FIELD AND MODELLING INVESTIGATIONS OF ACID SHOCK FROM SNOWMELT AT GUELPH

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ABSTRACT

Acid shock loadings to streams and lakes can occur as contaminants, built up in the snowpack during the winter season, are released with the initial melt waters. In this paper a physically-based model is described which determines the transport of pollutants through the unsaturated and saturated zones of the snowpack for an unsteady snow-surface-melt condition. The model has been tested against field observations from a plot (22.1 m x 4.57 m) at Guelph, Ontario. The model results for runoff flowrates matched the observed runoff reasonably well. The model predicted much lower pH in runoff than was observed. The discrepancy is probably due to buffering of the percolating water by dust in the basal layer of the snowpack.

Sensitivity tests of the model indicated that the grain diameter in the unsaturated snow is the critical factor controlling the shape of the hydrograph of runoff, and also the peak concentration of pollutant in runoff.

INTRODUCTION

Polluted snow occurs in some areas of Canada and in other northern countries. During winter periods with air temperatures continuously below freezing, contaminants contained within the precipitation, or deposited on the snow surface, are accumulated within the snow. The impact of collected contaminants on the local environment can be intense during the melting process since the pollutants held within the snowpack are released with significantly higher concentrations in the first melt waters than would be predicted from bulk concentrations (Johannessen and Henriksen, 1978, Colbeck, 1981).

The metamorphism of a snowpack plays a major role in concentrating pollutants in the first fractions of runoff water. Pollutants are not incorporated into the crystalline lattice during recrystallization, and the resulting separation concentrates the impurities on the grain surface (Colbeck, 1981). During the initial melt, water from melted ice and rain percolates downwards, removing soluble impurities from the snow grain surfaces. This creates an increased pollutant concentration in the water as it drains down through the pack. Once enough water has entered the pack to satisfy capillary retention, enriched melt water exits from the snowpack and becomes available for infiltration into the soil and/or overland runoff.

Although the above-noted release of pollutant to stream and lakes has been recognized in recent years, there is not a fully satisfactory description of the physical processes involved in the transport of pollutant with initial melt water. An
empirical model by Louie et al. (1984) and calculations by Colbeck (1974) and by Hibberd (1984) have been used to determine the transport of pollutant with the initial melt water. Colbeck's and Hibberd's models omitted the saturated basal layer at the bottom of the unsaturated zone of the snowpack and in Colbeck's unsaturated pollutant transport theory, pollutant hydrodynamic dispersion is omitted. In Hibberd's model, an unrealistic boundary condition of steady snow-surface melt is used to simulate the transport of pollutant with the melt water.

The snowmelt and acid shock model presented in this paper provides simulation of snowmelt at the top of snow, water and pollutant movement through the unsaturated snow layer and estimation of early flushing of pollutant at the downstream end of the snowpack saturated zone. The model is a physically-based model and uses unsteady snow surface melt conditions as a top boundary condition which is realistic in nature.

The water movement calculations are based on Colbeck's presentation (Colbeck, 1972) and the pollutant transport theory uses both convective and dispersion (Chalam, 1986). Inputs to the model are readily available meteorological observations and pH measurements of the bulk contents of the snowpack.

**LIQUID WATER RUNOFF MODEL**

The liquid water model is based on the formulations given by Colbeck (1971, 1972 and 1974). Only the summary equations to be applied to the field situations are given here.

Percolation of water through the snowpack is treated in two steps (see Figure 1). Melting and rain at the upper surface of the snow release a wave of water which travels vertically through the unsaturated snowpack. This water accumulates at the base of the pack and travels downslope in a thin saturated zone to the lower end of the slope.

