

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

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Background & Motivation

Nonpoint-source groundwater contamination threatens to gradually degrade the quality of vast quantities of groundwater on time scales of decades to centuries in many parts of the world.

The past half century has witnessed the emergence of non-point source pollutants that challenge conventional models of contaminant transport, which initially evolved to address field-scale point-source pollutants.

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, 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.

While previous work shows that the appropriate phenomena can be modeled through detailed modeling of geologic heterogeneity and resultant transport processes, this is not feasible at the basin scale.

Methods of modeling regional-scale solute transport, including the effects of heterogeneity that produce non-Fickian transport, are urgently needed to ascertain what contamination source and groundwater quantity management actions are needed to avert irreversible degradation of groundwater quality.

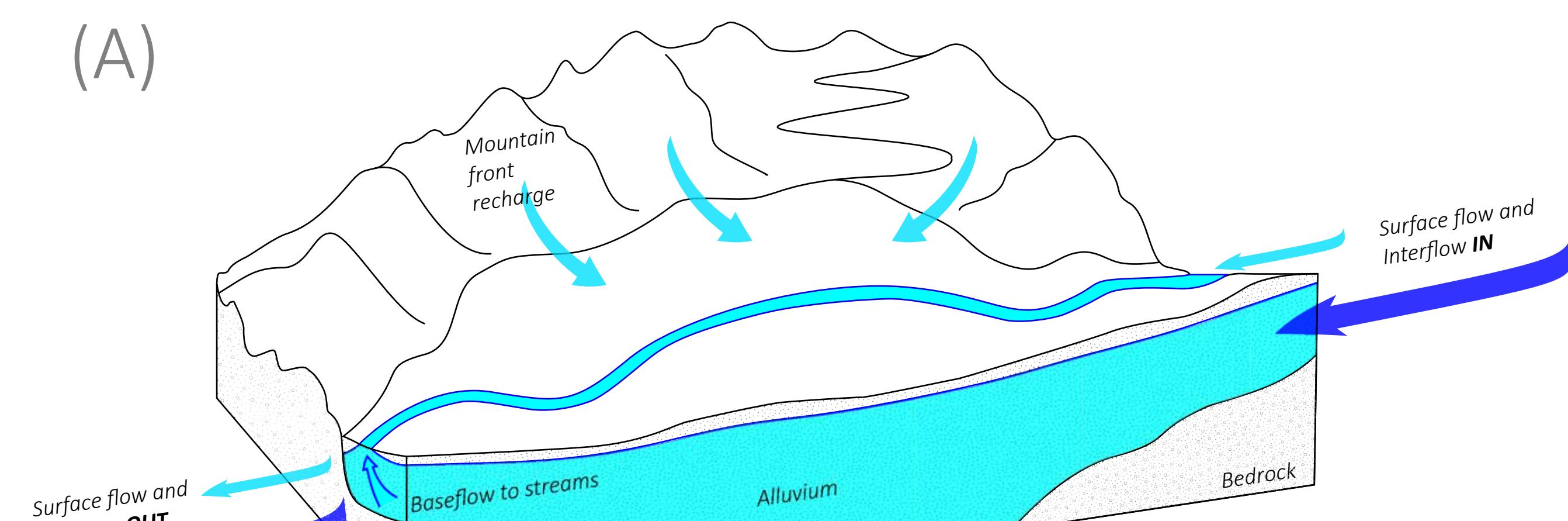
CORE QUESTION:

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

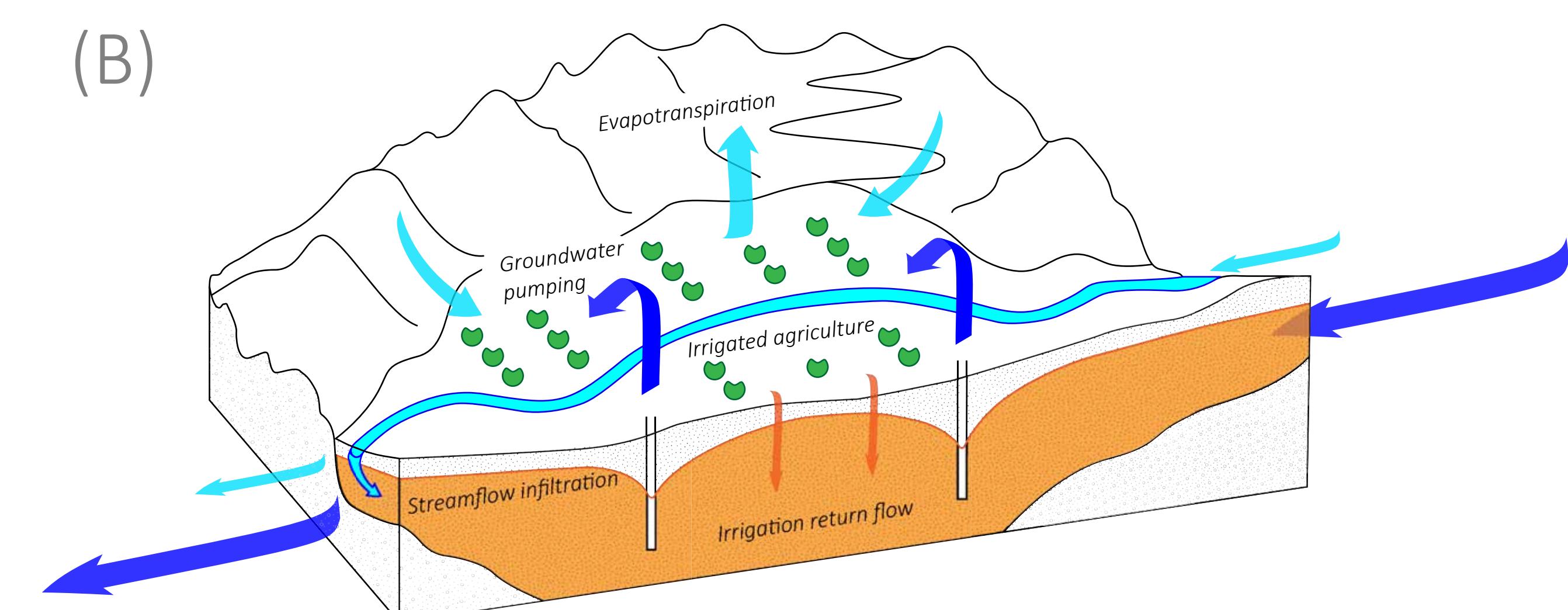
Approach

1. Generate a 3D hydraulic conductivity domain from thousands of well logs and a transition probability geostatistical approach (T-PROGS)¹ in the King's River Fan in California, USA. Derive 2D realizations from this domain.
2. Simulate regional-scale, steady state groundwater flow with finite difference groundwater modeling in MODFLOW for the 3D domain and all 2D realizations.
3. Simulate advection-dispersion in the 3D domain and all 2D realizations with the particle tracking code RW3D. Measure breakthrough curves for a pulse injection of particles and compare.
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

