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Validations of a Numerical Model of Solute Transport in a Snowpack

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눈 속에서 용질이동을 모사하기 위한 수치모델의 검증

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겨울철동안 쌓여 봄에 놓은 눈 녹은 물(snowmelt), 즉 융설의 유출은 북반구 및 산간지역에서 매우 중요한 것으로 여겨지고 있다. 이러한 지역에서 융설로 인한 유동 및 이온의 이동에 대한 이해는 매우 중요하며 전세계적으로 꾸준하게 연구되고 있다. Lee *et al*. (2008a)와 Lee *et al*. (2008b)연구에서는 대기로부터 수송된 이온 및 오염원이 융설에 의해 눈 속을 이동하는 것을 모사하기 위한 Mobile-Immobile water Model (MIM)을 개발하였다. 이 연구에 사용된 모델을 검증하기 위해서 물질수지계산(mass balance calculation) 및 해석해(analytical solution)를 이용한 모델결과와의 비교를 수행하였다. 일정시간동안 눈 속에서의 물질의 질량변화는 눈 표면에서 들어온 물질과 눈 기저부에서 빠져나간 물질의 질량 차이와 같아야한다는 사실을 이용하여 물질수지를 계산하였다. 파면(wave front)의 이동속도 및 기존문헌에서 알려진 해석해를 이용하여 모델결과와의 비교도 시도하였다. 모델의 물질수지계산결과 질량 차이가 거의 발생하지 않았으며 모델결과와 해석해와의 비교 역시 두 결과가 거의 일치하였다.

주요어 : 융설, Mobile-Immobile Model, 물질수지계산

Snowmelt from seasonal snow covers can be significant in many environments of northern and alpine areas. Water flow and chemical transport resulting from snowmelt have been studied for an understanding of contributions to watersheds or catchments. A Mobile-Immobile water Model (MIM) was developed to describe the movement of ionic tracers through a snowpack by Lee *et al*. (2008a) and Lee *et al*. (2008b). To validate the model used in the studies, mass balance calculations of the model were conducted and comparisons were made between model results and analytical solutions in this work. Mass balance was calculated based on the fact that change in total mass within a snowpack with time is equal to sum of any change in the flux of water or ionic tracers into and out of the snowpack. Calculations of both water and ionic mass show almost perfect agreement between changes of two water and solute mass fluxes. Comparisons between model results and analytical solutions including wave velocity and effective saturation show almost perfect agreement.

Key words : snowmelt, Mobile-Immobile Model, mass balance calculation

1. Introduction

Precipitation is of major interest in the water cycle, and is the ultimate source of water to catchments or watersheds. Seasonal snow covers over 25% of the Earth's land surface, distributing mostly at high latitude and at high altitude areas (Rodhe, 1998). This stored water of precipitation in snowpack greatly affects the hydrological regime through melting processes. This winter storage and spring release of precipitated water has important consequences for the water resources of catchments in many alpine areas (Meixner *et al*., 2004). Seasonal snow supplies to water reservoirs and recharges groundwater aquifers during spring. Therefore, snowmelt is a major component of the hydrological cycle in many regions and is an important consideration for water resourses (Singh *et al*., 1997).

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Seasonal snow covers can be significant in the chemical dynamics of ecosystems in many regions. For example, terrestrial nitrogen export (N) during snowmelt to aquatic ecosystems is linked to nitrogen saturation and freshwater acidification. An exponential decrease of solute concentration (i.e., an ionic pulse) has been reported through the melting season and so have diurnal variations that were negatively related to the melting rate (Lee *et al*., 2008a). The solutes tend to leave the snowpack with the first meltwater, which may be much higher in solutes than the original snowfall during snow metamorphism or snow redistributions, which causes low pH values in the streams with health hazards for the biota (Williams *et al*., 1995).

