

Fields Institute RSC New Fellows Symposium University of Toronto, November 14, 2005

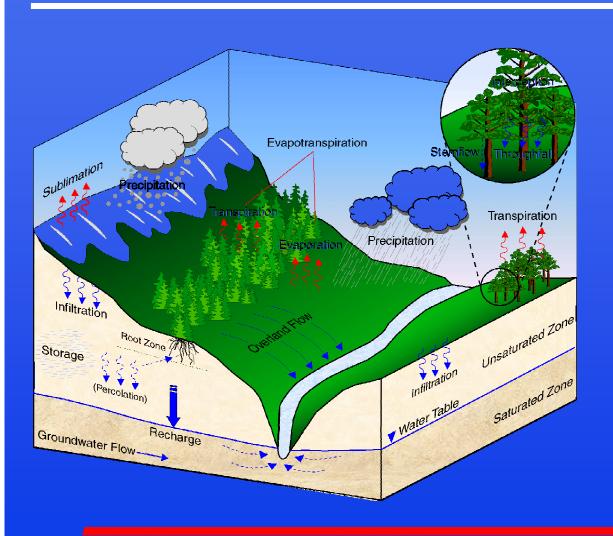
On the Challenge of Simulating Integrated Surface-subsurface Flow and Contaminant Transport at Multiple Catchment Scales

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Integrated Surface/Subsurface Hydrologic Modelling: A Grand Challenge in Water Resources Simulation



- S Attempt to account for all interactions between the surface and subsurface flow regimes
- Simultaneously solve surface and subsurface flow & transport equations
- Simulate the complete hydrologic cycle

Motivation

- Surface water models commonly lack rigor in the treatment of 3D subsurface variably-saturated flow and solute transport processes, especially in complex geologic settings
- Groundwater models typically ignore dynamics of overland/stream/wetland flow processes & surface water quality issues
- Coupling between surface/subsurface models commonly performed via sources/sinks without feedback or weakly through simple iteration

Some Issues

- Quantify spatial/temporal distribution of GW recharge, surface water/groundwater interactions in streams and wetlands
- Impacts of groundwater extraction on surface water
- Ø Effects of urbanization/land-use change on water quantity & quality, health of aquatic ecosystems
- Restoration of adversely-impacted streams, wetlands, etc.
- Subsurface versus overland migration pathways of contaminants & pathogens

Waterloo/Laval "HydroGeoSphere" Model

First Generation Code – <u>Integrated Hydrologic Model (InHM,</u> VanderKwaak, U of Waterloo, PhD Thesis, 1999), Evolved from FRAC3DVS (Therrien & Sudicky, JCH, 1996)

Consortium of "HydroGeoSphere" developers/researchers:

- Therrien et al. (Geology, Univ. Laval, Quebec)
- Sudicky et al. (Earth Sciences, Univ. Waterloo, Ontario)
- Sykes et al. (Civil Engineering, Univ. Waterloo, Ontario)
- Forsyth (Computer Science, Univ. Waterloo, Ontario)
- Panday, Guvanasen & Huyakorn et al. (HydroGeoLogic, Inc., Herndon, VA)
- Matanga et al. (US BOR, Sacramento, CA)



Overview of Current HydroGeoSphere Features

- 2D overland/stream flow (Diffusion-wave equation), including stream/surface drainage network genesis
- 3D variably-saturated flow (Richards' equation) in porous medium
- Ø 3D variably-saturated flow in macropores, fractures and karst conduits (dual-porosity, dual-permeability for macropores/fractures or discrete fracture networks)
- Advective-dispersive, reactive solute/thermal transport in all continua
- Allows for complex topography, irregular surface & subsurface properties, density-dependent flow, pumping wells, tiles, etc.
- Fully-coupled, simultaneous solution of surface/subsurface flow and transport via Control-Volume Finite Element Method

Challenges

- Ø Disparate time frames between surface/subsurface flow and transport regimes
- Very large unstructured grids, irregular topography, complex boundary conditions, surface properties & geological features
- Strong nonlinearities in governing equations
- Data availability and upscaling issues
- Applicability of governing equations & constituitive relations at watershed & larger scales

Flow Equations

Porous Medium (3D): Richards' Equation

$$-\nabla \cdot \omega_m \bar{q} + \sum_{s} \Gamma_{ex} \pm Q = \omega_m \frac{\partial \theta_s S_w}{\partial t}$$

Darcy Equation:

$$\vec{q} = -\vec{K} \cdot k_r \nabla \left(\psi + z \right)$$

Surface Water Flow (2D): Diffusion Wave Equation

$$-\nabla \cdot d_o \bar{q}_o - d_o \Gamma_o \pm Q_o = \frac{\partial \phi_o h_o}{\partial t}$$

Manning Equation (2D):

$$\vec{q}_o = -\frac{d_o^{2/3}}{\vec{n}\vec{\phi}^{1/2}} k_{ro} \nabla \left(d_o + z_o \right)$$

 ψ = pressure head

 d_o = water depth

z = elevation

 $S_w = \text{saturation}$

 $\theta_{\rm s}$ = porosity

 ω_m = pm volume fraction

 \vec{K} = permeability

 $k_r, k_{ro} = \text{rel. perm.}$

 $Q, Q_o = \text{source/sink rate}$

 Γ_{ex} , Γ_o = exchange fluxes

 $\vec{n} = \text{roughness}$

 $\vec{\Phi}$ = sw gradient

Flow Equations: Integrated Solution

Coupled Equations:

$$-\nabla \cdot \omega_{m} \vec{q} + \Gamma_{o} \pm Q = \omega_{m} \frac{\partial \theta_{s} S_{w}}{\partial t}$$

$$\uparrow \qquad \qquad \uparrow \qquad \qquad \uparrow$$

$$-\nabla \cdot d_{o} \vec{q}_{o} - d_{o} \Gamma_{o} \pm Q_{o} = \frac{\partial \phi_{o} h_{o}}{\partial t}$$

- interact via water exchange relations
- → feed-back
- convergence difficulties eliminated
- exchange relationships need explicit definition

First-Order Exchange:

$$d_o \Gamma_o = k_{rso} K_{so} \left(h - h_o \right)$$

 K_{so} = surface/subsurface conductance

 k_{rso} = coupling rel. perm./rill storage

Transport Equations: Integrated Solution

Coupled Advection-Dispersion Equations:

$$\omega_{m} \left[\frac{\partial \theta_{s} S_{w} RC}{\partial t} + \theta_{s} S_{w} R\lambda C \right] = -\nabla \cdot \omega_{m} \left[\bar{q} C - \theta_{s} S_{w} \bar{D} \nabla C \right] + \left[R\lambda C \right]_{par}$$

$$\pm Q_{c} + \Omega_{o}$$

$$\begin{split} &\frac{\partial \phi_{o} h_{o} R_{o} C_{o}}{\partial t} + \phi_{o} h_{o} R_{o} \lambda C_{o} = -\overline{\nabla} \cdot \psi_{s} \left[\overline{q}_{o} C_{o} - \overline{D}_{o} \phi_{o} h_{o} \overline{\nabla} C_{o} \right] \\ &+ \left[\phi_{o} h_{o} R_{o} \lambda C_{o} \right]_{par} \pm Q_{co} - d_{o} \Omega_{o} \end{split}$$

- interact via advective and diffusive transport processes
- → feed-back
- distinct surface and subsurface concentrations
- exchange relationship need explicit definition

Solute Exchange Flux (e.g.):

$$\Omega_o = C_{ups} \Gamma_o + \alpha_o (C - C_o)$$



Tracer-Based Hydrograph Separation Techniques to Quantify Groundwater Contributions to Streamflow

OR

Where Does the Water Go When it Rains?



Tracer-based Separation

ü Methodology

$$C_{\text{stream}}Q_{\text{stream}} = C_{\text{event}}Q_{\text{event}} + C_{\text{unsat}}Q_{\text{unsat}} + C_{\text{gw}}Q_{\text{gw}}$$
 (1)

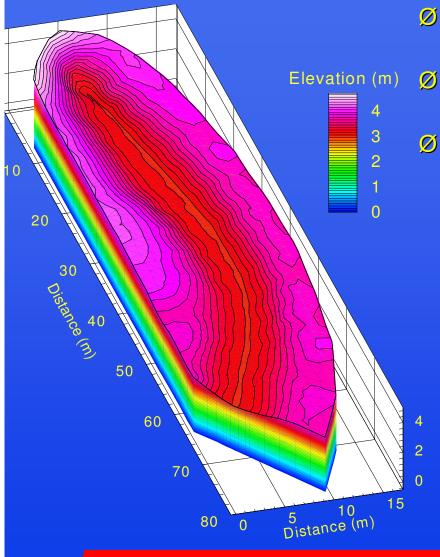
- ü Assumptions
- ü Potential problems

Example 2-Component Separations

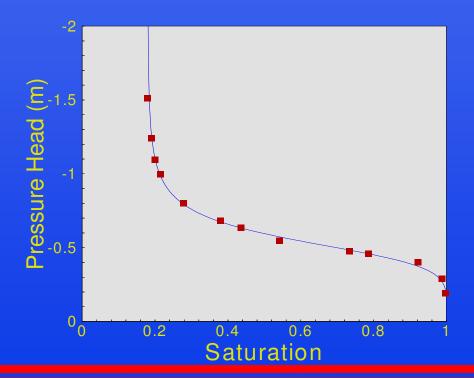
Reference	Catchment		Geological Setting	Pre-Event Contribution to Total Discharge Volume (%)
	Area (Km²)	Tracer		
Jordan, 1994	0.036	18O	Shallow Soils	45, 75
McDonnell et al., 1990	3.1	D	8 5	24
Fritz et al., 1976	22	18O	Clay-loam Glacial till	90
Fritz et al., 1976	1.8	18O	Shallow sands, silts and clays	40-45
McGlynn and McDonnell, 2003	0.0264	18O	Silt loams	53-96
Buttle and Peters, 1997	0.0322	18O	Sandy till	77
Hill and Waddington, 1993	1.57	18O	Glacial deposits	59-89
Kendall et al., 2001	0.00049	18O	Shallow silty loam	10
Leopoldo et al., 1987	1.58	18O	Sandy soils	55-93
Leopoldo et al., 1987	3.27	18O	Sandy soils	47-87
Bottomley et al., 1984	1.24	18O, D	Glacial deposits	40
Turner et al., 1987	0.82	18O, D, Cl	_ 7	60-95
Blowes and Gillham, 1988	0.0075	18O, Cl	Fine sands and silts	22- 50
Nolan and Hill, 1990	10.6	D	Clays, stony loams	57, 89
Crouzet et al., 1970	0.57	T		97
Crouzet et al., 1970	15	T T	i .	99
Crouzet et al., 1970	91	T	(2	46
Kennedy et al., 1986	620	D, T	Gravelly to clayey loam	50-80
DeWalle et al, 1988	2.08	18O	Silt loams	75
Loye-Pilot and Jusserand, 1990	0.33	18O		60-90
Sklash, 1990	0.038	¹⁸ O, D	Shallow Humic soil	75-85
Turner and Macpherson, 1990	27	D	Deeply weathered granite	58
Turner et al., 1991	6	D	Shallow Soils	25
Turner et al., 1991	10	D	Shallow Soils	37
Abdul et al., 1989	0.1	Br	Medium sands	37

Table 1. Results of previous two-component tracer-based hydrograph separation studies. Note: D = Deuterium, T = Tritium, ¹⁸O = Oxygen-18 and Br = Bromide.

