, method B), which facilitated simulation of overland flow and down-slope infiltration. Only dissolved constituents could be considered with method B, but less post-processing was required because all water and solute output as seepage by HYDRUS included the runoff component.

Some characteristics of the catchments simulated are summarised in Table 1. Hypothetical variations were also tested, including the hypothetical scenarios of Evans and Davies (1998).

Table 1. Some characteristics of the two catchments simulated as hillslopes**.**

Characteristic	**Padez**	**Montagu**
Country, latitude	Slovenia ,45° North	Australia, 41° South
Area (ha)	4210	11.9
Hillslope length (m)	515	13.2
Rainfall annual (mm/year)	1440	1283
Rainfall events (mm)	34.5, 18.2	54.4
Rainfall peak intensity (mm/15 minutes)	1.2, 1.5	6.0
Land-use	forest 92%, pasture 18%	Pasture 100%
Geology	Marine sediments	Colluvium and alluvium
Soil depth (m)	1	2
Soil surface texture	silty clay	sandy loam over clay
Soil saturated 3D hydraulic conductivity (cm/d)	31	60 over 6
Soil solid-liquid phase partition coefficient (mL/g)	0	0
References	Rusjan et al (2008)	Holz (2008, pers. comm.)

3. RESULTS AND DISCUSSION

3.1. Scenarios based on the Padež catchment

Rusjan et al. (2008) provided two quite contrasting measured hysteresis patterns. The first type was shown in both their March and April events (Figs. 6a and 6b in Rusjan et al., 2008), in which 2- to 5-fold increases in discharge occurred with little change in concentration except a slight anticlockwise increase. These patterns occurred with a 34.5 mm rainfall event on relatively dry soil at the end of winter. We simulated a similar pattern (Fig. 1) using hillslope, soil profile, soil water, and rainfall as described by Rusjan et al (2008), and assuming initial concentrations of NO_3 in soil water decreased from 2.5 mg/L at the soil surface to 0 mg/L at the bottom of the profile. The simulated concentration was 1.4-1.5 mg/L, compared to 1.8-2.4 mg/L, suggesting that the assumed initial condition for the concentration profile were not quite correct.

Changing to a high soil water content and uniform concentration of 5.8 mg/L NO_3 down the profile, with an 18 mm rainfall event (as indicated by Rusjan et al 2008 for their August II-5 event), similar temporal patterns of discharge and concentration were produced to those observed, i.e. sharp increase and return in flow accompanied by a concurrent decrease and return in concentration (Fig. 2). The resulting C(Q) plot showed no hysteresis while runoff occurred, and was followed by a steady but less substantial increase in discharge while concentration remained constant at 5.8 mg/L, which reflected high NO_3 concentrations observed during late spring.

We used this scenario to demonstrate how hypothetical patterns of concentration in runoff could produce contrasting patterns of hysteresis, i.e. C(Q). By assuming the concentration in runoff peaked at 15 mg/L 1 h before peak discharge, a clockwise hysteresis was simulated (Fig. 3 left). Conversely, by assuming concentration in runoff peaked at 15 mg/L 0.5 h after peak discharge, an anticlockwise hysteresis was simulated (Fig 3 right). Because concentrations in runoff are important for predicting C(Q) patterns, further advances in these predictions will only be made if we develop a sufficient understanding of the mechanisms contributing to concentrations of dissolved and particulate constituents in runoff and the resultant temporal patterns of concentration in discharge. Some progress has been made, but generalised mechanistic predictions are not yet available (Robertson and Nash, 2008; Vadas et al., 2008).