Hibberd (1984) simulated the ionic pulse using a standard advection-dispersion model, which was unable to simulate the long-tail following initial solute arrival. This limitation was improved by a mobile-immobile model (MIM), which provided one simple conceptualization for modeling preferential flow in snow (Harrington and Bales, 1998). In the MIM, solutes in the mobile water are transported by advection and dispersion, and those in the immobile water are transported only by exchange between immobile and mobile water (Harrington and Bales, 1998; Feng *et al*., 2001; Lee *et al*., 2008a). In early model (e.g., Harrington and Bales, 1998), the exchange between mobile and immobile water was parameterized by first order kinetics with an invariant exchange rate constant. Feng *et al*. (2001) discovered that an invariant exchange rate constant cannot explain their observed results in a rain-on-snow experiment, in which tracer concentrations positively associated with the input flux. Lee *et al*. (2008b) monitored chemical compositions of both natural and artificial tracers flowing fresh snow, snow profile and snowmelt. They observed that natural tracers showed negative concentration-discharge relationship while artificial tracers showed positive relationship under same hydrological condition.

To better understand how hydrological conditions control solute transport and redistribution in a snowpack, it is, however, limited to use the model by Feng *et al*. (2001) to simulate both types of concentration-discharge relationship with a common set of hydrological parameters. Lee *et al*. (2008a) described artificial rain-on-snow experiments onto a snowpack to understand how hydrological and chemical conditions cause a positive or negative relationship between meltwater in discharge and solute concentration based on observations from the experiments and those of Feng *et al*. (2001). Lee *et al*. (2008a) tested the necessity of having a flow-dependent exchange rate coefficient as proposed by Feng *et al*. (2001) under different hydrological and chemical conditions for simulating both the positive and negative concentration-discharge relationships using the MIM. Here we present a validation of the MIM used by Lee *et al*. (2008a) and Lee *et al*. (2008b), which has never been discussed elsewhere. Our objective in doing this is to develop and validate the capability to investigate the solute transport in a snowpack, and thence to use this model to explore concentration-discharge relationships under various hydrological and chemical conditions. In this paper, we first describe how to validate the model and then compare results from the model with analytical solutions and mass balance calculations.

2. Theoretical Background

Both flow and transport model can be verified using mass balance and analytical solutions. Change in total mass within snowpack with time is equal to sum of any change in the flux of water or ionic tracers into and out of snowpack. For flow model, we can compare the wave front velocity at the surface under a certain circumstance. On the other hand, van Genuchten and Wierenga (1976) derived analytical solution for mobile and immobile water exchange. The analytical solution will be used to verify the accuracy of mobile and immobile model (MIM) presented here. The variables used in these and following equations are described in Table 1.

2.1. Mass balance

As introduced earlier, Eq. (1) describes that total water mass change within the snowpack with time is equal to sum of any changes in the flux ($q=\rho KS^n$) of water and ice into and out of snowpack.

$$\int_{z=surface}^{z=bottom}(a+b)_{t=t_1}dz-\int_{z=surface}^{z=bottom}(a+b)_{t=t_2}dz = \int_{t=t_1}^{t=t_2}[(\rho KS^n)_{z=surface}-(\rho KS^n)_{z=bottom}]dt \tag{1}$$

