

# Upscaling Regional, 3D, Non-Fickian Solute Transport with 2D Equivalent Models

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## Background & Motivation

The past half century has witnessed the emergence of non-point source pollutants [1, 2] that challenge conventional models of contaminant transport in porous media, and demand regional groundwater quality management models [3].

For example, decreasing water quality associated with increases in Total Dissolved Solids (TDS) has been documented at regional scales in aquifers across the United States in the past half century [4], yet to our knowledge, no models of regional groundwater quality management have been developed to appropriately describe the transport dynamics and the groundwater quality and quantity management options needed to protect against loss of fresh groundwater resources.

Previous work emphasizes the importance of geologic heterogeneity, and in particular the presence of connected pathways, in accurately modeling non-Fickian solute transport phenomena (early arrival and tails) [5, 6, 7, 8], but at the basin scale, this problem becomes computationally intractable. Therefore, this research proposes developing up-scaled 2D equivalent models that reproduce non-Fickian transport.

Upscaled non-Fickian solute transport models are urgently needed to ascertain regional scale groundwater quality and the management strategies that will avert or remediate the degradation of fresh groundwater resources.

### CORE QUESTION:

Can non-Fickian contaminant transport effects produced by 3D heterogeneity be represented in 2D, and at what information loss?

## Approach

1. Weissmann (1999) developed a 3D hydraulic conductivity domain from thousands of well logs and a transition probability geostatistical approach (T-PROGS) in the King's River Fan in California, USA [9]. Derive 63 2D realizations from this domain by taking "slices" along the zy plane. Let the set of all slices be called  $S$ , and individual slices,  $s_i$ . Then,

$$S = \{s_1, s_2, s_3, \dots, s_{63}\}$$

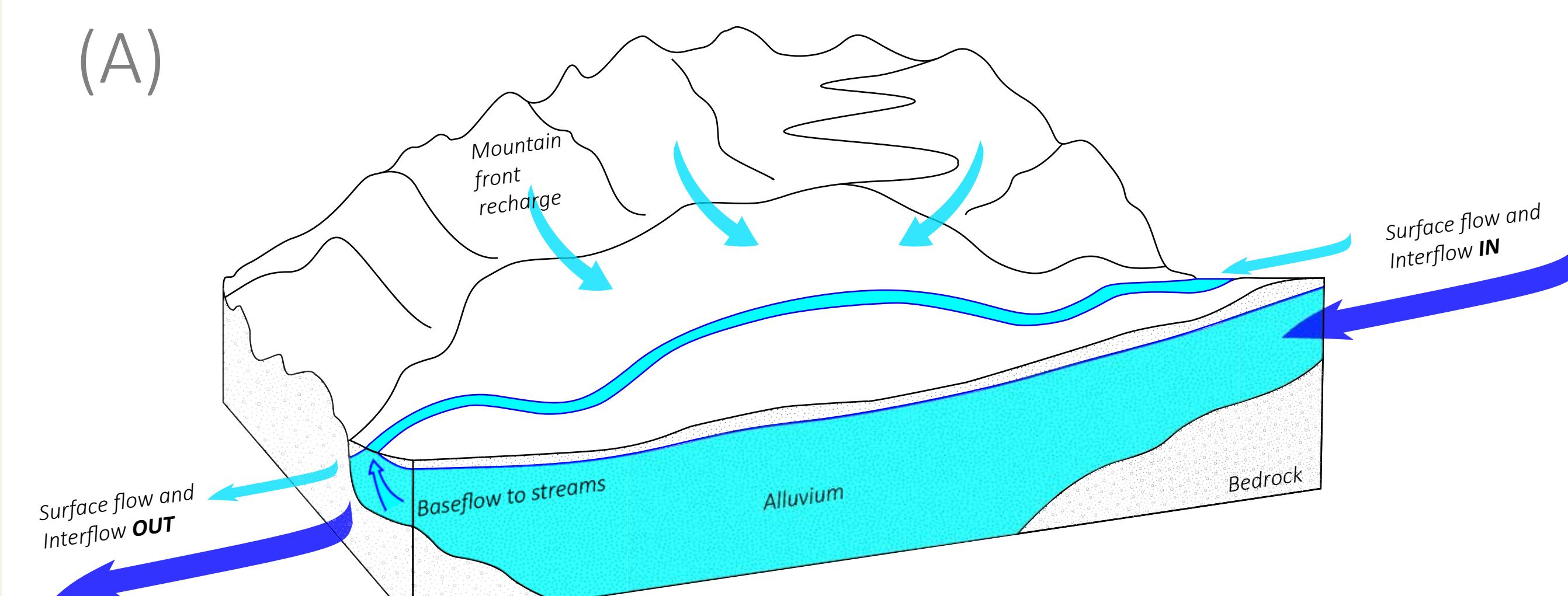
2. Solve the regional-scale, steady state groundwater flow problem with finite difference groundwater modeling in MODFLOW for the 3D domain and all 2D realizations.