Borden Field Experiment (Abdul, 1985)

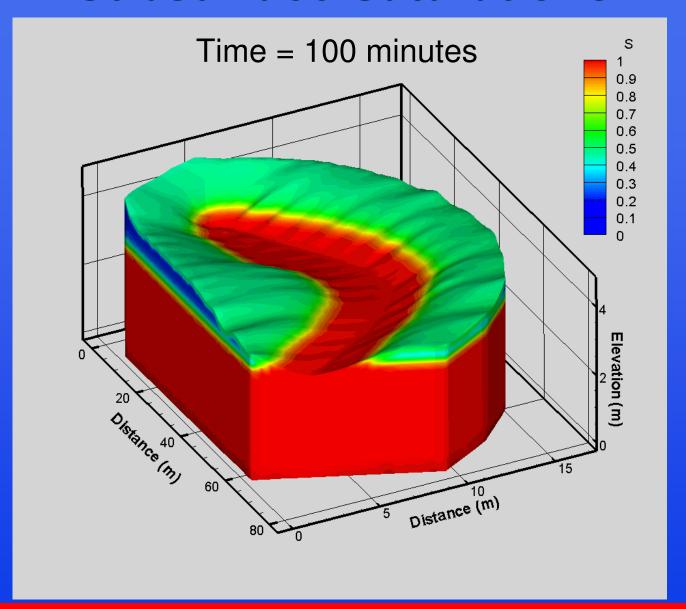


- © Capillary fringe intersects land surface along stream axis (initial head about 22 cm below stream
- Rainfall containing a conservative tracer applied for 50 minutes at 2 cm/hr
- Ø Hydrologic response observed and measured



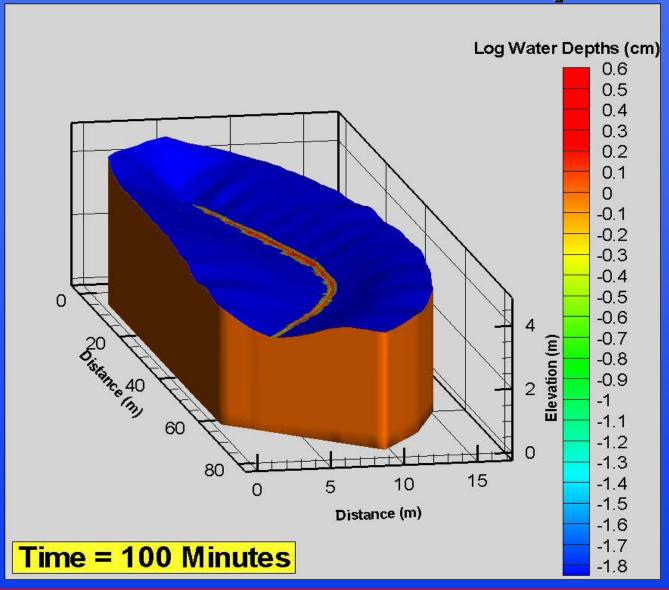


Subsurface Saturations



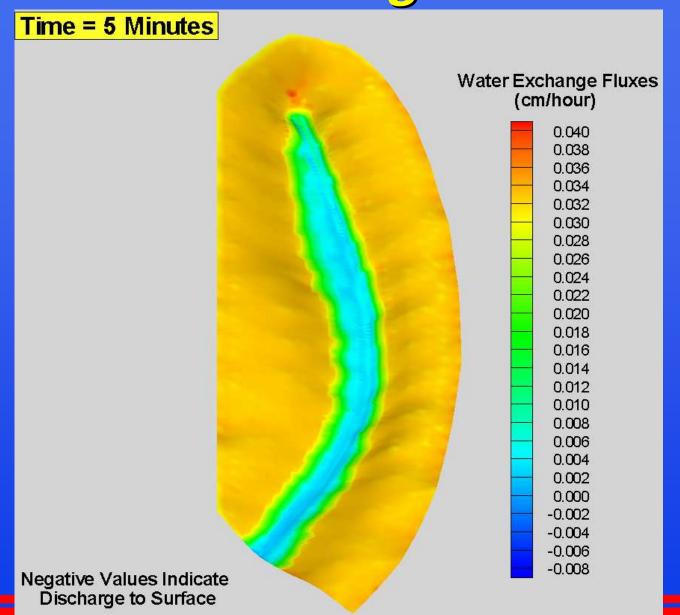


Surface Water Depths



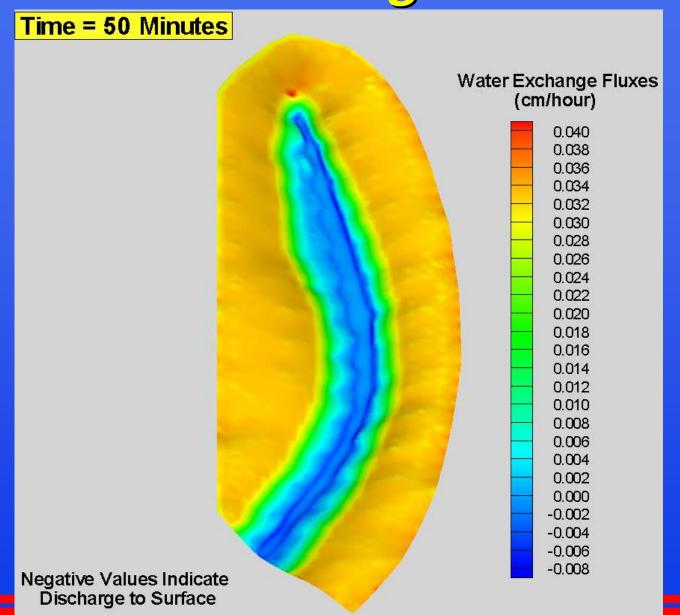


Waiter Exchange Fluxes



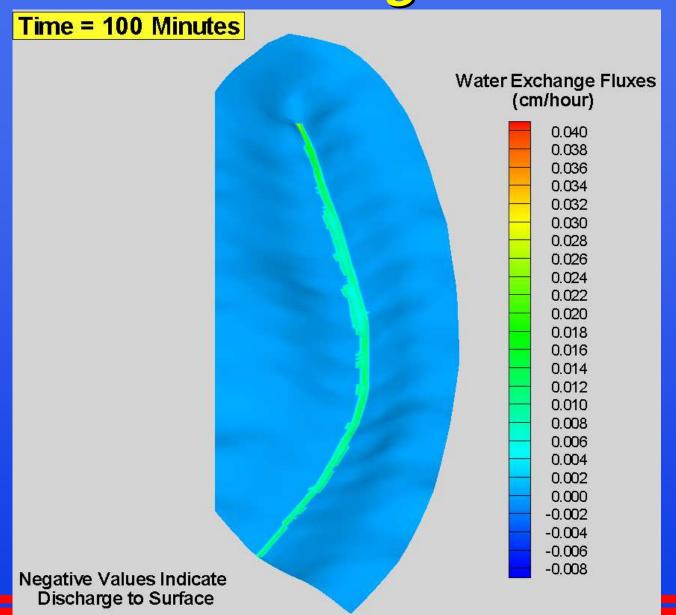


Waiter Exchange Fluxes



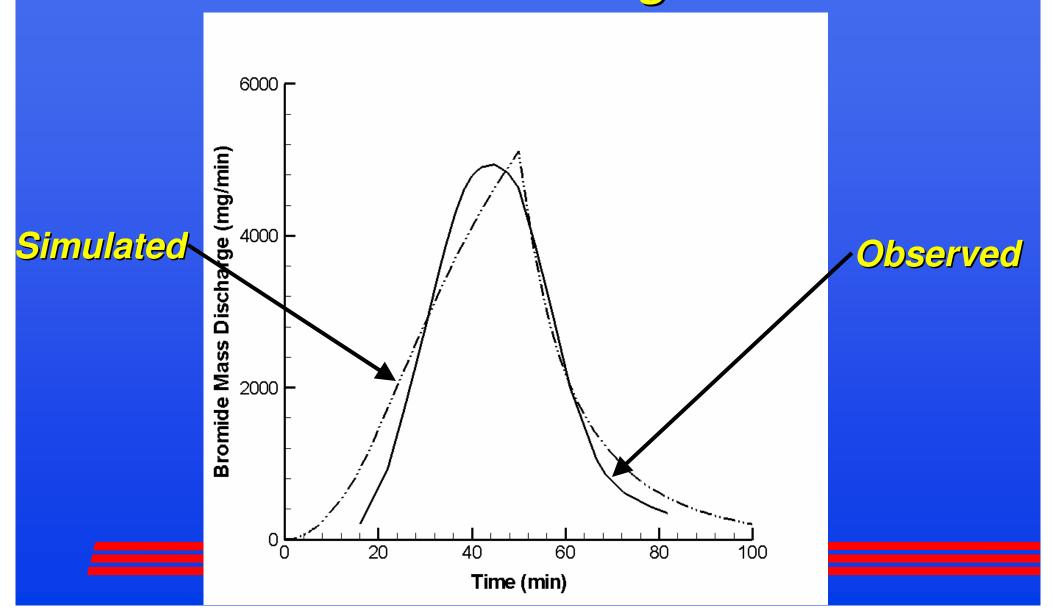


Waiter Exchange Fluxes

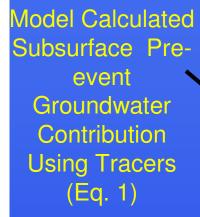




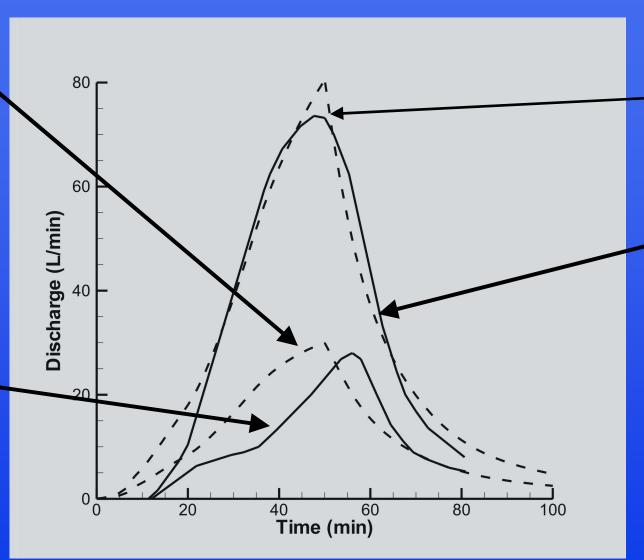
Simulated vs. Observed Bromide Mass Discharge



Measured versus Model Results



Field Interpreted
Subsurface Prevent Groundwater
contribution Using
Tracers (Abdul,
1985, Eq. 1)