Table 1. Snowpack properties and symbols used in this study

	Meaning (Values used in the simulations if not otherwise specified)	Units	Dimension
α	total mass of water per unit snow volume	g cm^{-3}	g of total water/ cm^{3}snow
α_i	mass of immobile water per unit snow volume	g cm^{-3}	g of immobile water/ cm^{3}snow
α_m	mass of mobile water per unit snow volume	g cm^{-3}	g of mobile water/ cm^{3}snow
b	mass of ice per unit snow volume	g cm^{-3}	g of ice/ cm^{3}snow
C_i	tracer concentration in immobile phase	g/cm^{-3}	g of solute mass/cm^{3}ofimmobilewater
C_{ice}	initial concentration in ice ($C_{ice} = 0$)	g/cm^{-3}	
C_m	tracer concentration in mobile phase	g/cm^{-3}	g of solute mass/cm^{3}ofmobilewater
C_r	tracer concentration when sprayed	g/cm^{-3}	g of solute mass/cm^{3}ofwater
D	dispersion coefficient	cm^2/h	
d	dynamic dispersivity ($d = 0.05$)	cm	
g	gravitational acceleration	cm h^{-2}	
K	hydraulic conductivity	cm h^{-1}	
k	intrinsic permeability	cm^2	
n	exponent		3
q_z	specific discharge	cm h^{-1}	$q_z = KS^3$ cm of snow*cm^{3}water/(cm^{3}snow*h)
S	effective water saturation $(S_w - S_i)/(1 - S_i)$		cm^{3}of(totalwater-immobile) volume / cm^3 of (pore-immobile) volume
S_i	irreducible water content: irreducible volume of water over pore volume		cm^{3}ofimmobilewatervolume/cm^3 of pore volume
S_w	total water content: total water volume over the pore volume		cm^{3}oftotalwatervolume/cm^3 of pore volume
t	time	h	
u	water velocity	cm h^{-1}	cm snow/s
V_{melt}	melting rate	cm h^{-1}	cm^{3}ofsnowvolume/(cm^2 of snow*h)
V_{rf}	spraying rainfall rate	cm h^{-1}	cm^{3}ofwatervolume/(cm^2 of snow*h)
z	depth ($z = 200$)	cm	
β	$S_i/(1 - S_i)$		
θ	volumetric water content		cm^{-3}ofwatervolume/cm^3 of pore volume
ρ_{ice}	density of ice	g cm^{-3}	g of ice/ cm^{3}ofice
ρ_w	density of water	g cm^{-3}	g of water/ cm^{3}ofwater
ϕ	porosity		cm^{-3}ofporevolume/cm^3 of total volume
ω	exchange rate coefficient	h^{-1}	

where K is saturated hydraulic conductivity, S is effective saturation, n is empirical exponent, a is the mass of water and b is the mass of ice per unit snow volume, z is the depth into the snowpack, t is time and ρ is the density of water.

2.2. Analytical Solutions for Flow

2.2.1. Wave velocity

The model can be verified using the wave velocity. When there is a discontinuity of water content (wave front) in the snowpack, the position of wave front can be determined by the wave velocity, V_s (Hibberd, 1984; Feng *et al.*, 2001),

$$V_s = \frac{K}{\phi(1-S_i)}\frac{S_+^n - S_-^n}{S_+ - S_-} \tag{2}$$

where the subscripts plus and minus represent values directly behind and preceding the wave front, ϕ is the porosity, S_i is irreducible water content in the snowpack and S is the effective water saturation.

2.2.2. Solutions of S

When two wave fronts move through the snowpack, water content (S) between two wave front that have different water content (S_1, S_2) can be presented in literature (Feng *et al.*, 2001) as following,

$$S=\left[\frac{z}{n(t-t_2)}\right]^{\frac{1}{n-1}} \tag{3}$$

This solution can be applied when S_2 is less than S_1, which means a sudden decrease of water content at the surface. t_2 is when the water content changes at the surface. One-dimensional water percolation in snow is as following,

$$\phi(1-S_i)\frac{\partial S}{\partial t}+\frac{\partial(KS^n)}{\partial z}=0 \tag{4}$$

2.3. Analytical solutions for transport

2.3.1. Solutions of C_m

van Genuchten and Wierenga (1976) developed a mathematical model to describe the chemical transport. The following general system of equations (Eqs. 4 to 8) depicts the mobile and immobile phases, resulting from a pulse input of solute.

$$\theta_m\frac{\partial C_m}{\partial t}+\theta_{im}\frac{\partial C_{im}}{\partial t}=\theta_m D\frac{\partial^2 C_m}{\partial z^2}-v_m\theta_m\frac{\partial C_m}{\partial z} \tag{5}$$

$$\theta_{im}\frac{\partial C_{im}}{\partial t}=\alpha(C_m-C_{im}) \tag{6}$$

$$\lim_{z\to 0^+}\left[v_m C_m-D\frac{\partial C_m}{\partial z}\right]=\begin{cases} v_m C_0 & 0\le T<T_1 \\ 0 & T\ge T_1 \end{cases} \tag{7}$$

$$\lim_{z\to\infty}[C_m(z,t)]=0 \tag{8}$$

$$C_m(z,0)=C_{im}(z,0)=0 \tag{9}$$

where θ_m and θ_{im} are mobile and immobile water content, respectively, v_m is average pore-water velocity in dynamic region, D is dispersion coefficient and α is mass transfer coefficient. The following analytical solutions were presented for the relative concentrations in the mobile and immobile liquids in van Genuchten and Wierenga (1976).