3. Using the flow from 2., solve the advection-dispersion equation in the 3D domain and all 2D realizations with RW3D [10]. For 3D domain and all 2D realizations, compare breakthrough curves, and Bianci and Pedretti's (2006) transport connectivity indicator [11].

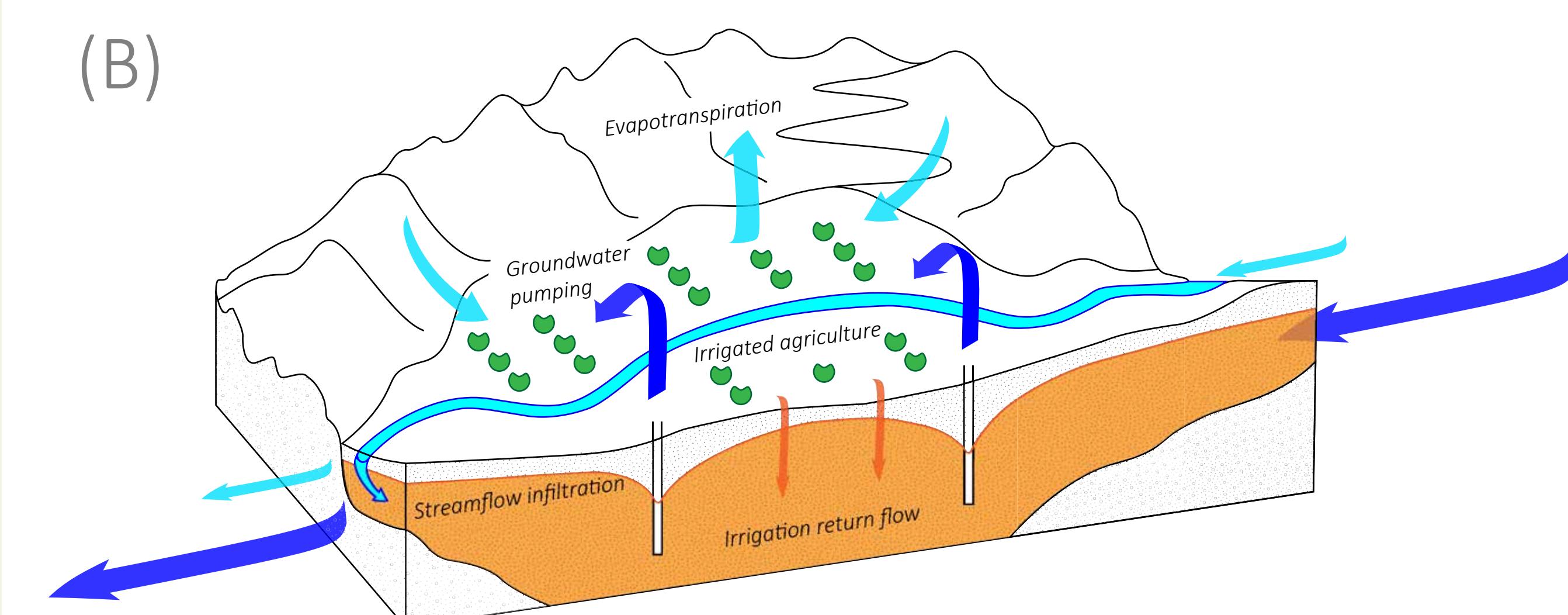
4. If 2D transport can approximate 3D transport, use the developed T-PROGS model to simulate multiple 2D basin-scale realizations.