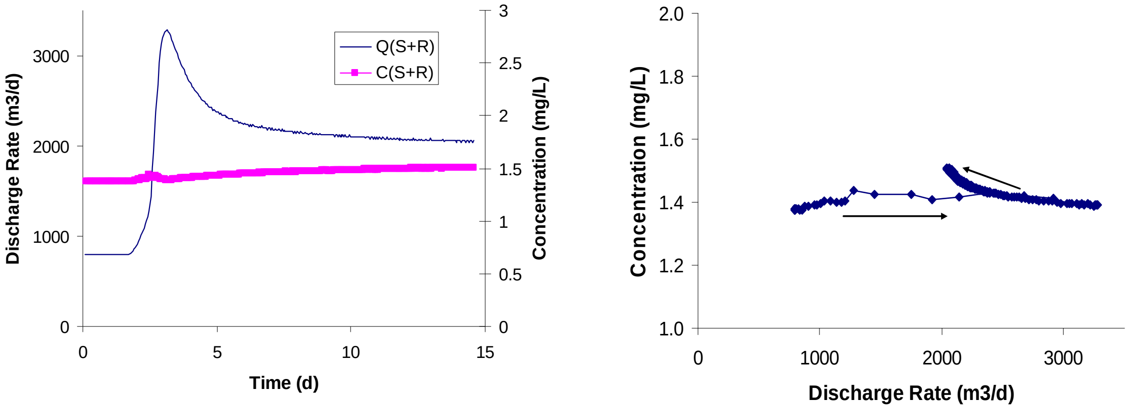

Fig. 1. Simulated temporal patterns of discharge and concentration (left) and the resultant discharge-concentration pattern (hysteresis; right), which are similar to those patterns described by Rusjan et al. (2008) for their March and April rainfall events. Q = discharge, C = concentration, S+R = combined seepage and runoff. Runoff method A was used, but insignificant runoff occurred during this event (observed and simulated). The direction of hysteresis is indicated by arrows.

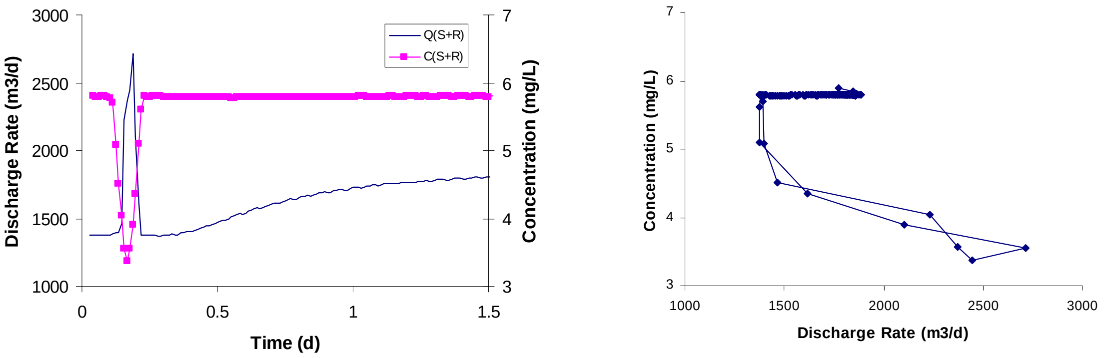

Fig. 2. Patterns of C(Q) simulated for the Rusjan et al. (2008) August II-5 rainfall event in Slovenia. Significant runoff occurred during this event (observed and simulated). Simulated flow (left) shows the separate influence on flow of runoff that lasted a few hours and longer-term seepage at an increased rate due to infiltration. Runoff method A was used.

We also tested the use of an artificial runoff layer (method B) for the scenario presented in Fig. 2, but because most ‘runoff’ water reinfiltrated the profile, a very different C(Q) pattern was predicted to that observed, i.e. in this case it simulated a slow increase in discharge and only a minor change in concentration (data not shown).

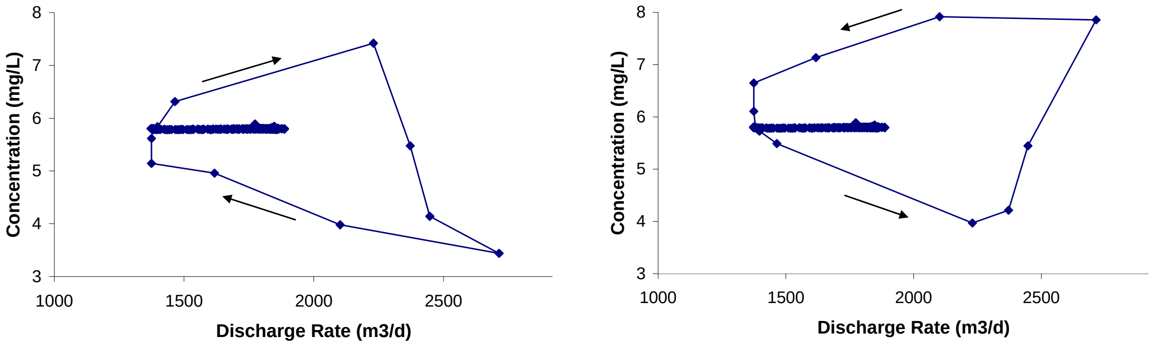

Fig. 3. Patterns of C(Q) simulated for the Rusjan et al (2008) August II-5 rainfall event assuming peak concentrations preceded (left) or followed (right) peak discharge. The direction of hysteresis is indicated by arrows. Runoff method A was used.