$$c_m(x,T)=\begin{cases} c_1(x,T) & 0\le T<T_1 \\ c_1(x,T)-c_1(x,T-T_1) & T\ge T_1 \end{cases} \tag{10}$$

$$c_{im}(x,T)=\begin{cases} c_2(x,T) & 0\le T<T_1 \\ c_2(x,T)-c_2(x,T-T_1) & T\ge T_1 \end{cases} \tag{11}$$

$$c_1(x,T)=G(x,T)\exp(-\overline{\alpha}T/\beta)+\frac{\overline{\alpha}}{R}\int_0^T G(x,\tau)H_1(T,\tau)d\tau \tag{12}$$

$$c_2(x,T)=\overline{\alpha}\int_0^T G(x,\tau)H_2(T,\tau)d\tau \tag{13}$$

$$G(x,T)=\frac{1}{2}erfc\{(P/4\beta T)^{1/2}(\beta x-T)\}$$
$$-\frac{1}{2}(1+Px+PT/\beta)\exp(Px)erfc\{(P/4\beta T)^{1/2}(\beta x+T)\}$$
$$+(PT/\pi\beta)^{1/2}\exp\{-P(\beta x-T)^2/4\beta T\} \tag{14}$$

$$H_1(T,\tau)=\exp(-u-v)\{I_0(\xi)/\beta+I_1(\xi)(u/v)^{1/2}/(1-\beta)\} \tag{15}$$

$$H_2(T,\tau)=\exp(-u-v)\{I_0(\xi)/(1-\beta)+I_1(\xi)(v/u)^{1/2}/\beta\} \tag{16}$$

$$u=\overline{\alpha}\tau/\beta \tag{17}$$

$$v=\overline{\alpha}(T-\tau)/(1-\beta)R \tag{18}$$

$$\xi=2(uv)^{1/2} \tag{19}$$

where c_m and c_{im} are relative concentrations of mobile and immobile water, respectively, $\beta=\phi R_m/R$, R is average retardation factor, and I_0 and I_1 are modified Bessel functions of the second kind of 0 and 1.

2.3.2. Wave velocity

The chemical composition of wave front can be derived in Feng *et al* (2001). So the position of wave front is determined by the wave velocity, V_c

$$V_c=\frac{K}{\phi(1-S_i)}\frac{C_m^+S_+^n-C_m^-S_-^n}{C_m^+S_+-C_m^-S_-}-S_+D_+\frac{\partial C_m^+}{\partial z}+S_-D_-\frac{\partial C_m^-}{\partial z} \tag{20}$$

In this model, water that percolates through the snowpack can be from rainfall and snowmelt. Therefore mass balance calculations and analytical solutions are divided into part of rainfall and snowmelt.

3. Model Verification

3.1. Rainfall

3.1.1. Mass balance calculation

The snowpack properties and modeling parameters were described in Lee *et al*. (2008a). The initial condition of snowpack is dry (S=0). Rainfall was applied 2.5 days later and the rainfall rate was 3 cm/hr. Figs. 1 and 2 show mass balance calculation of water and solute caused by the rainfall. The snowpack has a constant thickness. There is a sudden increase of water mass right after 2.5 days. When the rainfall is applied, the water mass in the snowpack increases so that the two changes show positive values. It shows almost perfect agreement between change of water mass in the snowpack and change of water flux. Discrepancy between change of water mass in the snowpack (14.994 g/cm^2) and change of water flux (15.003 g/cm^2) is 0.06% of the change of water flux (Fig. 1). Total mass change of ionic tracer within the snowpack (149.9 g/cm^2) with time is equal to sum of any changes in the flux of ionic tracer into and out of snowpack (150.01 g/cm^2). It also shows almost perfect agreement between changes of two solute mass fluxes (Fig. 2). The error is 0.07% of the change of solute flux.