Calculated Outflow Stream Hydrograph

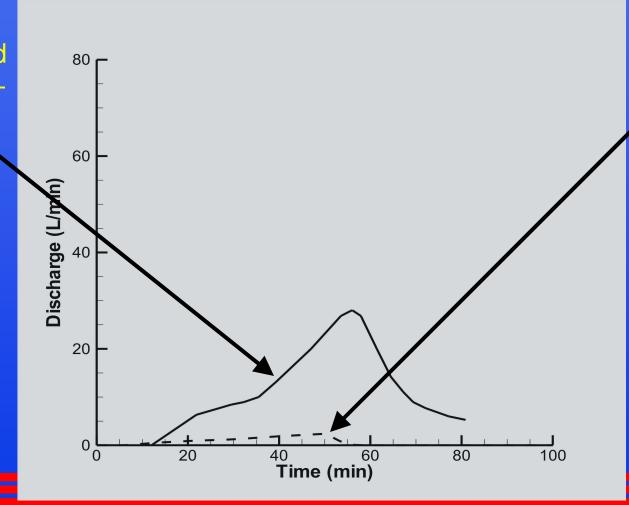
Measured
Outflow Stream
Hydrograph



Tracer-Based (Eq. 1) vs Hydraulically-based Groundwater Contribution: The Discrepancy

Field Interpreted
Subsurface Preevent
Groundwater
Contribution
Using Tracers
(Eq. 1)

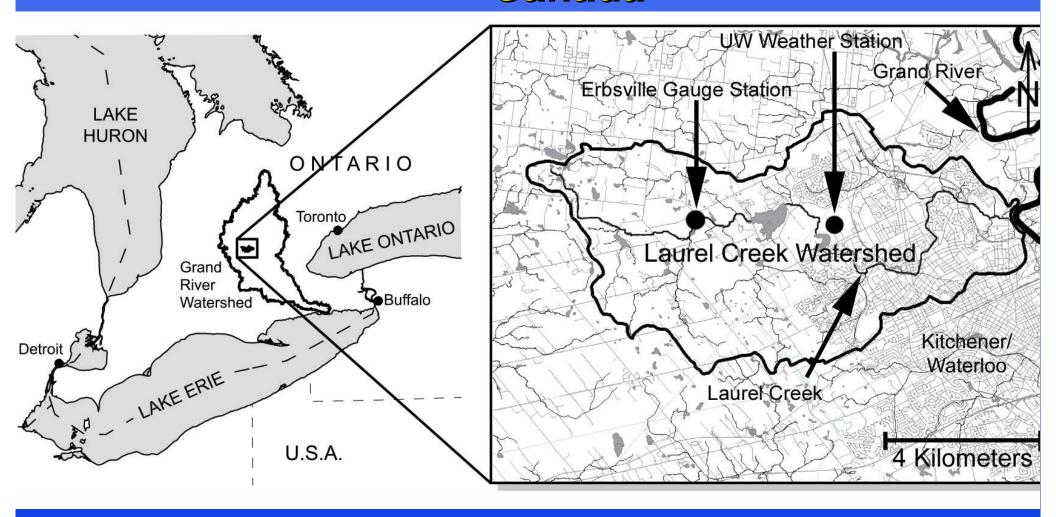
(Abdul, 1985)



Calculated
Subsurface Pre
event
Groundwater
Contribution



Laurel Creek Watershed, Waterloo, Ontario, Canada



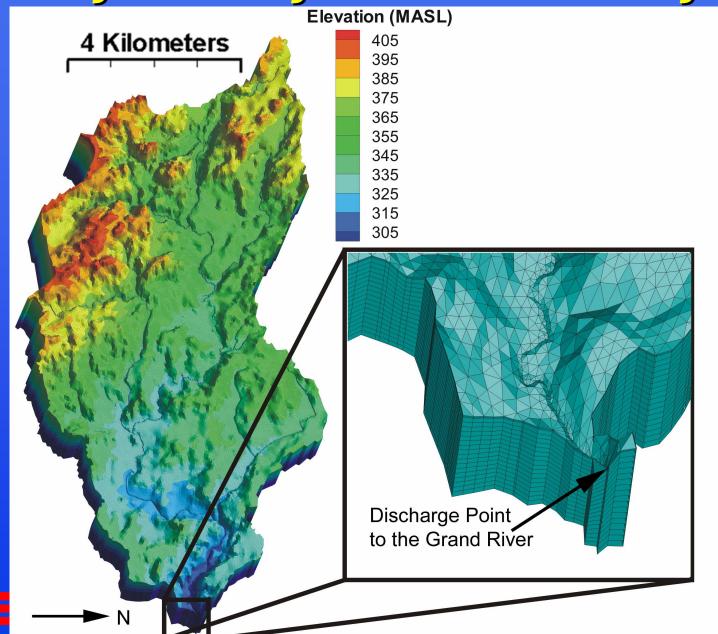
Laurel Creek







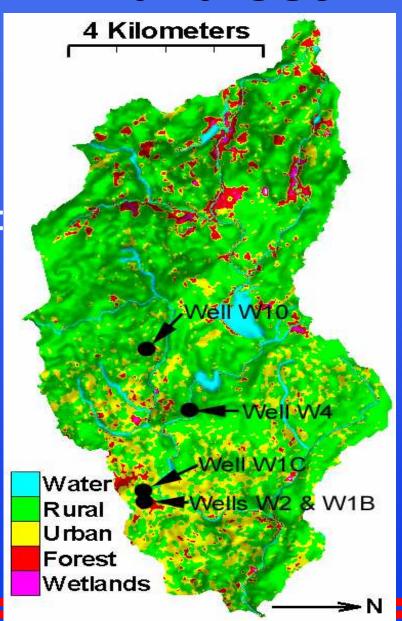
Physical System Geometry Elevation (MASL)



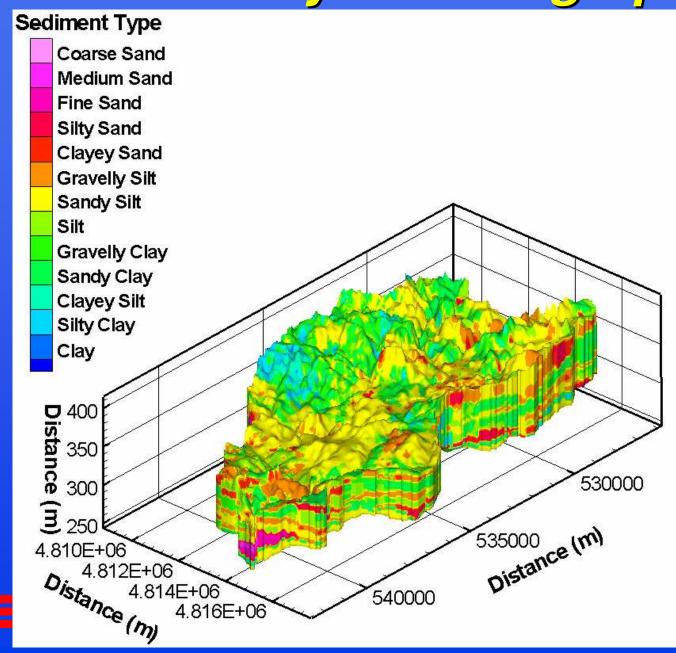
Land Use

lanning Coefficients:

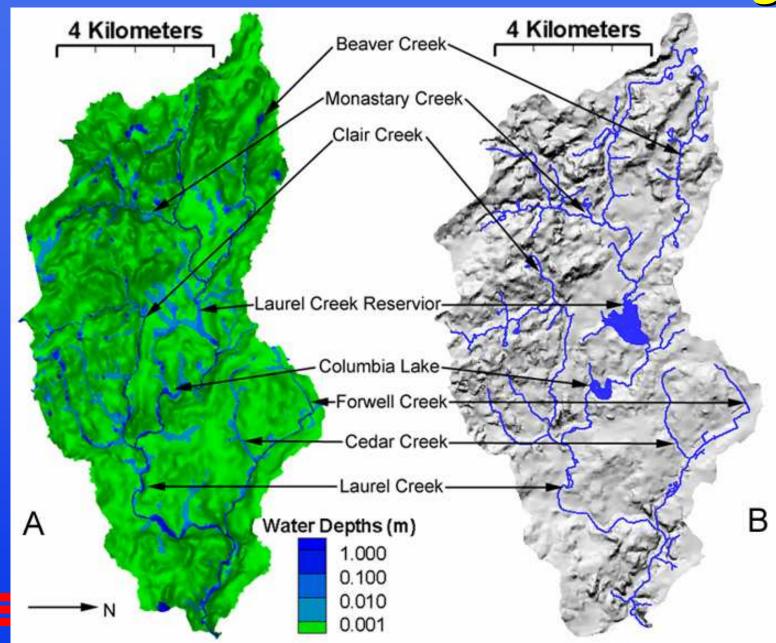
- Water 0.04
- Wetland 0.05
- Forest 0.6
- Urban 0.012
- Agricultural 0.2