The unsaturated zone

In considering the liquid water (melt water + rain) released at a flux rate $U_w$ at any time, and ignoring capillary effects Colbeck (1971) shows that the vertical rate of movement of this value of flux is given by:

$$V_u = \frac{(ak_u)^{1/3}}{P_e} [\left(\frac{U_w}{U_{w+}}\right)^{2/3} + \left(U_w - U_{w+}\right)^{1/3} + \left(U_{w+}\right)^{2/3}] \quad \text{(1)}$$

where

- $a = (d g/u_w) = \frac{5470000 \text{ m}^{-1} \text{s}^{-1}}{993 \text{ kg/m}^3 \times 9.81 \text{ m/s}^2} = 9.81 \text{ m/s}^2$ and $\mu_w = 1.78 \times 10^{-3} \text{ kg m}^{-2} \text{s}^{-1}$ at 0°C
- $k_u$ = the intrinsic permeability of the snow (m²)
- $P_e$ = the effective porosity of the snow defined as total porosity minus the water-filled porosity when gravity flow ceases
- $U_{w+}, U_w$ = the flux above and below the wave front respectively
- $V_u = \text{the propagation velocity of the wave front caused by the flux } (\text{m/s})$

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The time-varying input flux is represented by a sequence of time steps with \( U_w \) held constant within each time step. Within each time step, the constant \( U_w \) value at the snow surface (\( Z = 0 \)) produces a step-in-flux wave which moves downward into the snow with a constant characteristic velocity given by equation (1). The depth of penetration of the wave as a function of time can be calculated directly as a product of this characteristic velocity multiplied by elapsed time. Between the snow surface and the penetrating wave, the flux is constant with depth and equals \( U_w \) for that step.

The hydrograph of outflow from the unsaturated zone, \( I(x,t) \) that is created by the arrival of the various flux rates at the bottom of the snowpack is the input to the saturated layer.

The saturated layer

For the strip of hillside of unit width with constant small angle, \( i \), Colbeck (1974) expressed the continuity equation for the saturated layer as:

\[
K_s \frac{\partial h}{\partial x} + \theta_s \frac{\partial h}{\partial t} = I(x,t) \quad \text{(2)}
\]

where

- \( \theta_s \) = the water content in the saturated basal layer
- \( K_s \) = permeability of the saturated layer (cm/s),
- \( i \) = slope of the hillslope,
- \( h \) = thickness of the saturated layer (cm),
- \( x \) = distance along the hill slope, (cm), and
- \( t \) = time (s).

This equation indicates that the thickness of the saturated layer increases with distance downslope and varies with time in response to the input of water percolating from the unsaturated zone. In the case of daily cycles of snowmelt from a pack of uniform thickness the input is constant along the slope at any one time but varies throughout the day in response to varying melt and rain rates.

Another approach to represent the flow in the basal layer is to represent the layer as a series of continuous stirred tank reactors (CSTR) (see Figure 2). The total length of the saturated layer is divided into a number of cells and flow through the reactors is solved simultaneously for all time steps. The output from the \((n-1)\)st reactor will be the input to the \(n\)th reactor and the mass balance is given by equations 3 and 4.

\[
\theta_s \frac{\Delta h(I,J)}{\Delta t} = \theta_s \frac{\Delta h(I,J-1)}{\Delta t} = I(\Delta x, t) \Delta x \Delta t + Q(I-1,J) \Delta t - 0.5 \left[ Q(I,J-1) + Q(I,J) \right] \Delta t \quad \text{(3)}
\]

\[
Q(I,J) = K_s \frac{\partial h(I,J)}{\partial x} \quad \text{(4)}
\]

where

- \( \theta_s \) = water content in the saturated basal layer,
- \( \Delta x \) = length of each cell (cm),
FIG 1 Schematic representation of water flow through the unsaturated and saturated zones of the snowpack.

FIG 2 Schematic diagram showing the layout of continuous stirred tank reactors in the saturated snow.
\( Q(I,J) \) = discharge at the outlet of cell I at time \( (J) \) \((\text{cm}^3/\text{s})\) and,
\( h(I,J) \) = depth of the saturated zone cell I at time \( J \).