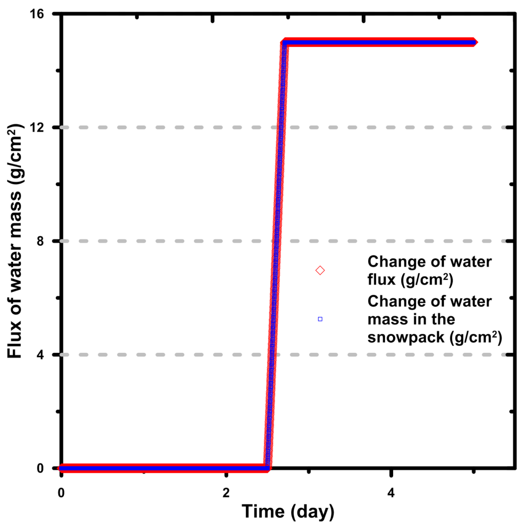

Fig. 1. Mass balance calculation for water only considering rainfall.

3.1.2. Wave velocity

Eqs. (2) and (19) describe water and chemical wave velocities. First, water wave velocity in Eq. (2) is 40 cm/hr and it takes 5 hours for water front to reach at the bottom, theoretically. Therefore, the wave front will be at the bottom after 0.208 days

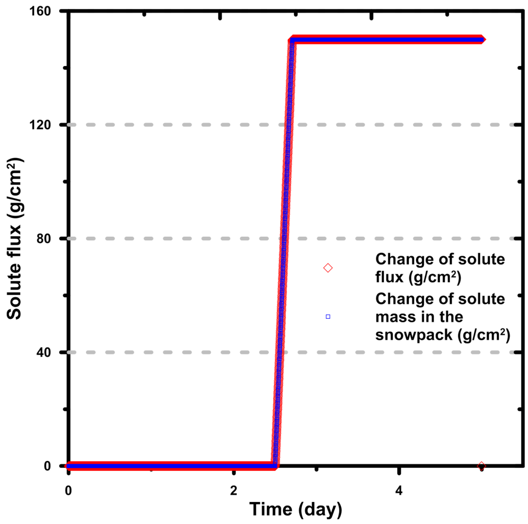

Fig. 2. Mass balance calculation for solute by rainfall.

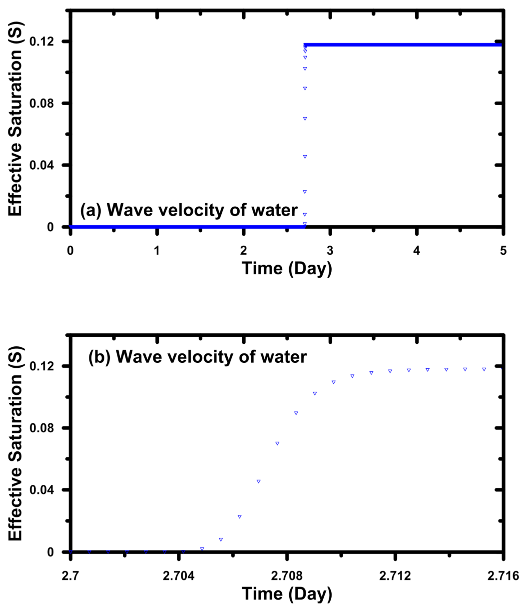

Fig. 3. Water wave front velocity calculation by rainfall.