Subsurface Hydrostratigraphy

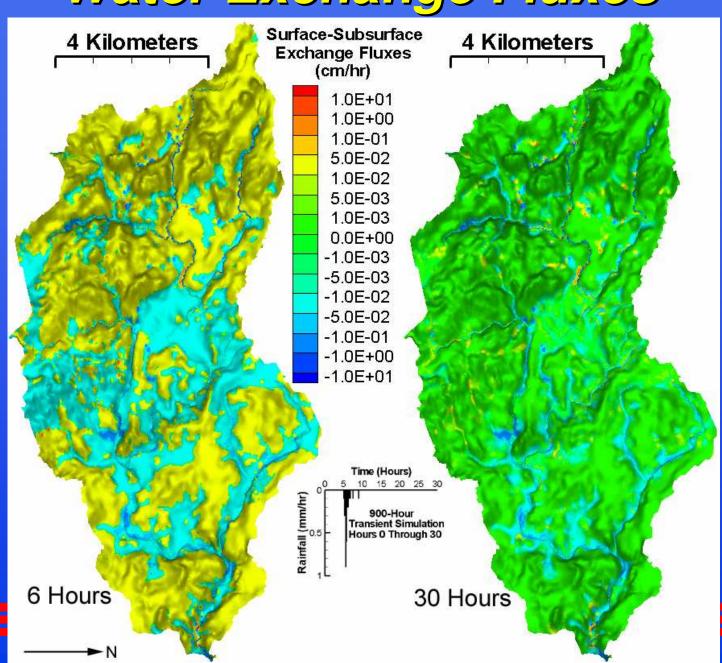


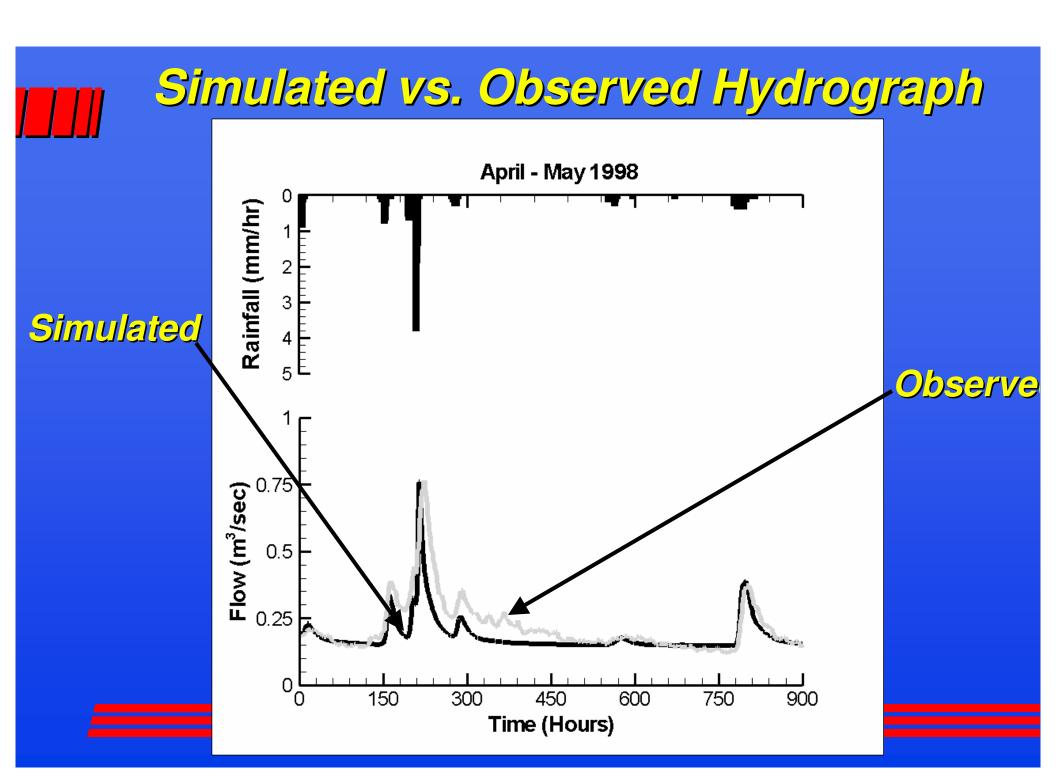
Simulated vs. Observed Drainage



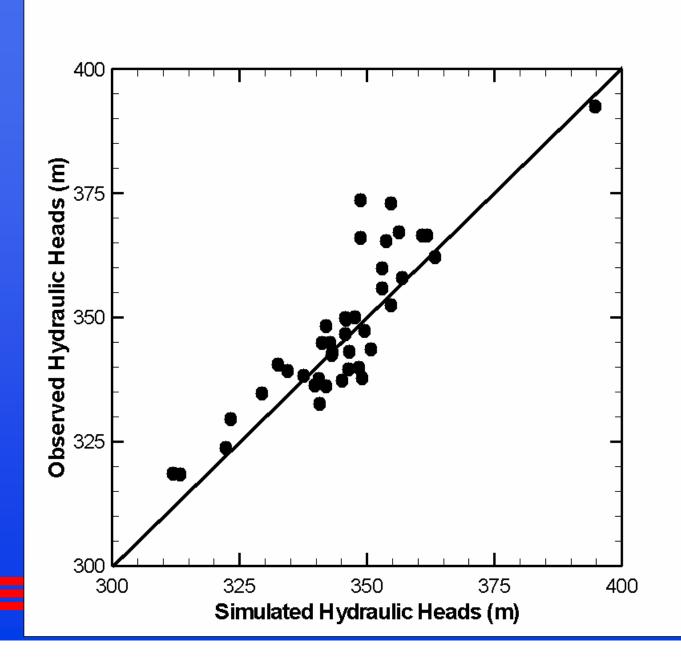
Water Exchange Fluxes

lote: negative values denote ischarge from subsurface to surface

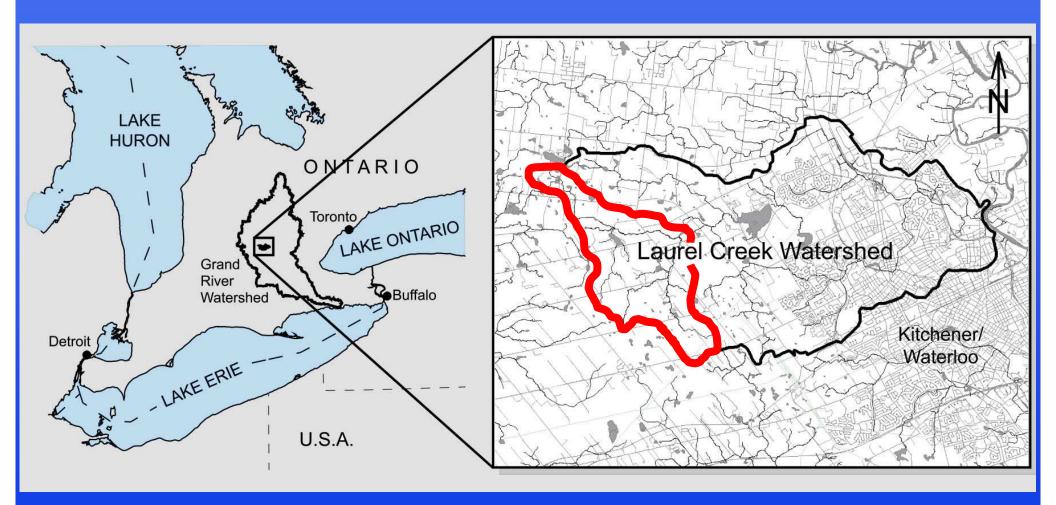




Simulated vs. Observed Subsurface Heads



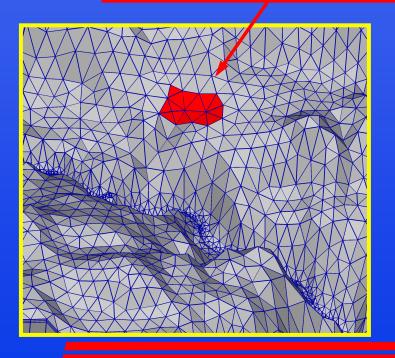
Sub-Catchment of Laurel Creek Watershed, Contaminant Transport Example

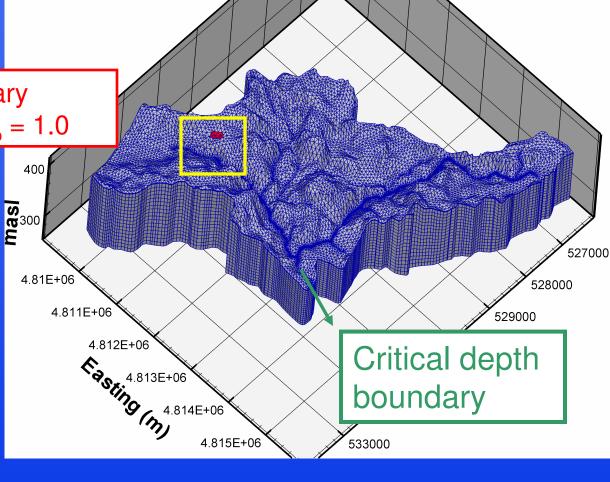


Surficial Contaminant Source

Rainfall to the surface is the only water into to the system

First-type solute boundary condition on surface, $C_o = 1.0$

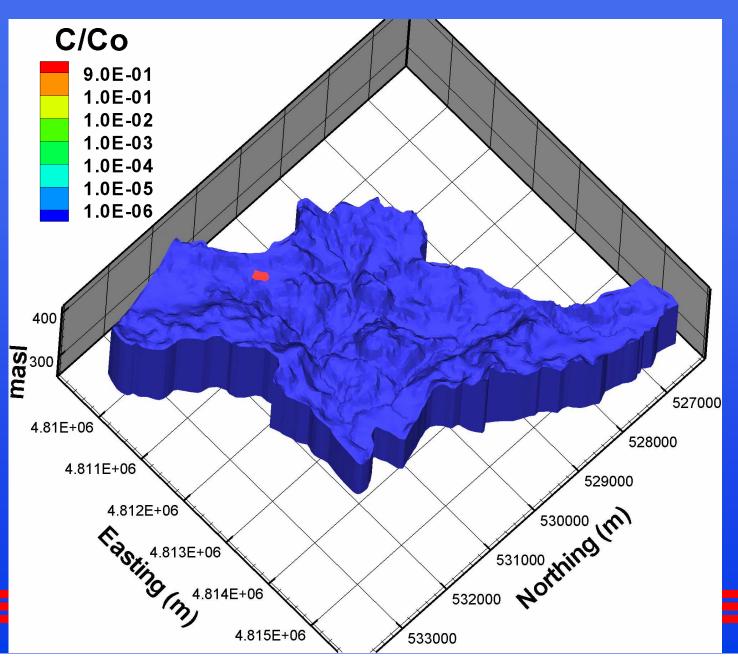




Plume Migration on Land Surface

t = 0

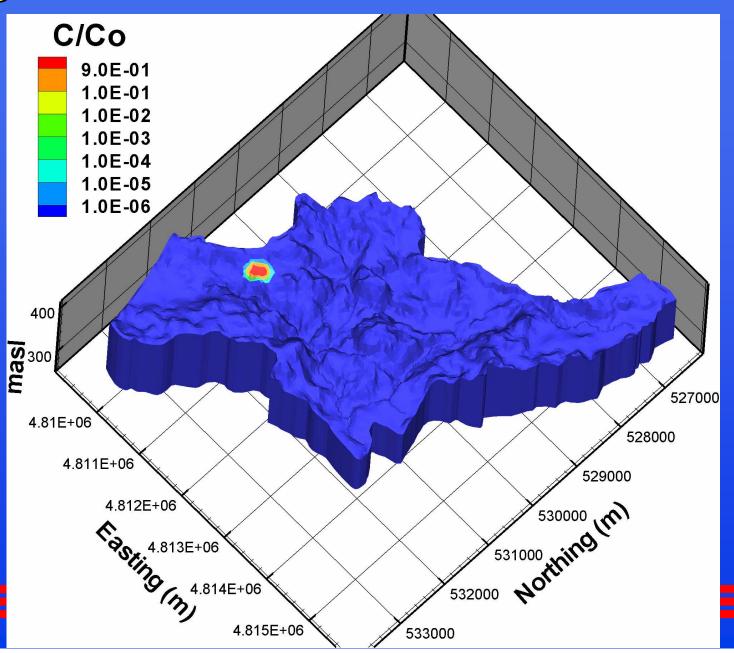
Under mean annual rainfall of 0.36 m/year



Plume Migration on Land Surface

t = 1 year

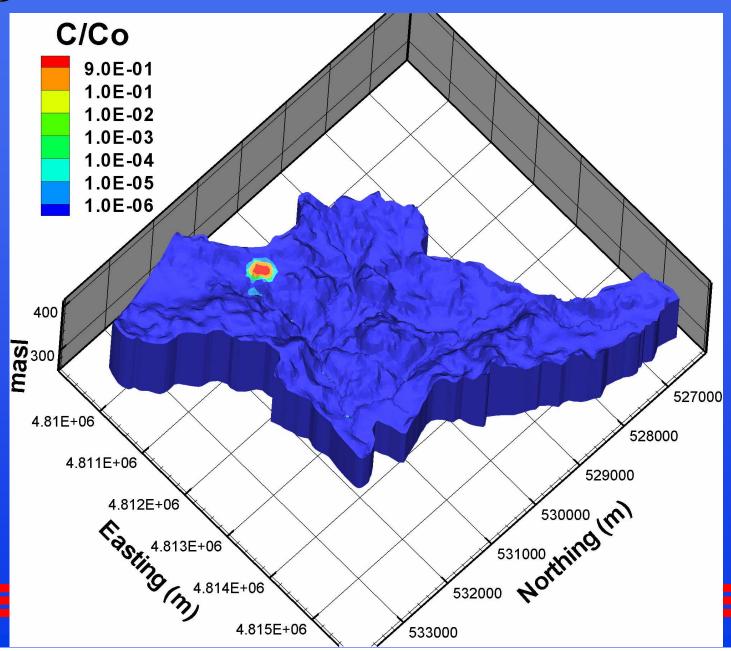
Under mean annual rainfall of 0.36 m/year