**POLLUTANT TRANSPORT MODEL**

The pollutant transport with percolating water is treated in two steps. Firstly, transport through the unsaturated zone is simulated followed by transport through the saturated zone. Simplification is gained by noting that most pollutant present within a snowpack is in solution within a liquid water film around the ice crystals.

**The unsaturated zone**

The continuity equation for solute transport in an unsaturated media is very well established. The differential equation governing dispersion of a non-reacting solute in a one-dimensional profile with no source and sink is:

\[
\theta \frac{\delta c}{\delta t} = \frac{\delta}{\delta z} \left( \theta D \frac{\delta c}{\delta z} \right) - u \frac{\delta c}{\delta z} \tag{5}
\]

where

\( \theta \) = water content,
\( c \) = concentration of pollutant \((\text{mg/cm}^3)\),
\( D \) = dispersivity \((\text{cm}^2/\text{s})\).

The solution of equation (5) must be coupled with the liquid water conservation equation (1) and to proper initial conditions and boundary conditions at the top of the snowpack. The conditions used to solve equation (5) are:

\[
t = 0; \quad x > 0; \quad c = c_i \quad t > 0; \quad x = 0; \quad c = c_0
\]

where

\( c_i \) = pollutant concentration in the irreducible water \((\text{mg/cm}^3)\)
\( c_0 \) = pollutant concentration in the input water \((\text{mg/cm}^3)\)

The solution of equation (5) with the above boundary conditions under conditions of varying surface flux is quite complex. In the model the solution is approximated by assuming that dispersion occurs around the position of the moving front formed by the penetrating melt and rain water following a procedure given by Rose et al. (1982). This "solute front" separates water with concentration \( c_0 \) above and \( c_i \) below. The position of this front at time \( t \) is determined by calculating the depth of snow measured downward from the surface, which contains the total amount of water that has entered the pack at time \( t \). Dispersion of pollutant on either side of the front then is allowed for by an error function solution of the form

\[
\frac{c - c_i}{c_0 - c_i} = 0.5 \text{erf} \left[ \frac{2 - \frac{\lambda}{2D(t)^{\frac{1}{2}}}}{2(Dt)^{\frac{1}{2}}} \right] \tag{6}
\]

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where

\[ C = \text{concentration of pollutant in the percolating water (mg/cm}^3), \]
\[ \lambda = \text{depth to solute front (cm), and} \]
\[ D = \text{dispersion coefficient (cm}^2/\text{s}). \]

The pollutograph obtained at the base of the snowpack becomes the input, \( C(x,t) \), to the saturated snow.

The saturated snow

The CSTR technique, once proved efficient in determining the water transport, was used to determine the pollutant transport in the basal layer. The final form of solute balance for the saturated zone using CSTR technique is:

\[
\theta_s \Delta x \left[ c(I,J)h(I,J) - c(I,J-1)h(I,J-1) \right] =
\]
\[
c(\Delta x,J)I(\Delta x,J)\Delta x\Delta t + c(I-1,J)Q(I-1,J)\Delta t - 0.5 \left[ c(I,J)Q(I,J) + c(I,J-1)Q(I,J-1) \right] \Delta t \]

\[ \text{where} \]
\[ h(I,J) = \text{saturated layer thickness of the I th cell at the J th time step, (cm)}, \]
\[ c(I,J) = \text{concentration of pollutant in the I th cell at J th time step, (mg/cm}^3), \]
\[ Q(I,J) = \text{is the outflow from the I th cell at the J th time step (cm}^3/\text{s}), \]
\[ \Delta x = \text{length of cell (cm), and} \]
\[ \Delta t = \text{time step (s)}. \]

MODEL INPUTS

To make the simulation model widely applicable, it was structured to require data that can be readily obtained. The water transport submodel requires data on rate of rain and of snowmelt and porosity of the snowpack. Pollutant concentration in bulk snow and in rain are needed for the pollutant transport submodel.