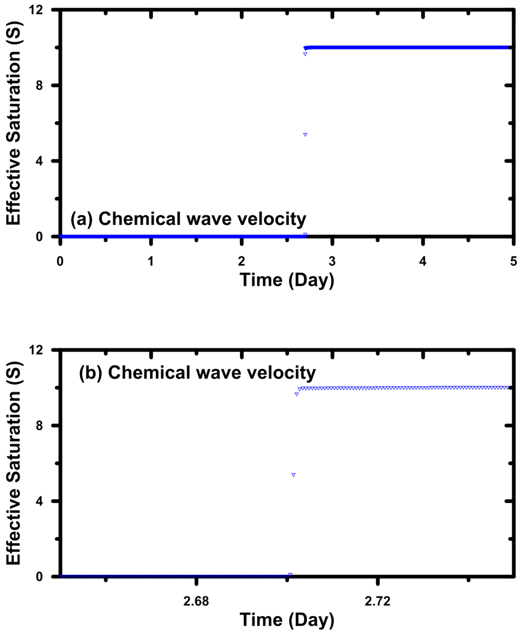

Fig. 4. Chemical wave front calculation by rainfall.

because of the change of water saturation at the surface. The rainfall was applied after 2.5 days, so we can observe the wave front 2.708 days later at the bottom. This agrees well with the model calculation (Fig. 3). Using chemical wave velocity in Eq. (20), chemical wave velocity is 40.01 cm/hr and it takes 0.207 day for chemical front to be at the bottom. So we can observe the wave front 2.707 days later at the bottom. This also agrees well with the model calculation (Fig. 4).

3.2. Snowmelt

3.2.1. Mass balance calculation

Figs. 5 and 6 show mass balance calculation of water and solute only due to snowmelt. The water mass in the snowpack decreases because it loses water mass when snow melts. In Fig. 5, it shows perfect agreement between change of water mass in the snowpack (–5.478 g/cm^2) and change of water flux (–5.4874 g/cm^2). Mass balance error between two changes of water is 0.17%. Total mass change of ionic tracer within the snowpack (–317.43 g/cm^2) with time is equal to sum of any changes in the flux of ionic tracer into and out of snowpack (–316.42 g/cm^2). It also shows almost perfect agreement between changes of two solute

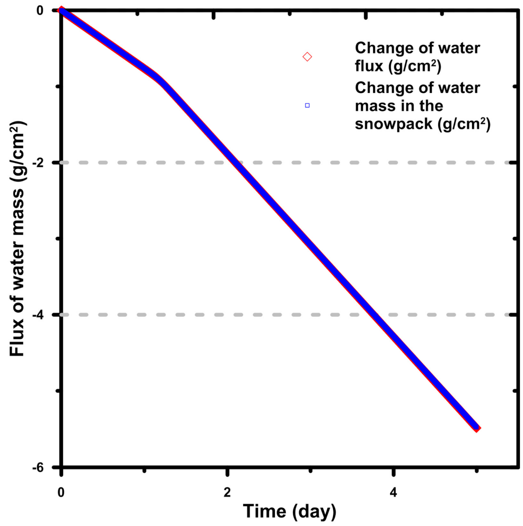

Fig. 5. Mass balance calculation of water caused by snowmelt.

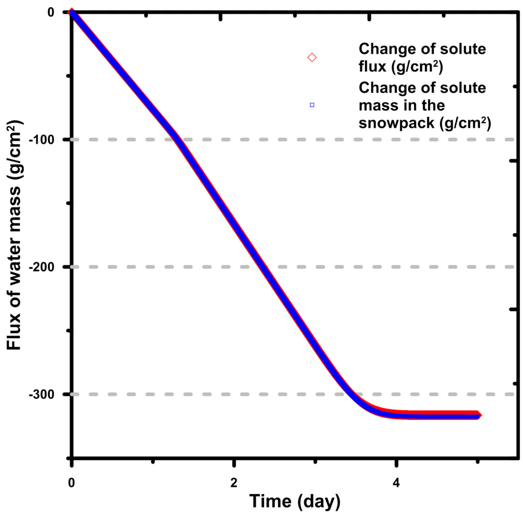

Fig. 6. Mass balance calculation of solute by snowmelt.

mass fluxes. The error is 0.32% of the change of solute flux (Fig. 6).

2.2.2 Wave velocity

Figs. 7 and 8 show the wave front position calculated by model. As discussed earlier, Eqs. (2) and (20) confirm the wave velocity. Two equations results in 1.286 days and 3.593 days for each wave front to reach at the bottom. Like rainfall, calculations of wave velocity by snowmelt agree well with model calculations.