Plume Migration on Land Surface

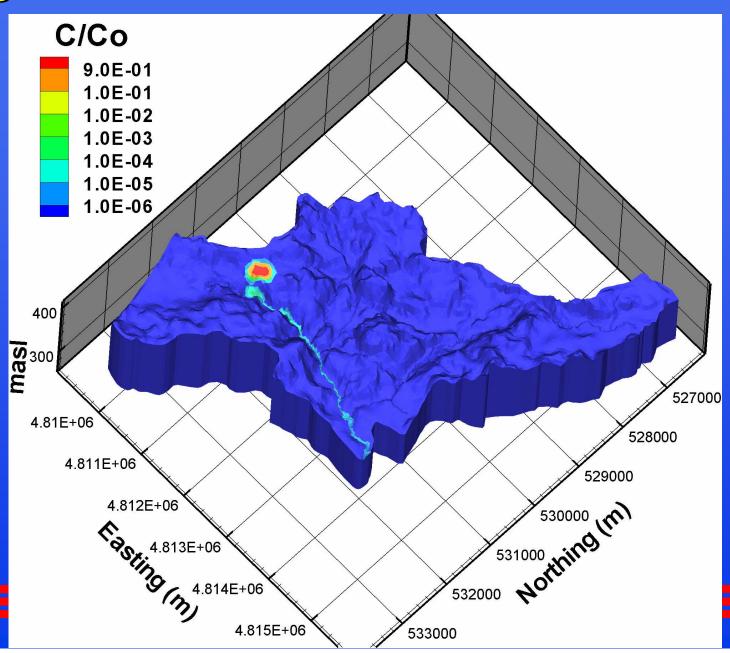
t = 2 years

Under mean annual rainfall of 0.36 m/year



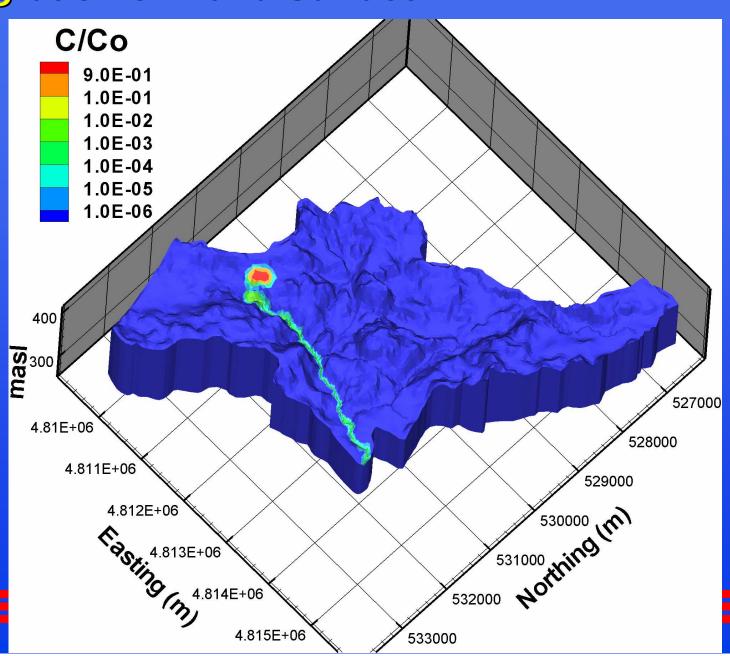
Plume Migration on Land Surface

t = 3 years



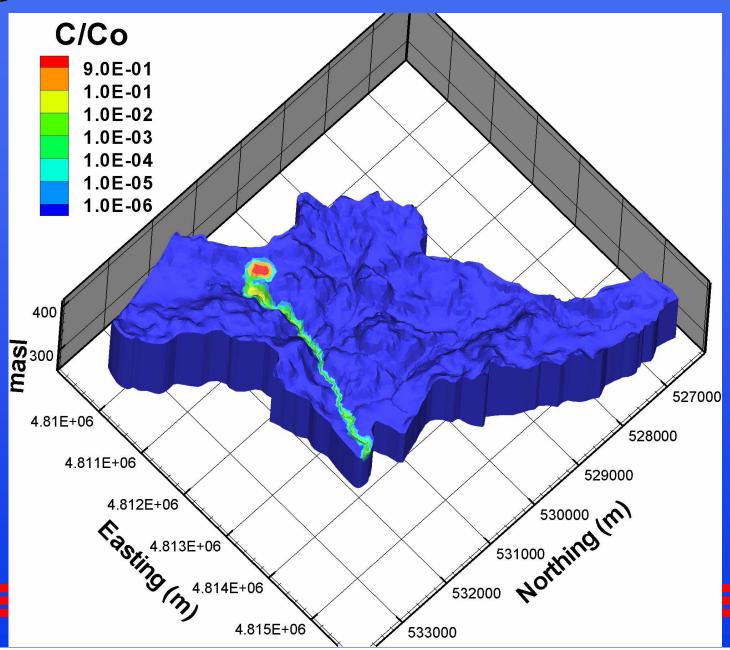
Plume Migration on Land Surface

t = 5 years

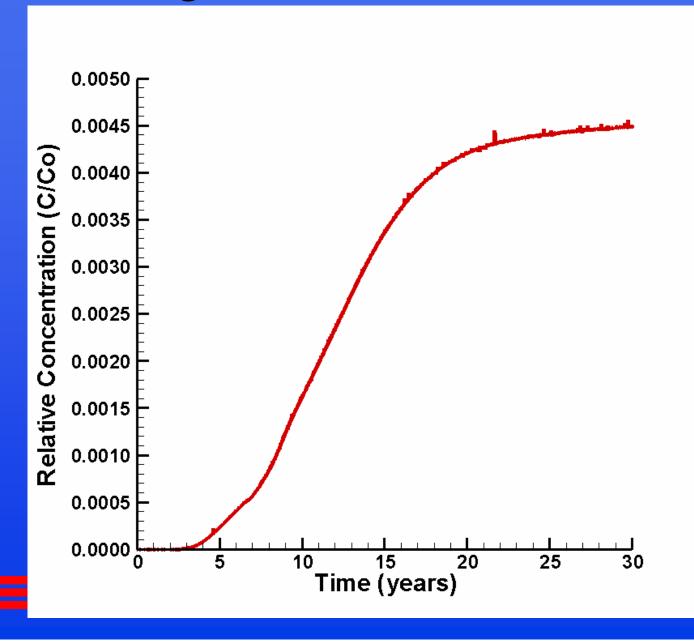


Plume Migration on Land Surface

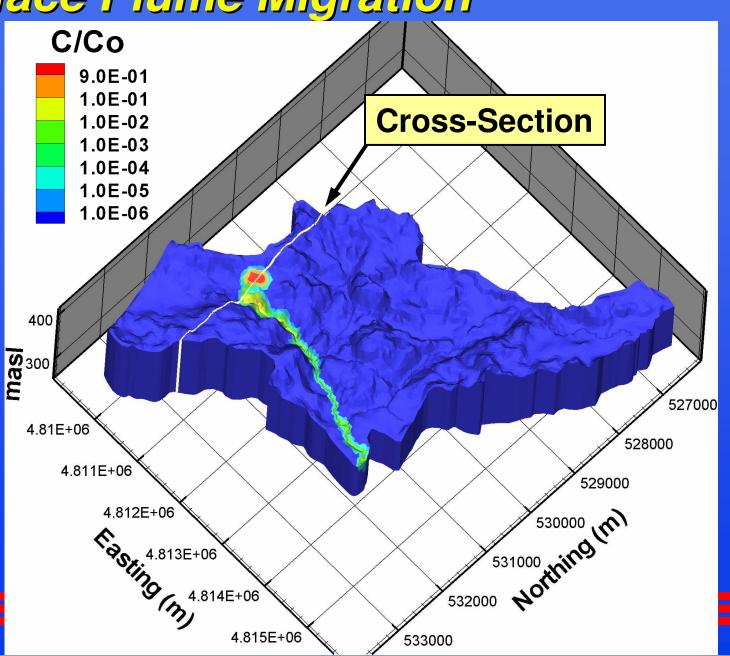
t = 10 years



Breakthrough Curve at Stream Outlet

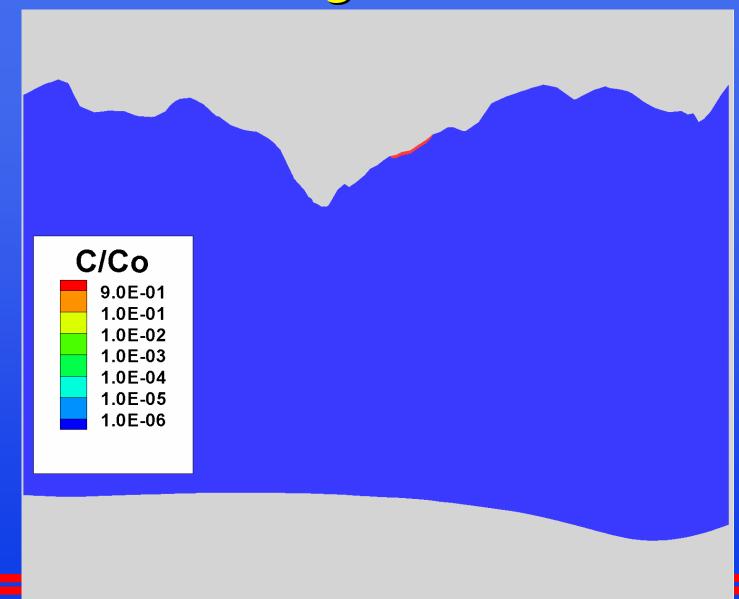


| Subsurface Plume Migration



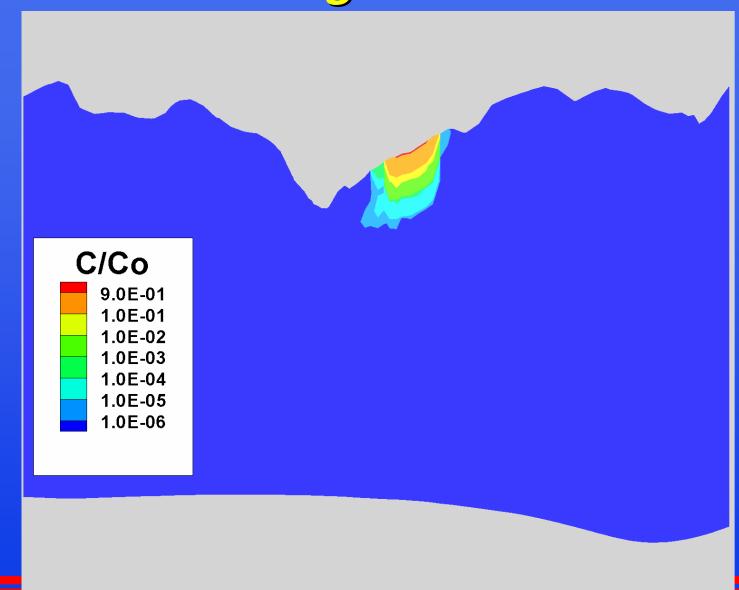
📕 Subsurface Plume Migration