5. Using MODFLOW and RW3D, simulate:  
 (a) business as usual groundwater quality evolution  
 (b) climate change impacts to groundwater quality  
 (c) effects of mitigative practices (clean recharge via MAR)  
 (d) water budget required to reverse closed basin salinization

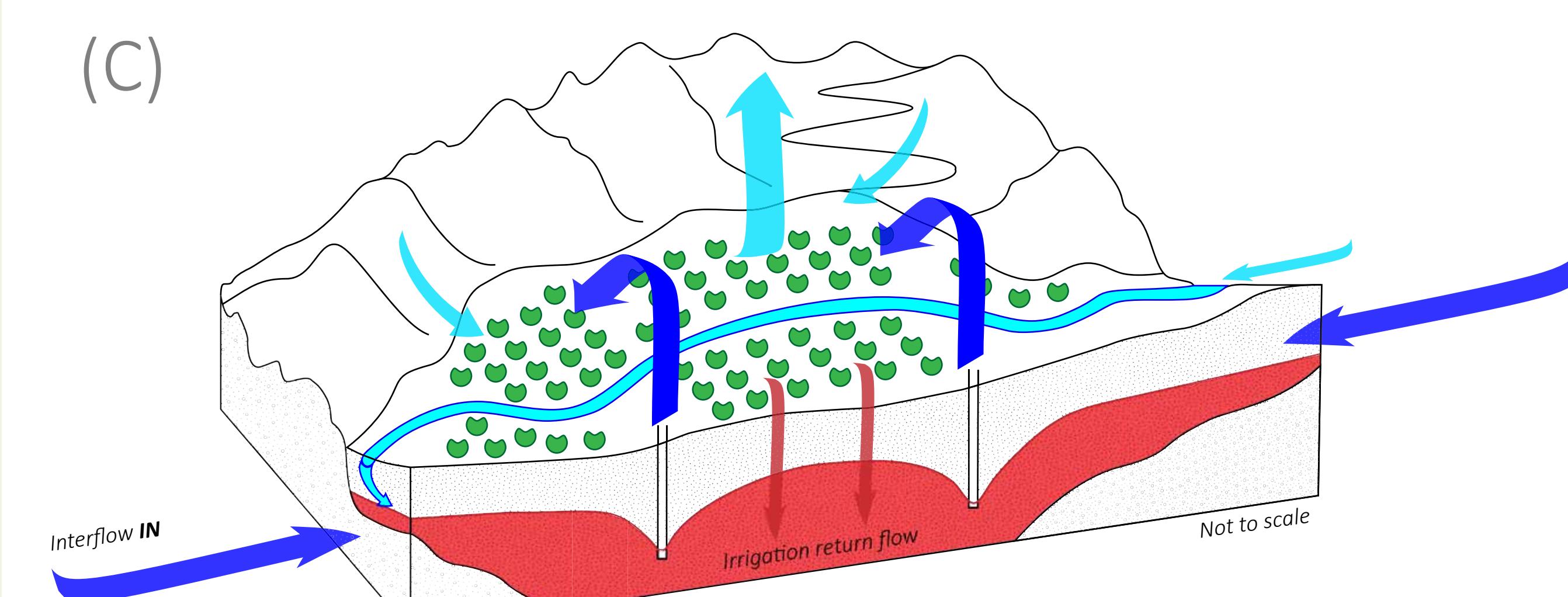
## Closed Basin Groundwater Salinization



Open basin, pre-groundwater development: surface and groundwater systems connect. Groundwater discharges dissolved solids into surface water which exit the basin. Groundwater at this stage is predominantly fresh (e.g., < 1,000 mg/L).