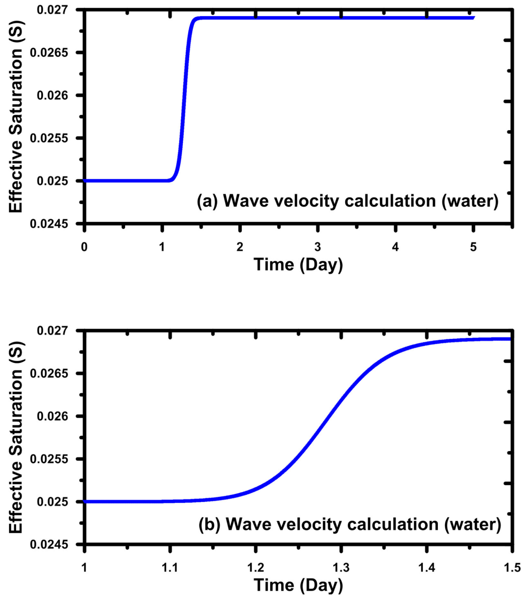

Fig. 7. Water wave front calculation by snowmelt.

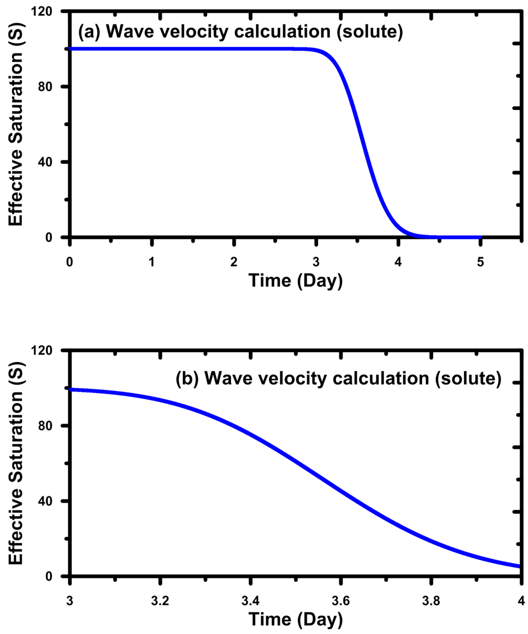

Fig. 8. Chemical wave front calculation by snowmelt.

4. Examples

There are two examples will be concerned to verify the MIM. First, flow part will be examined using Eq. (3). As discussed earlier, the analytical solutions suggested by van Genuchten and Wierenga (1976) will be also examined.

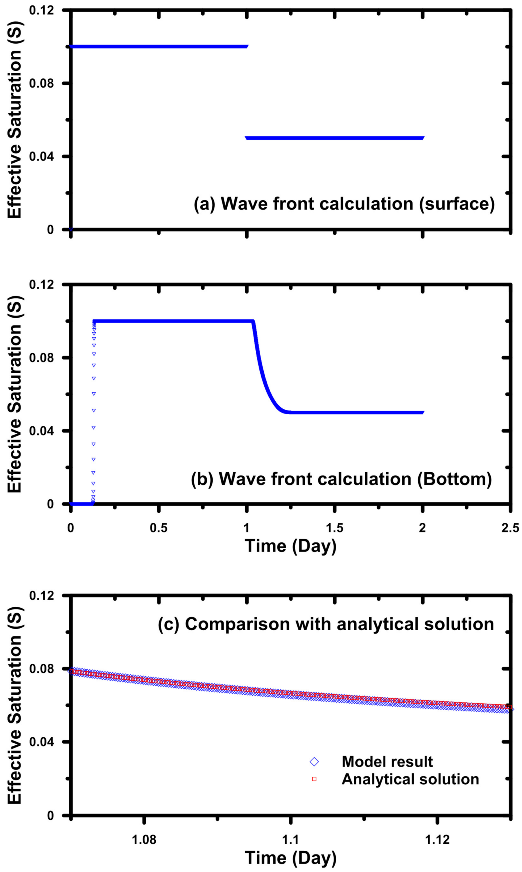

Fig. 9. Comparison with analytical solutions.