The concentration of pollutant in the irreducible water is calculated by assuming that liquid water fills 7% of the voids and that this water contains all the pollutant present in the snowpack. The parameters intrinsic permeability in the unsaturated and the saturated zones, and dispersion coefficient, are calculated with the established equations given in literature (Shimizu (1970), Bear (1972)). The unsaturated and saturated snow grain diameters which are required for these equations were assumed due to a lack of field measurements.

MODEL VERIFICATION

The suitability of the model, was tested using field measurements of snowmelt from plot No. 10 (Figure 3) on the University of Guelph campus in Guelph, Ontario. Two melt events, one a rain-on-snow event and the other a sequence of sunny-days, were observed during the plot study in February and March, 1985. The model has been tested for only the rain-on-snow event so far.
Fig 3  Diagrammatic plan of the runoff plots.
Snow depth and density measurements were made before and after the melt event in order to estimate the snow water equivalence in mm on the plot. The liquid water runoff from the snowpack was measured at a flume at the downstream end of the plot. Measurements for pH and specific conductance in the runoff were made throughout the study period. Samples were analysed within 24 hours of their removal from the snowpack.

**Snow surface melt condition**

The snow surface melt for the observed rain-on-snow event used to check the model was calculated by an empirical equation (8) given by Richard Kettleman of Central Sierra Snow Laboratory in California (personal communication).

\[ M = 0.46 \times T_a + 0.25 \]  \hspace{1cm} (8)

where

- \( M \) = daily reduction in snow water equivalent (cm),
- \( T_a \) = air temperature in °C.

Kettleman's equation gives daily water-equivalent reduction in cm. It is modified to hourly values in mm by multiplying with an appropriate constant (0.417). Further, Kettleman's equation was calibrated against measurements of reduction in water equivalent and \( M \) includes the liquid water released as ice crystals melt. \( M \) was reduced by multiplying it by the thermal quality of the snow to get ice crystal melt.

The total liquid water in mm entering the snowpack is obtained by adding the reduced Kettleman's melt to the rain amounts. The total quantity of percolation water moving through the snowpack for each time step was then obtained by adding to the rain and melt amount the amount of liquid water released from storage in the snow by melt or compaction during that time step. Hourly air temperatures and hourly rain fall amounts for calculating the snow-surface melt condition were obtained from nearby observations of Elora and Wellington-Waterloo airport respectively.

**Pollutant concentration in bulk snow**

The pH and specific conductance of dry snow had been measured at the field site in the top 5 cm and in a 5 cm layer centred at 15 cm depth before the start of the melt event to assess the concentration variation in the snowpack. These measurements were averaged to obtain a value of concentration in the snowpack before the start of the melt event. Measurements of pH and specific conductance of snow at the bottom of the snowpack were not included in order to avoid any influence of soil interaction on the average initial pollutant concentration within the snowpack.

**Selection of snow grain diameters**

Since there is a great variability of grain diameters in unsaturated and saturated snow, to be sure that possible values of these important parameters were considered, a wide range of published values of snow grain diameters were considered. Selection of snow grain diameter is a crucial parameter since many other parameters such as intrinsic permeability in the unsaturated and saturated zones and the pollutant dispersion coefficient in the unsaturated zone are dependent on this value. To include possible values, a range of snow grain diameters from 0.25 mm to 2.0 mm in the unsaturated snow was used for simulation trials of the model.
RESULTS FROM VERIFICATION

Figures 4a to 4d represent comparison between predicted and observed fluxes at the end of the saturated zone for different grain diameters in the unsaturated and saturated snow. The simulated results for water flux at the end of the saturated zone obtained by using 0.5 mm grain size in both the unsaturated and saturated zone has given the closest representation of the general trend of the observed flux at the flume. Increasing grain size in the unsaturated zone causes sharp peaks in outflow as a result of the lower water-holding capacity and greater percolation velocity in this zone.