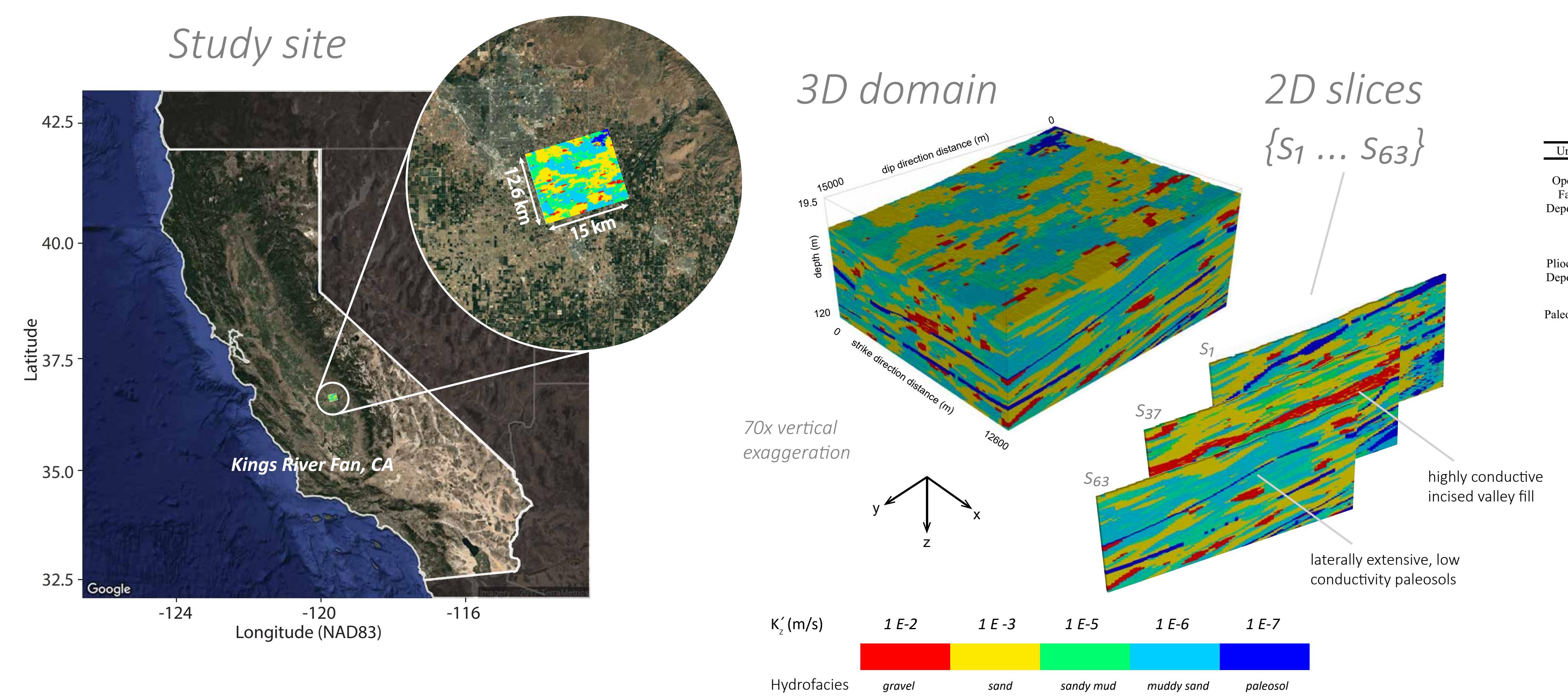
Partial closure of basin: groundwater pumping causes reduction or elimination of baseflow to streams. Pumped groundwater returns to the basin via irrigation return flow. Dissolved solids begin to accumulate in groundwater.



Closed basin: falling groundwater levels cause subsurface interflow to drain adjacent basins. Streams lose to groundwater. Water primarily exits via evapotranspiration, which further concentrates dissolved solids in groundwater.

Legend:  
 low TDS (blue)  
 medium TDS (orange)  
 high TDS (red)  
 groundwater well (grey circle)  
 water budget terms (blue arrow)  
 agriculture (green leaf)