3.2. Inclusion of high-resolution, measured rainfall for predicting NO_3 and PO_4 patterns

We simulated a transect of one half of a hump-and-hollow pasture system in the Montagu catchment described by Holz (2008 and pers. comm.). This pasture system is used in flat landscapes by moving soil from the hollows and depositing to construct the humps, thereby creating mini-catchments. Average annual rainfall was used to initialise water flow conditions, and solute concentrations in the profile were set at concentrations measured during baseflow. A particular period was selected for simulation because it included a complex pattern of rainfall events during a period of a few days, with an associated complex pattern of discharge and NO_3 and PO_4 concentrations. Hence, this period was chosen to test the behaviour of HYDRUS under complex rainfall patterns. The two methods of simulating runoff evaluated earlier were again tested here.

Using Method A, K_{sat} was varied within the measured range to achieve peak flow rates approximately 8.5 times higher than baseflow, i.e. similar to the measured ratio of peak flow to base flow. Using these conditions, the sharp rise and fall in runoff was matched by a decrease in NO_3 concentrations during peak runoff that was similar to those measured, which represented the expected dilution effect (Fig. 4 left). Conversely, assuming a pattern of PO_4 concentration variation with runoff that peaked at a similar value to that measured, a PO_4 concentration effect was simulated during this event (Fig. 4 right). However, simulated runoff did not occur during other rainfall events during this 3.4 day period, in contrast to that suggested by measured patterns of concentrations. This difference between observed and simulated behaviour might reflect the delays in surface drainage in this low-slope condition, which we did not simulate.

Method B provided two runoff events (not shown). However, using this method, the ratio of peak discharge to baseflow was much higher than measured and discharge returned to baseflow conditions between these two peaks, which did not match the measured pattern. Again, this difference between observed and predicted discharge patterns might be a reflection of differences in storage and the delay in drainage of overland flow in this low-slope catchment. Nitrate dilution was simulated using this method, but PO_4 patterns were not attempted. This result from the Montagu catchment and those above from the Padež catchment do not render method B unsuitable for all applications, but indicates that caution at least will be needed when it is used.

3.3. Hypothetical Scenarios That Included Groundwater

Various boundary conditions are provided as options in HYDRUS (e.g. constant or variable fluxes or heads), which allows scenarios to include ground water, i.e. water entering the catchment from outside its boundaries via an aquifer. Evans and Davies (1998) included ground water, soil water and runoff in a hypothetical 3-component mixing model to develop nine patterns of hysteresis using one particular temporal pattern of flows for these three components. Using runoff method A, we reproduced their type A3 pattern using HYDRUS, i.e. anticlockwise, concave and negative for $C_G>C_{SO}>C_{SE}$ (Fig. 5; see figure for symbol definitions), which indicates that groundwater was adequately simulated by HYDRUS, but attempts to reproduce another pattern (C1) were unsuccessful because, in a hill-slope scenario, we could not exactly reproduce the temporal patterns of discharge and concentration for the three water sources used in the hypothetical mixing model. Evans and Davies (1998) noted also that their patterns did not completely describe their own observed system nor those of some other authors. Hence, we abandoned attempts to reproduce the other seven patterns of these authors.

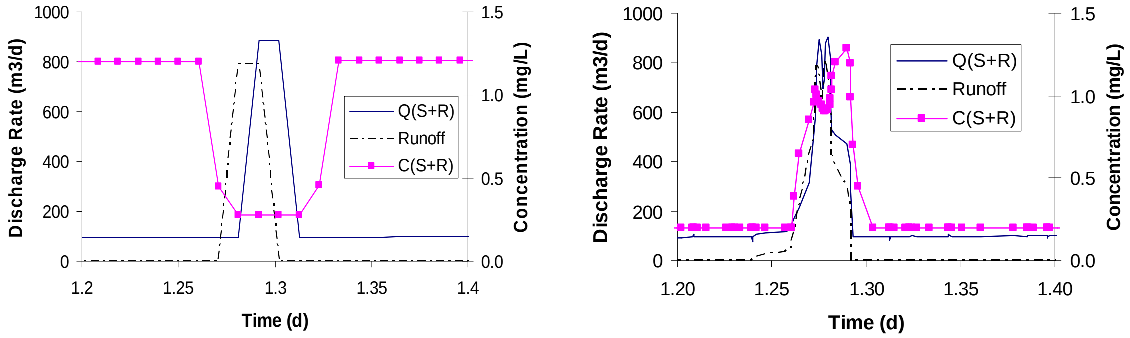

Fig. 4. Simulated temporal patterns of discharge and concentrations of NO_3 (left) and phosphate (right) during a complex rainfall event in the Montagu catchment that led to runoff.