Discrepancies in time-to-peak and peak rates between observed and model results are attributed to:

- differences in temporal pattern of rain between the Wellington–Waterloo airport and Guelph. The locations are 20 Km apart;

- addition of 1°C to the hourly temperature record at Elora to represent Guelph temperatures. This may not be appropriate for all time periods of the study;

- plot area calculations (the plot area was not well defined as boundary sheets fixing the plot sides had been removed for the winter);

- factors which were ignored in the present study such as ice blockage along the flow path and infiltration losses.

Figure 5 represents the comparison between the predicted and observed fluxes at the end of saturated snow for different saturated snow grain diameters. The results indicate that the grain diameter of 0.5 mm in both the unsaturated and saturated zones of the snowpack leads to model output corresponding to the general trend of the observed flux at the flume. The depth of the saturated zone needed to produce a given flux decreased with the increase of the saturated snow grain diameter and sharper peaks were observed in the simulation results.

Figure 6 represents the relative hydrogen ion concentration at the end of the saturated zone in relationship to the percentage of liquid water released. The results indicate that the initial 11% of water carries 80% of pollutant of the bulk snow. Johannessen et al., (1978) have reported that their laboratory and field lysimeter experiments showed a release of about 50 to 80% of pollutant load with the first 30% of the melt water. Similarly when Colbeck (1981) studied acid snowmelt in the laboratory, he observed a concentration of pollutant 5 times larger than the average pollutant concentration at the beginning of melt water outflow.

As a part of sensitivity analysis, results were obtained for the release of relative pollutant variation with liquid water outflow for different grain diameters (0.25, 0.5, 1.0, and 2.0 mm) in the unsaturated zone (with grain size in unsaturated and saturated snow the same). Figure 7 shows the variation of the release of relative pollutant with the melt water for different grain sizes in the unsaturated snow. The results indicate that, as the snow grain size in the unsaturated snow decreases, a longer time is required to wash the pollutant from the snowpack. With grain sizes of 1 mm, the first 11% of melt water released 80% of the pulse of elevated pollutant, whereas with 0.25 mm grain size, around 18% of melt water released the same 80% of the pollutant pulse. It is important to note the effect of unsaturated snow grain diameter on the release of pollutant from the snowpack.

CONCLUSIONS

While the model results for pH in runoff agree with published results for acid shock they do not correspond to the measured field values for pH of runoff at the flume.
Fig 4(a) Observed hydrograph and calculated outflow for a grain size of 0.25 mm in both unsaturated and saturated zones.

Fig 4(b) Observed hydrograph and calculated outflow for a grain size of 0.50 mm in both unsaturated and saturated zones.
Fig 4(c) Observed hydrograph and calculated outflow for a grain size of 1.0 mm in both unsaturated and saturated zones.

Fig 4(d) Observed hydrograph and calculated outflow for a grain size of 2.0 mm in both unsaturated and saturated zones.
Fig 5(a) Calculated outflow for a grain size of 0.5 mm in the unsaturated zone and 1.0 mm in the saturated zone.

Fig 5(b) Calculated outflow for a grain size of 0.5 mm in the unsaturated zone and 2.0 mm in the saturated zone.
Fig 6  Variation of relative hydrogen ion concentration with % of liquid water outflow from the snowpack for 0.5 mm grain size.

Fig 7  Variation of relative hydrogen ion concentration with % of liquid water outflow from the snowpack for different grain sizes.
The model predicted a pH in early runoff of 3.8 while the lowest observed pH in runoff was 5.9. It is believed that the discrepancy is due to the buffering of pH by dust contained in the basal snow layer in which the saturated zone formed.

The model represents the principal physical processes involved in pollutant transport in snow. The input parameters required to run the model are reasonably easy to measure or estimate. More testing of the model is required to establish the range of conditions for which it is applicable. The model would have to be expanded to include the effects of interaction of outflow water with basal dust and the ground surface, before it is applicable to modeling acid shock in areas with soils rich in carbonate.

BIBLIOGRAPHY