## Geostatistical Transition Probability Model



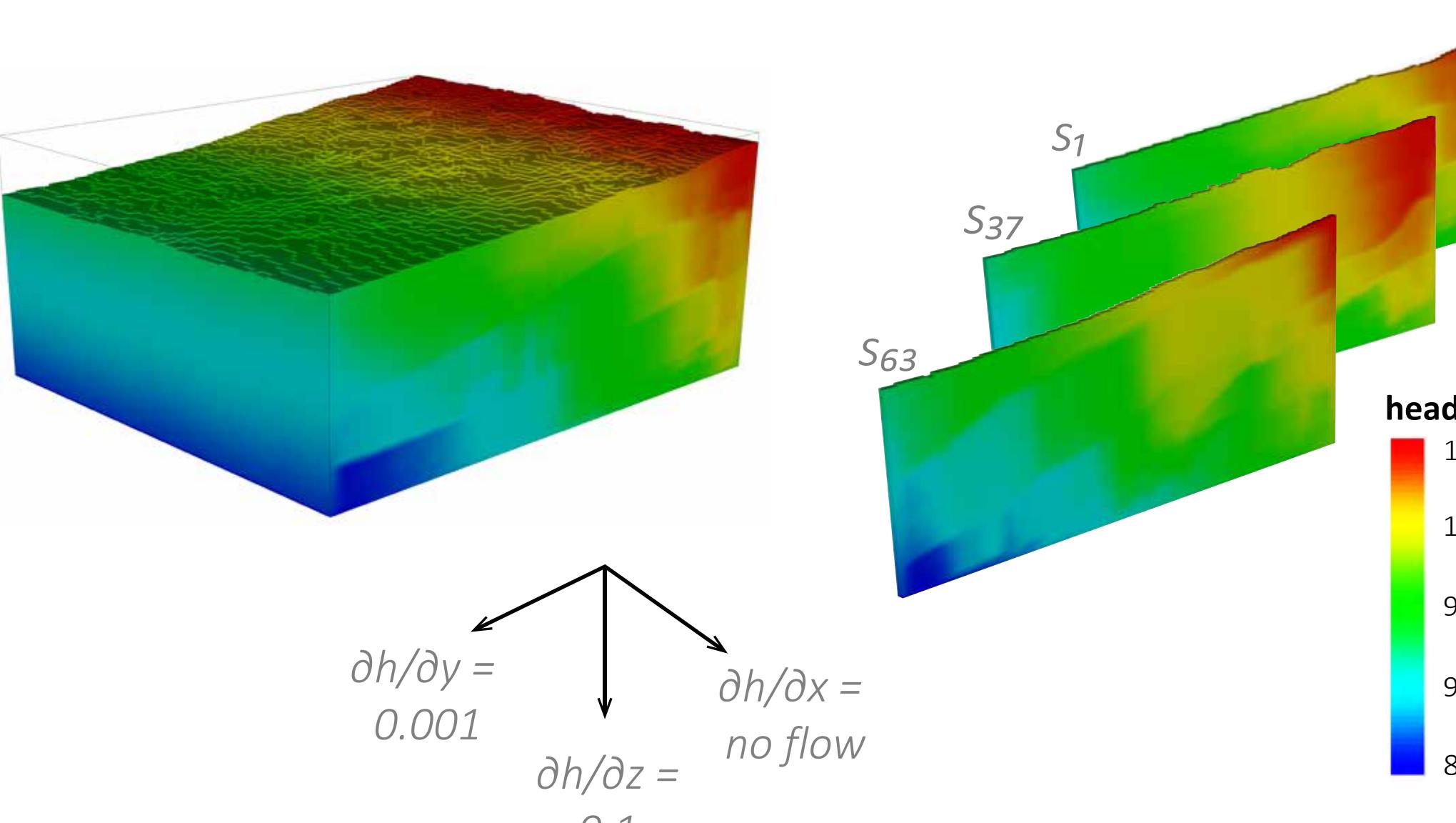
## Transition probability matrices

Unit	Vertical (z) direction	Strike (x) direction	Dip (y) direction
Open-Fan Deposits	$\begin{bmatrix} g & L=1.5m \\ s & 0.05 \\ m & 0.10 \\ np & 0.15 \end{bmatrix}$	$\begin{bmatrix} g & L=200m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$	$\begin{bmatrix} g & L=500m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$
Pliocene Deposits	$\begin{bmatrix} g & L=1.5m \\ s & 0.05 \\ m & 0.10 \\ np & 0.15 \end{bmatrix}$	$\begin{bmatrix} g & L=200m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$	$\begin{bmatrix} g & L=500m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$
Paleosols	$\begin{bmatrix} g & L=1.5m \\ s & 0.05 \\ m & 0.10 \\ np & 0.15 \end{bmatrix}$	$\begin{bmatrix} g & L=200m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$	$\begin{bmatrix} g & L=500m \\ s & 0.10 \\ m & 0.15 \\ np & 0.20 \end{bmatrix}$