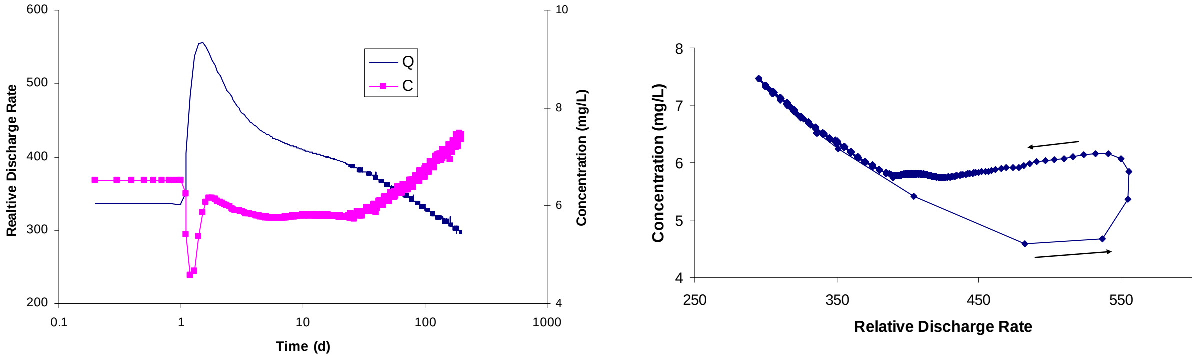

Fig. 5. A rainfall runoff event simulated with three water sources with contrasting concentrations. This scenario is akin to type A3 as described Evans and Davies (1998), i.e. ground-water concentration (C_G) > soil water concentration (C_{SW})> event concentration (C_{SE}). The direction of hysteresis is indicated by arrows.

3.4. Difficulties Encountered

Successful HYDRUS simulations require a sound knowledge of soil processes in combination with a working knowledge of numerical models generally, i.e. use of time steps and spatial nodes, and initial and boundary conditions. Failure of HYDRUS to reach a solution was not uncommon during the development of this paper, but sometimes failure was due to the user expecting the model to solve unrealistic situations, e.g. when extreme temporal or spatial gradients in pressure or concentration were unintentionally specified. Trial and error was required to develop solutions under many conditions.

HYDRUS requires boundary conditions to be set prior to a simulation, e.g. an atmospheric boundary condition is required for rainfall. Although HYDRUS simulates infiltration-excess runoff, simulation of saturation-excess runoff required progressive changing of surface nodes from an atmospheric boundary condition to a seepage face, which greatly complicated maintenance of the hydrological balance, because converted nodes no longer receive rainfall. Instead, we tested the approach of adding a runoff layer to the large catchment in the Rusjan et al. (2008) August II-5 scenario presented in Fig. 2. However, the simulation did not match observations or the simulation in Fig. 2 due to excessive down-slope infiltration. Although some rapid runoff was observed, it was minor and resulted in only a small dilution of seepage water. In contrast, when an artificial runoff layer was used to simulate the very small catchment of the hump-and-hollow system in Fig. 4, excessively rapid runoff occurred. Although use of an artificial runoff layer might be warranted under some conditions (perhaps longer time-scales and with appropriate tuning of surface soil and runoff layer K_{sat} values), results of these tests were not encouraging.

4. CONCLUSIONS

Using simple assumptions and measured values of soil, rainfall and solute characteristics, the HYDRUS model simulated some generalised aspects of C(Q) patterns, i.e. a large increase in discharge resulting from rainfall exceeding infiltration, and accompanying dilution or enrichment effects on solute concentrations. It was useful for evaluating hypotheses about concentration-discharge patterns that offers a means of improving upon those resulting from mixing model interpretations, because HYDRUS can mechanistically integrate many of the landscape processes that affect these patterns. Overall, HYDRUS was not easy to use in a hillslope context that included runoff. Two methods of simulating runoff and discharge (runoff plus seepage) were evaluated. Both methods had advantages and disadvantages, but method A was more useful for the applications tested. Applications of HYDRUS to the prediction of stream flow and water quality will be strongest where temporal patterns are dominated by processes within the soil profile rather than those affecting temporal patterns in the amount or quality of overland flow. HYDRUS simulations should not be expected to reflect high-resolution patterns of runoff or solute concentrations, but generalised, simulated longer-term patterns will probably be useful for testing some hypotheses about hillslope processes affecting stream flow and water quality. Efforts to find alternative approaches should continue.

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