t = 0



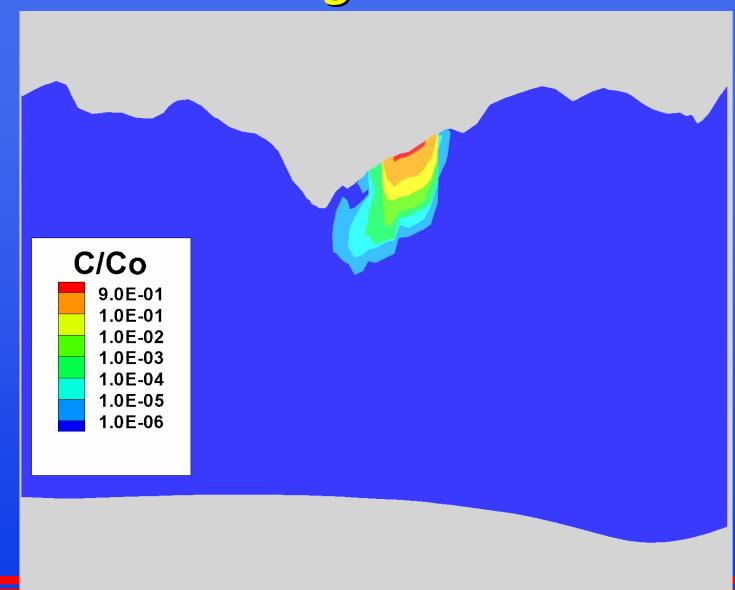
M Subsurface Plume Migration

t = 1 year



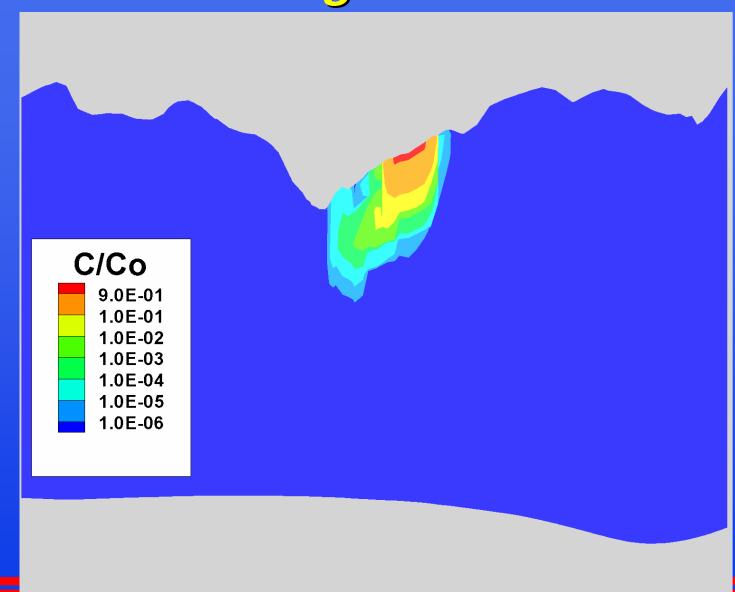
Subsurface Plume Migration

t = 2 years



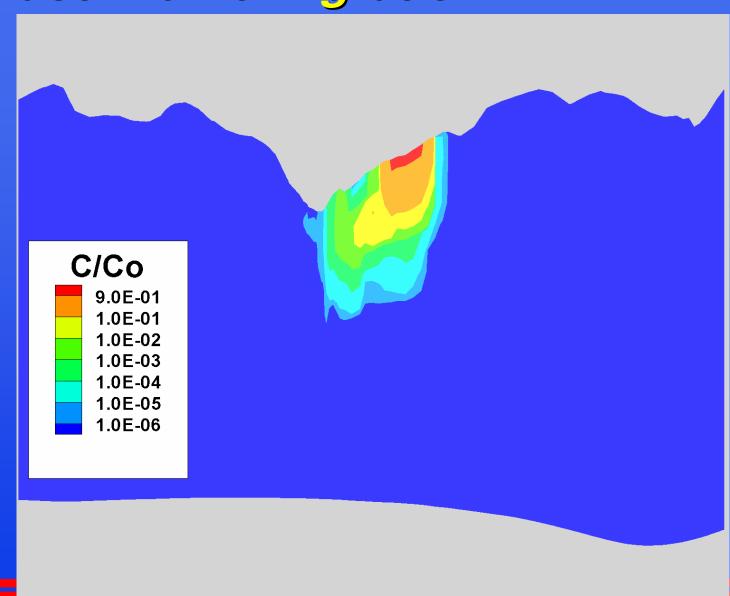
IIII Subsurface Plume Migration

t = 3 years



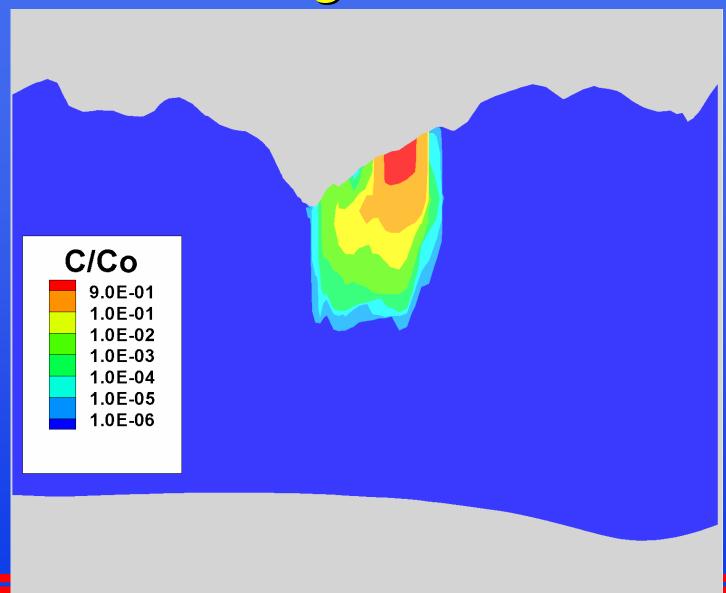
Subsurface Plume Migration

t = 5 years



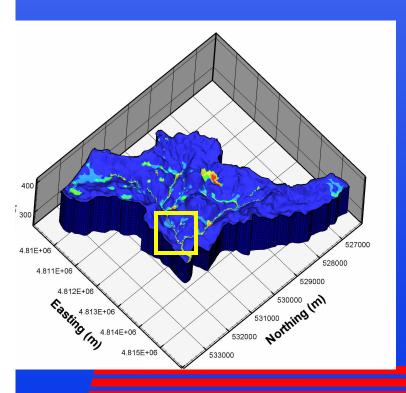
IIII Subsurface Plume Migration

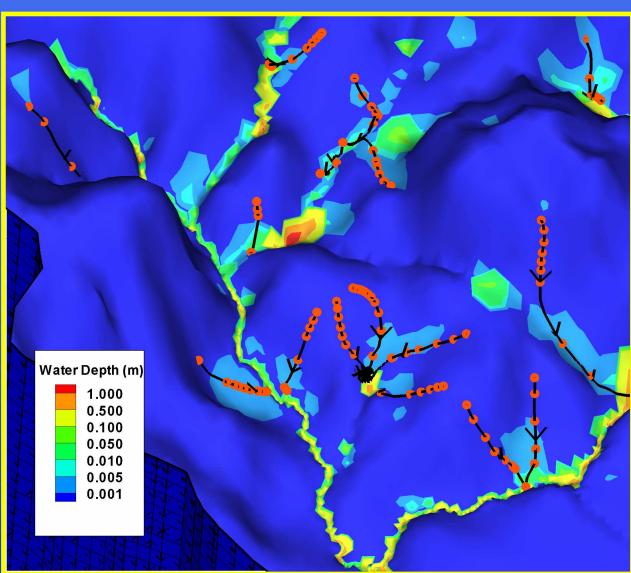
t = **10** years



Surface Particle Tracks

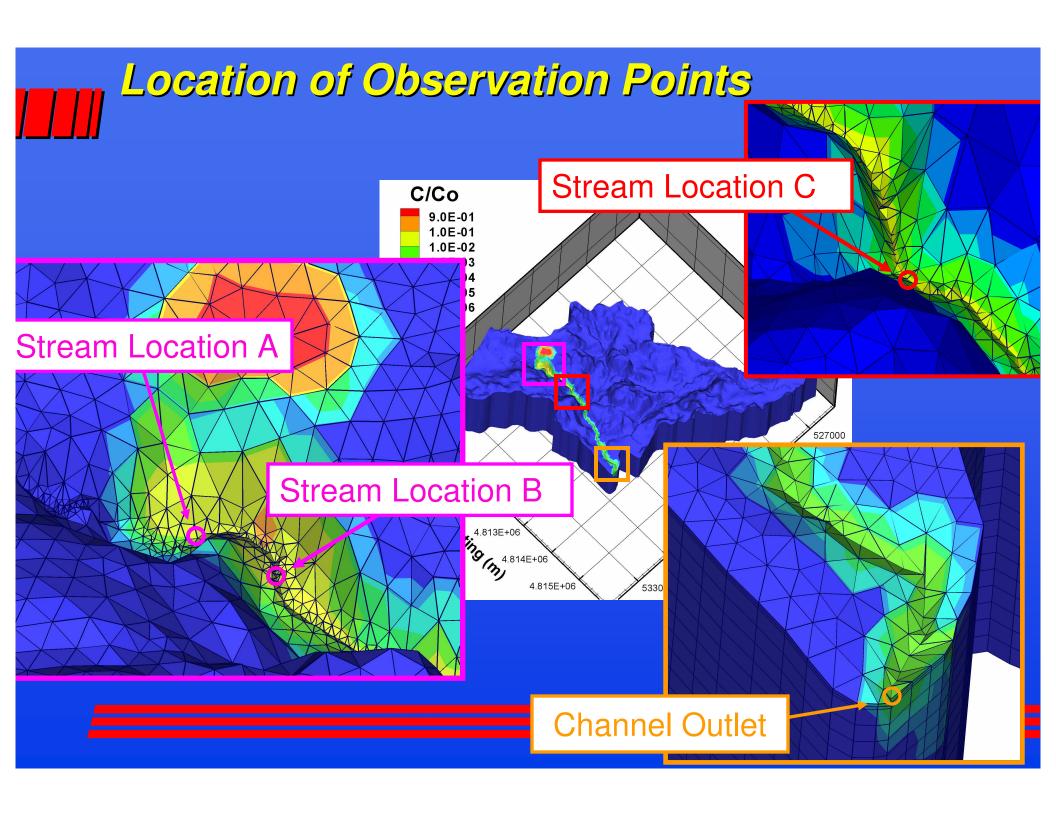
Particle track markers for $\Delta t = 2$ hours