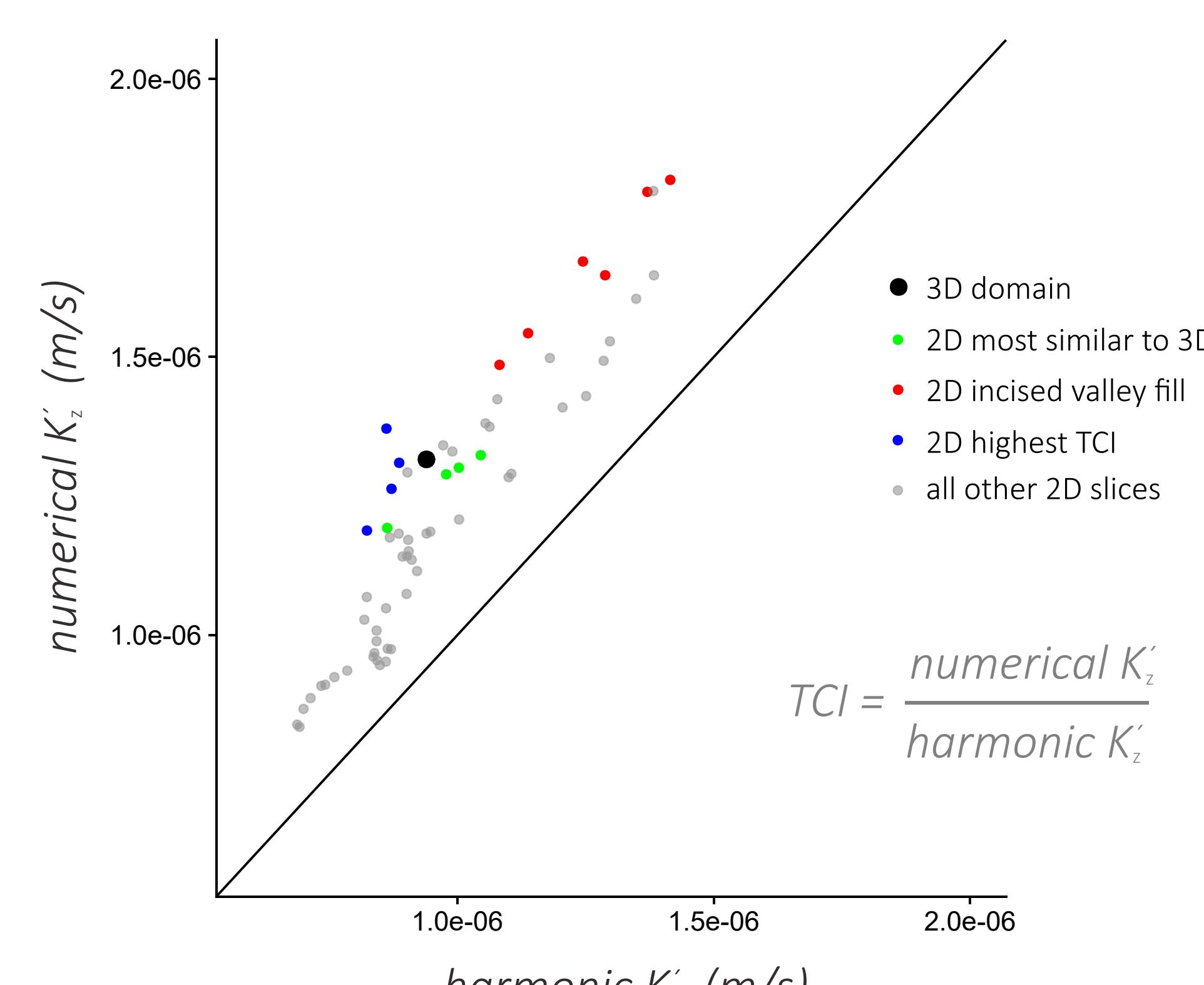
Embedded transition probability matrices for the Markov chain models of the open fan, Pliocene, and paleosol (from Weissmann and Fogg, 1999) [9].

Entries in the matrix diagonals indicate mean lengths ( $L$ ) for hydrofacies. Entries in the off-diagonal are the embedded probability values used to represent facies juxtaposition relationships. Facies abbreviations are  $g$  – gravel;  $s$  – sand;  $ms$  – muddy sand;  $m$  – mud;  $p$  – paleosol;  $np$  – no paleosol.  $b$  indicates the background category, and  $s$  indicates an assumption that the embedded transition probabilities are statistically symmetrical.