4.1. Wave front calculation

Eq. (3) predicts the effective water saturation at the bottom when boundary condition at the surface is changed, especially decrease of water content. The hydrological boundary condition at the snow surface equals the flux of water introduced to the snowpack as both rain and snowmelt (Lee *et al.*, 2008a; Lee and Ko, 2011),

$$KS_{surface}{}^{n}\rho_w = V_{rf}\rho_w + (a+b)V_{melt}$$
$$= V_{rf}\rho_w + V_{melt}[\phi(1-S_i)(S_{surface}+\beta)\rho_w + (1-\phi)\rho_{ice}] \quad (21)$$

where $\beta = S_i/(1-S_i)$ and ρ_{ice} is the density of ice. Here, as suggested Feng *et al.* (2001), boundary condition (effective saturation, S) at the surface will be changed from 0.1 to 0.05. Fig. 9 (a) shows that the effective saturation changed from 0.1 to 0.05 at the surface. Fig. 9 (b) shows the effective saturation at the bottom. Fig. 9 (c) shows comparison between model result (Eq. 4) and analytical solutions of effective saturation at the bottom for a certain period. The model results agree well with the analytical solution.

4.2 Analytical solutions for C_m

Eqs. (5) to (19) describe mathematical governing equations (Eqs. 5 to 9) and semi-analytical solutions (Eqs. 10 to 19) for mobile and immobile model that needs some assumptions. Fig. 10 shows comparison between model results and analytical solutions, especially changing with exchange rate coefficient between mobile and immobile phases (α=0 and 0.15). Feng *et al*. (2001) and Lee *et al*. (2008) confirmed that it is necessary for the exchange coefficient to increase with water velocity for the solute transport in a snowpack. The numerical calculations by the governing equations agree well with the analytical solutions suggested by van Genuchten and Wierenga (1976).

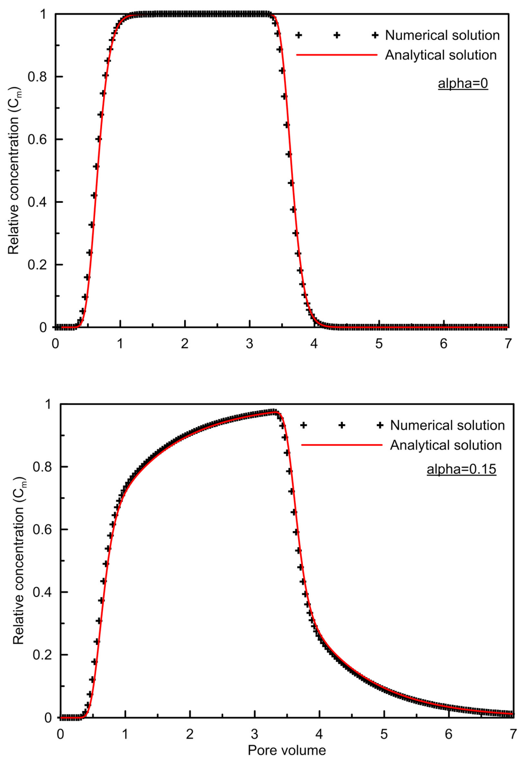

Fig. 10. Comparison with analytical solution.

5. Summary

A Mobile-Immobile water Model (MIM) was developed to describe the movement of ionic tracers through a snowpack by Lee *et al*. (2008a) and Lee *et al*. (2008b). In this work, we have validated the model using mass balance calculations and analytical solutions. Mass balances of both water and ion were calculated based on the fact that change in total mass within a snowpack with time is equal to sum of any change in the flux of water or ionic tracers into and out of the snowpack. Calculations of both water and ionic mass show almost perfect agreement between changes of two water and solute mass fluxes. Comparisons were made between model results and analytical solutions including wave velocity and effective saturation and show almost perfect agreement.

Chemical composition of a snowpack and its meltwater has never been investigated in Korea. Snowmelt-dominated systems in spring, for example, Jeju island and Ulleung island, should be studied to secure alternative water resources using snow chemistry. This work would be helpful to predict the chemical characteristics of a snowpack and its melt in those islands.

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