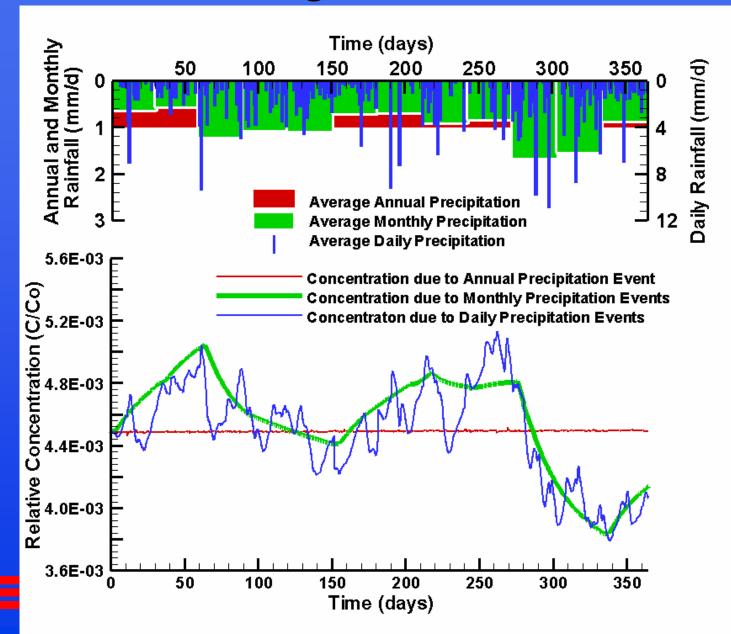


Response Due to Transient Rainfall Inputs

Ø t = 30 → 31 years: examine streambed water and solute exchange fluxes, and stream water concentrations, under various temporal averaging scales of input precipitation (daily, monthly, annual)



Solute Breakthrough at Channel Outlet

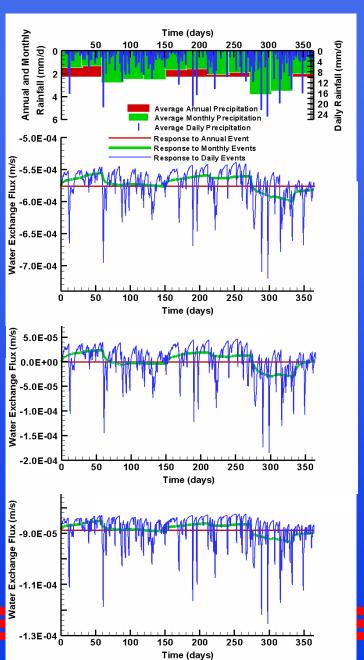


Water Exchange Fluxes at Stream Locations A, B and C

Location A

Location B

Location C

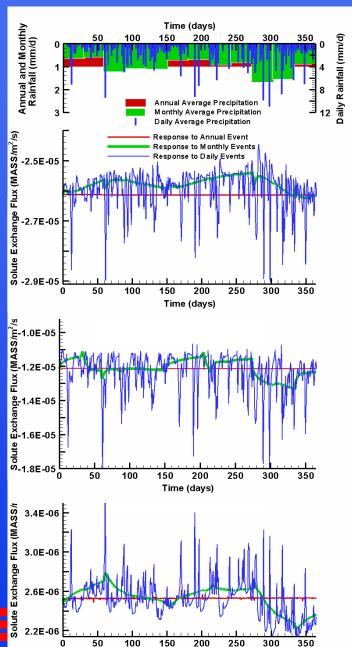


Solute Exchange Fluxes at Stream Locations A, B and C

Location A

Location B

Location C



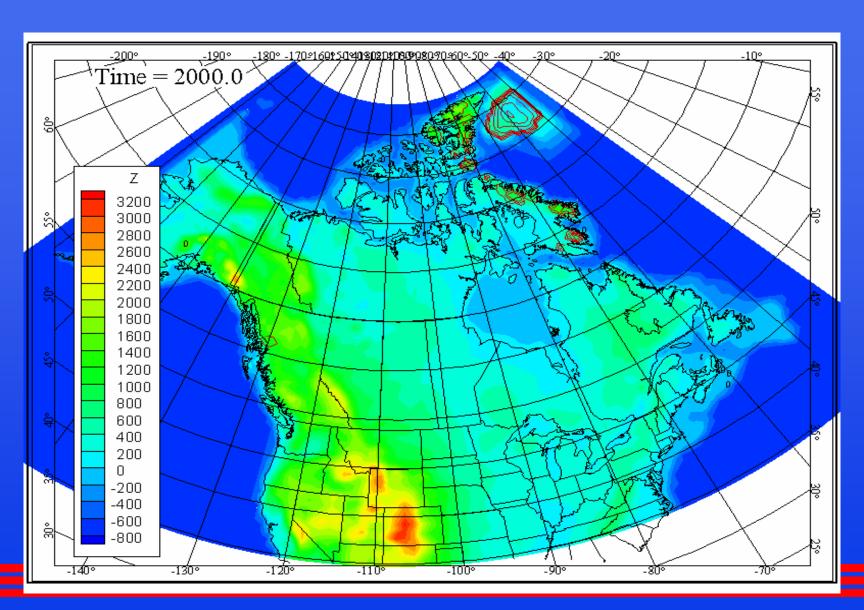
Time (days)



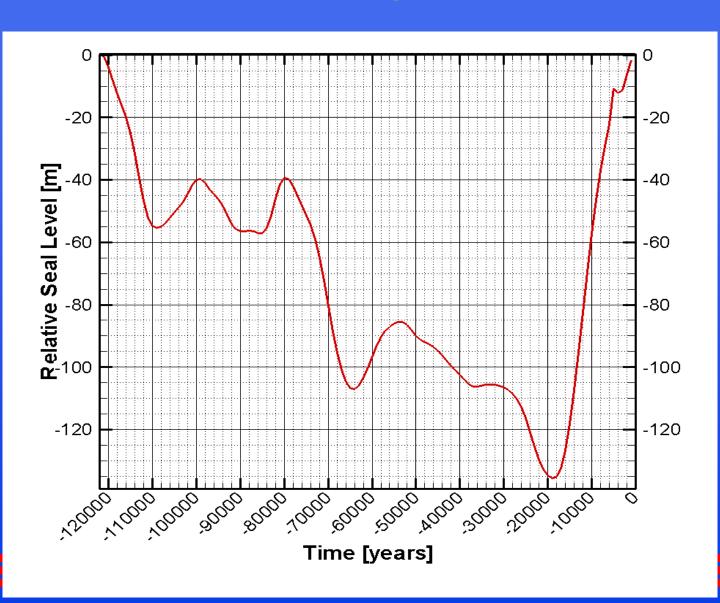
Continental-Scale Modelling of Coupled Surface-Subsurface Flow

- Impact of future climate-change scenarios on Canada's surface and groundwater resources
- Impact of advance & retreat of Laurentide ice sheet over last glacial cycle on groundwater flow over the Canadian landscape

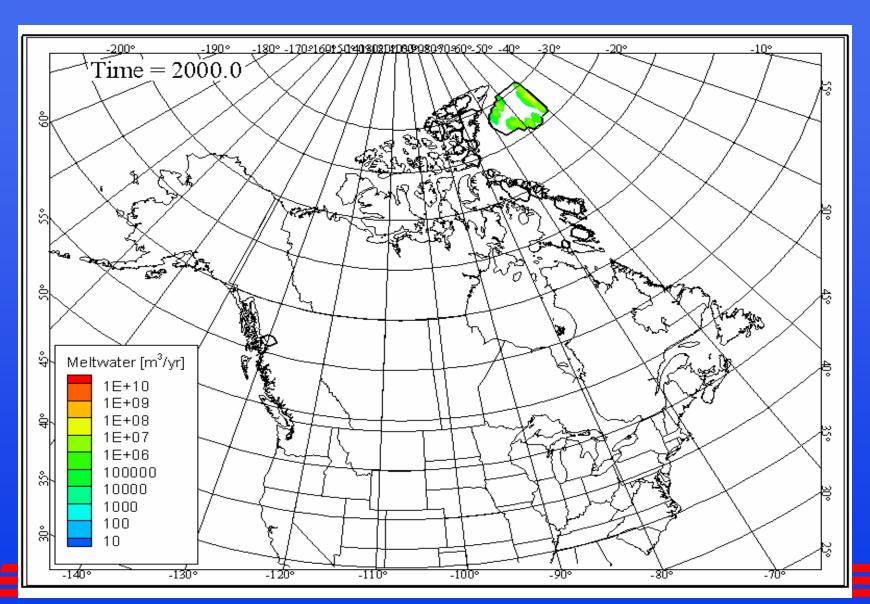
Topography & Ice Thickness (Tarasov and Peltier, 2005)



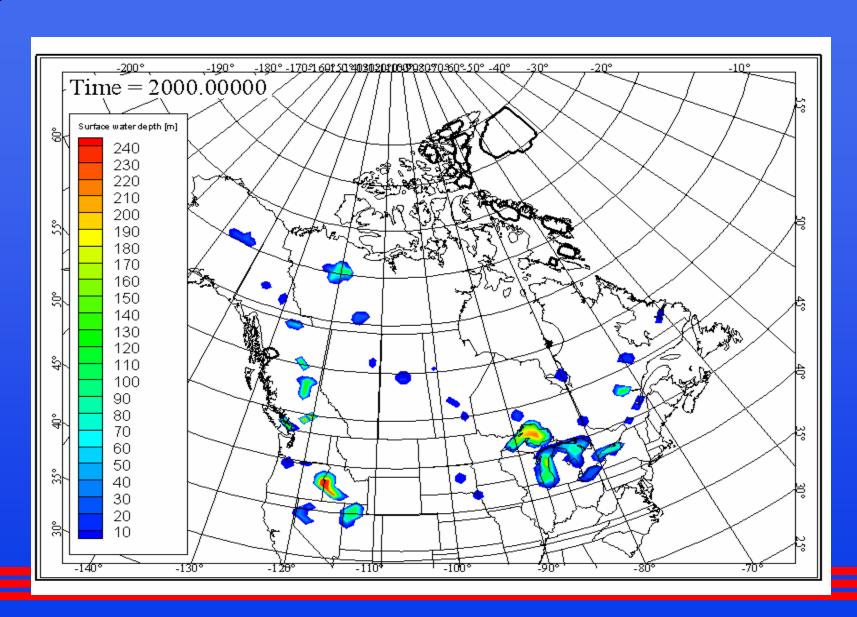
L. Sea Level Change



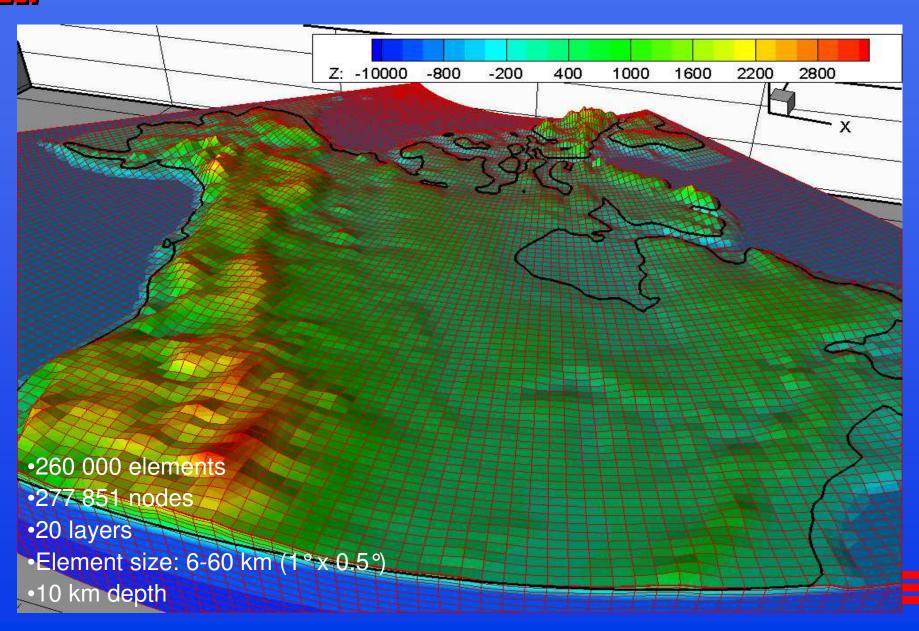
Subglacial Meltwater Flux (Tarasov and Peltier, 200:



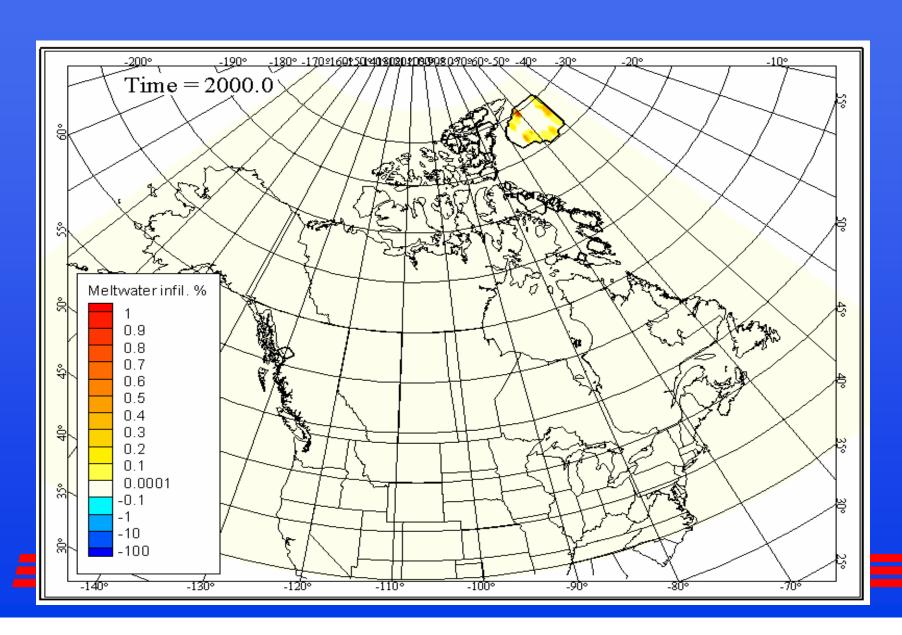
Surface Water Depths (Tarasov and Peltier, 2005)



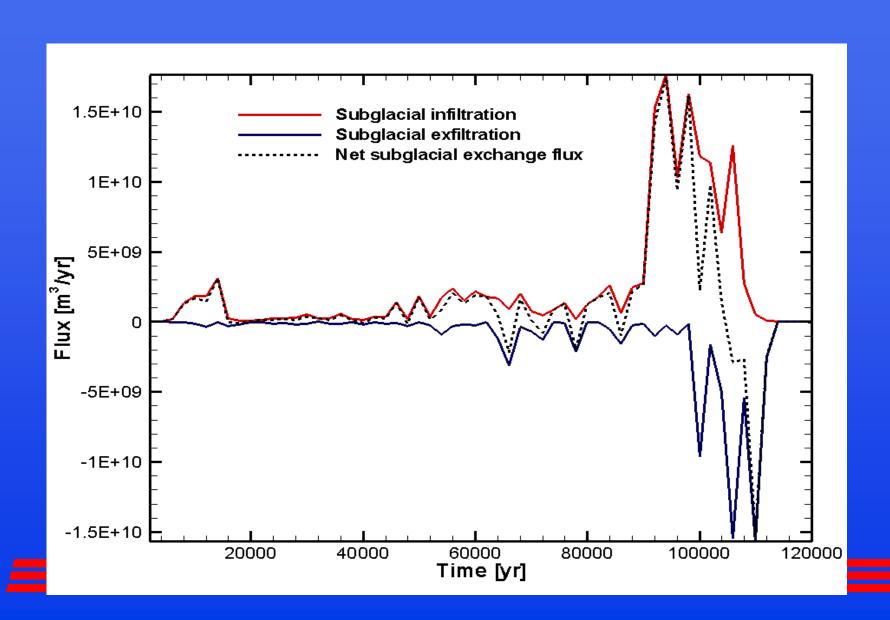
Model Discretization



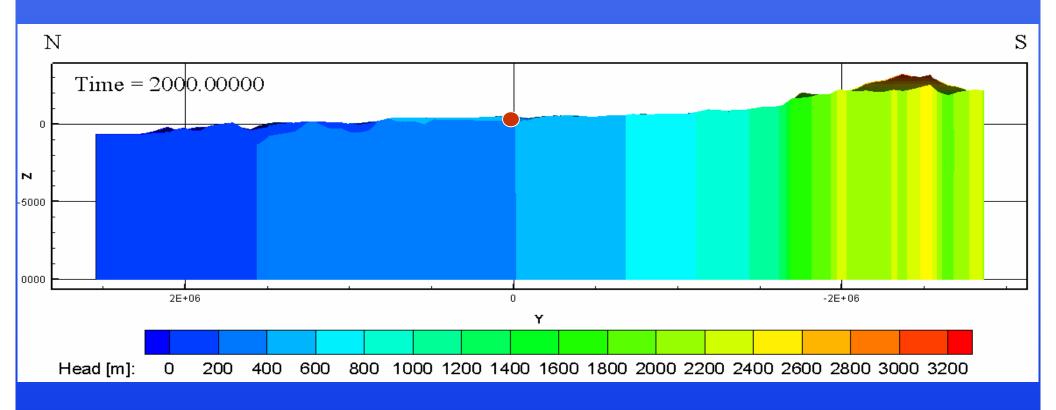
Subglacial Infiltration (% of Meltwater)



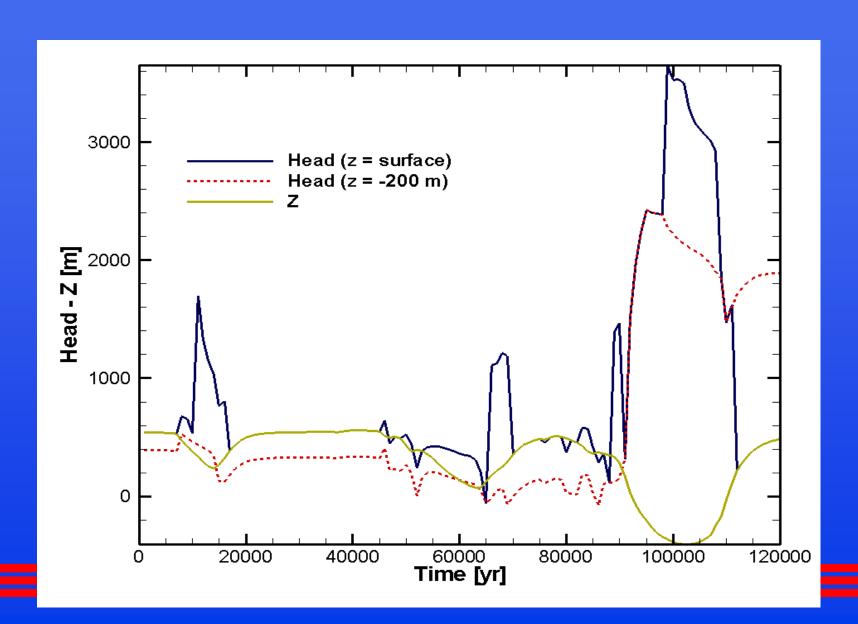
Integrated Subglacial Exchange Flux



IIII Hydraulic Head: N-S Cross Section

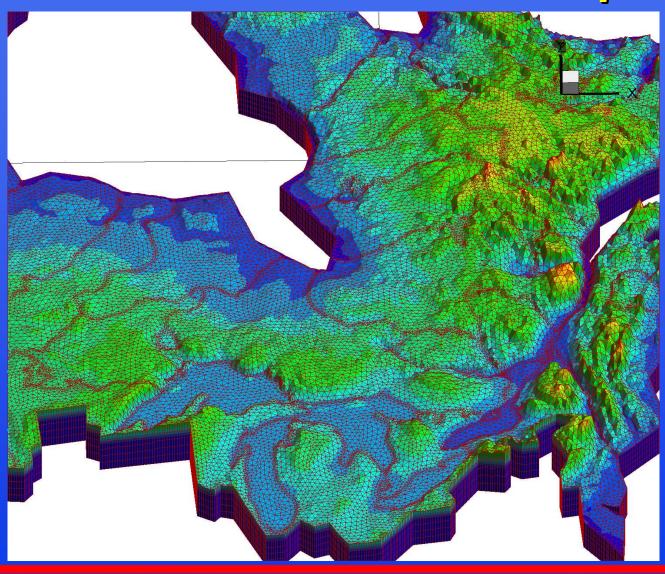


Hydraulic Head at Observation Point



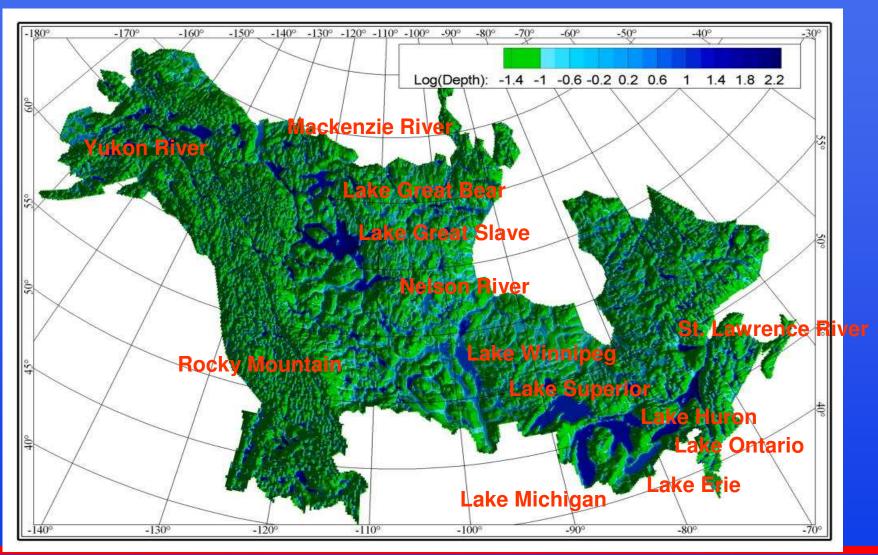


Grid for Future Climate Computations





"HydroGeoSphere" Computed (Hydrodynamic) Surface Water Depths For Present-Day Climate





Ongoing Extensions to HydroGeoSphere

- Energy transport with soil freeze-thaw cycles (phase change)
- Sediment erosion, transport & deposition
- Multi-species reactive transport (organic & inorganic, DO, etc.), pathogen transport
- Ø Forward and backward (adjoint) solution to ADE to predict water age pdf's, water-life expectancy pdf's, mean ages, etc., for both surface & subsurface waters
- Ø Domain decomposition, sub-gridding, sub-timing for large-scale problems

IIII Summary: Fully-integrated Model

- Solves one system of discrete CFVE equations
- Eliminates iteration between separate models or model components and need for "artificial" boundary conditions (e.g. seepage face BC)
- Does not a priori assume rainfall-runoff generation mechanisms
- Transport intimately linked to surface/subsurface hydrodynamics
- Water and solutes not "lost" from system in fullyintegrated modelling framework