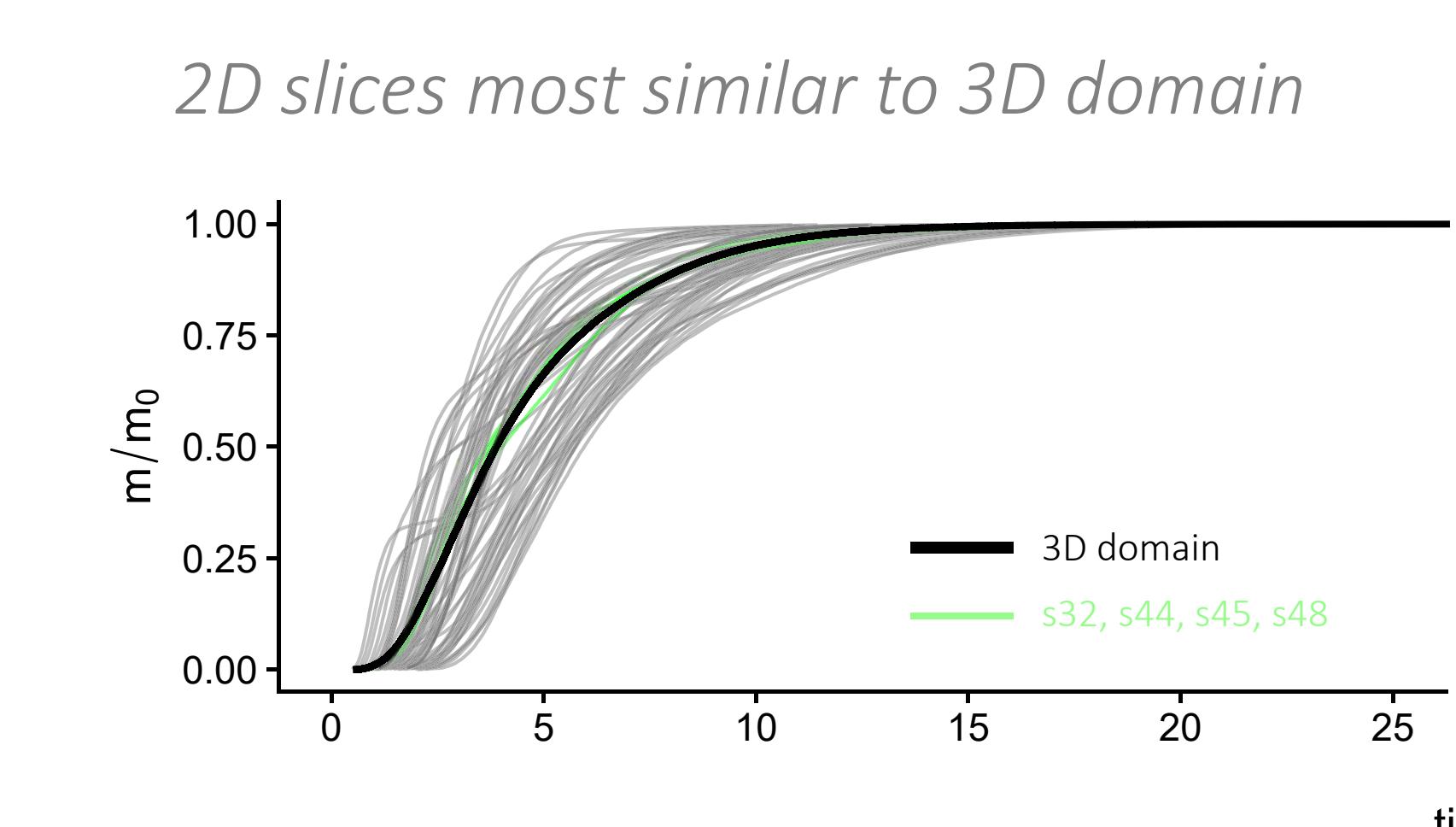
## Steady State Flow Model



## Transport Indicators

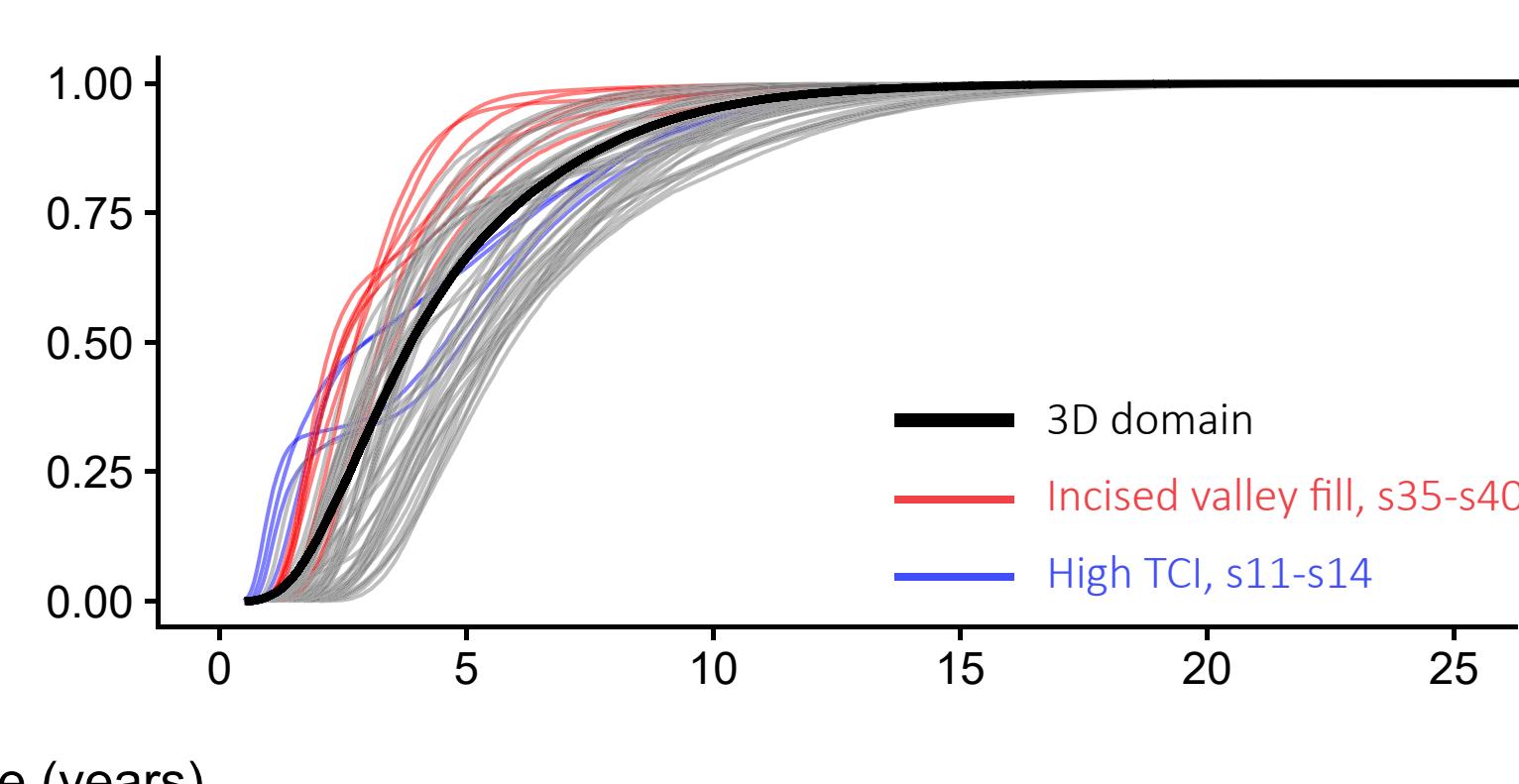


## Non-Point Source, Random Walk Particle Transport



Non-point source pulse injection of 100,000 particles at 10m below land surface. Simulation time = 10,000 days (27.4 years). Standard Random Walk with Eulerian integration of velocity. Dispersion in  $(x,y,z) = (2m, 2m, 0.05m)$ . No diffusion. No mass transfer.

## Early arriving particles



## Discussion & Future Research

Regional non-point source groundwater salinization threatens fresh aquifers worldwide. Solute transport models capable of simulating regional-scale, non-Fickian effects are needed to model this phenomenon.

These experiments suggest that 3D non-Fickian transport may be upscaled in 2D, and this upscaling hinges on characterization of the geologic heterogeneity, and the flow and transport boundary conditions.

Early arriving particles are explained by the presence of high-K facies, and high TCI, but the characteristics of 2D domains that mimic 3D transport behavior are not yet explained.

Graph based approaches are a promising avenue forward. It is hypothesized that 2D domains with similar graph efficiency to the 3D domain will exhibit similar contaminant breakthrough curves.

## Acknowledgements

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