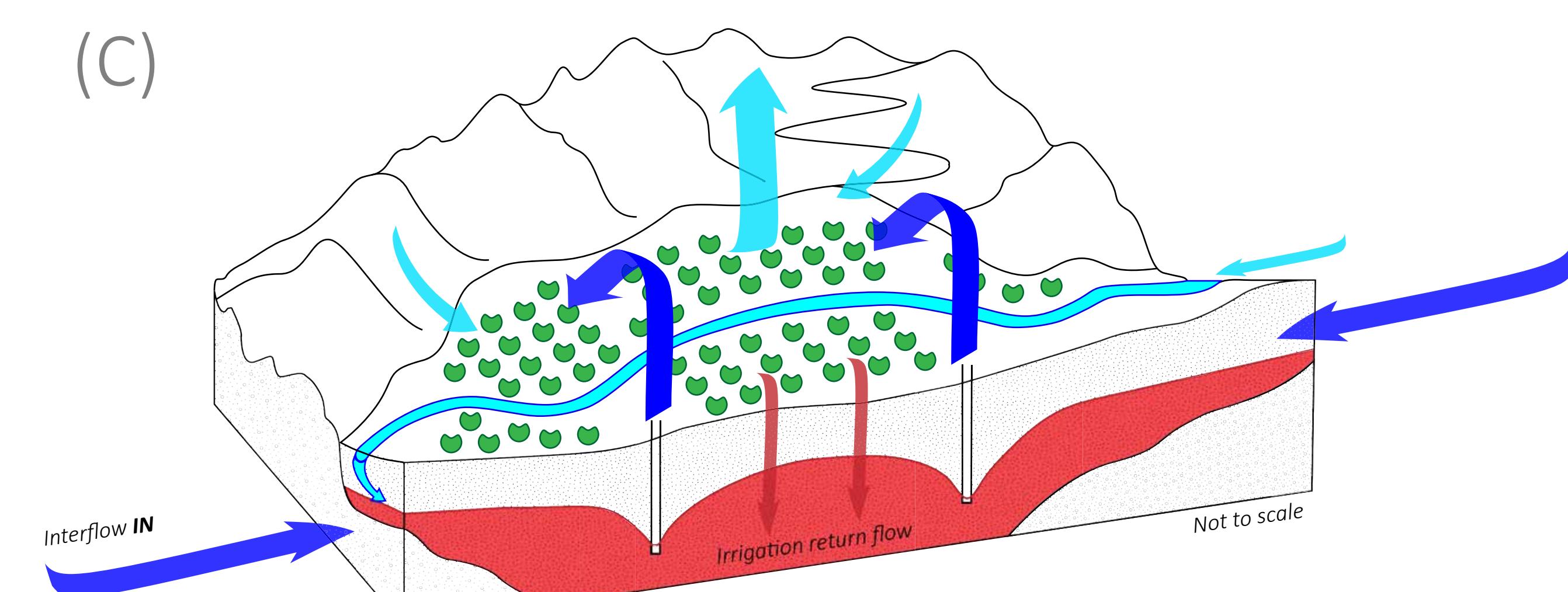
Closed Basin Groundwater Salinization



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).



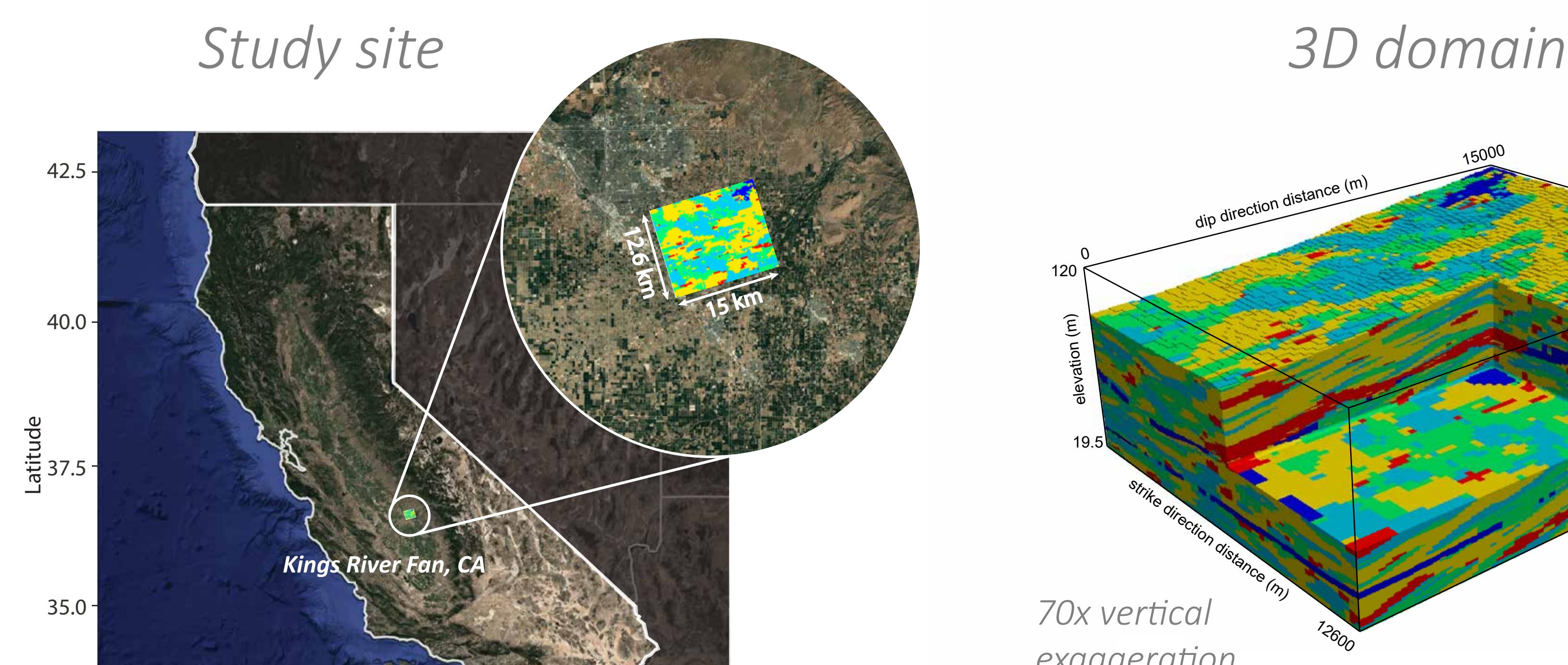
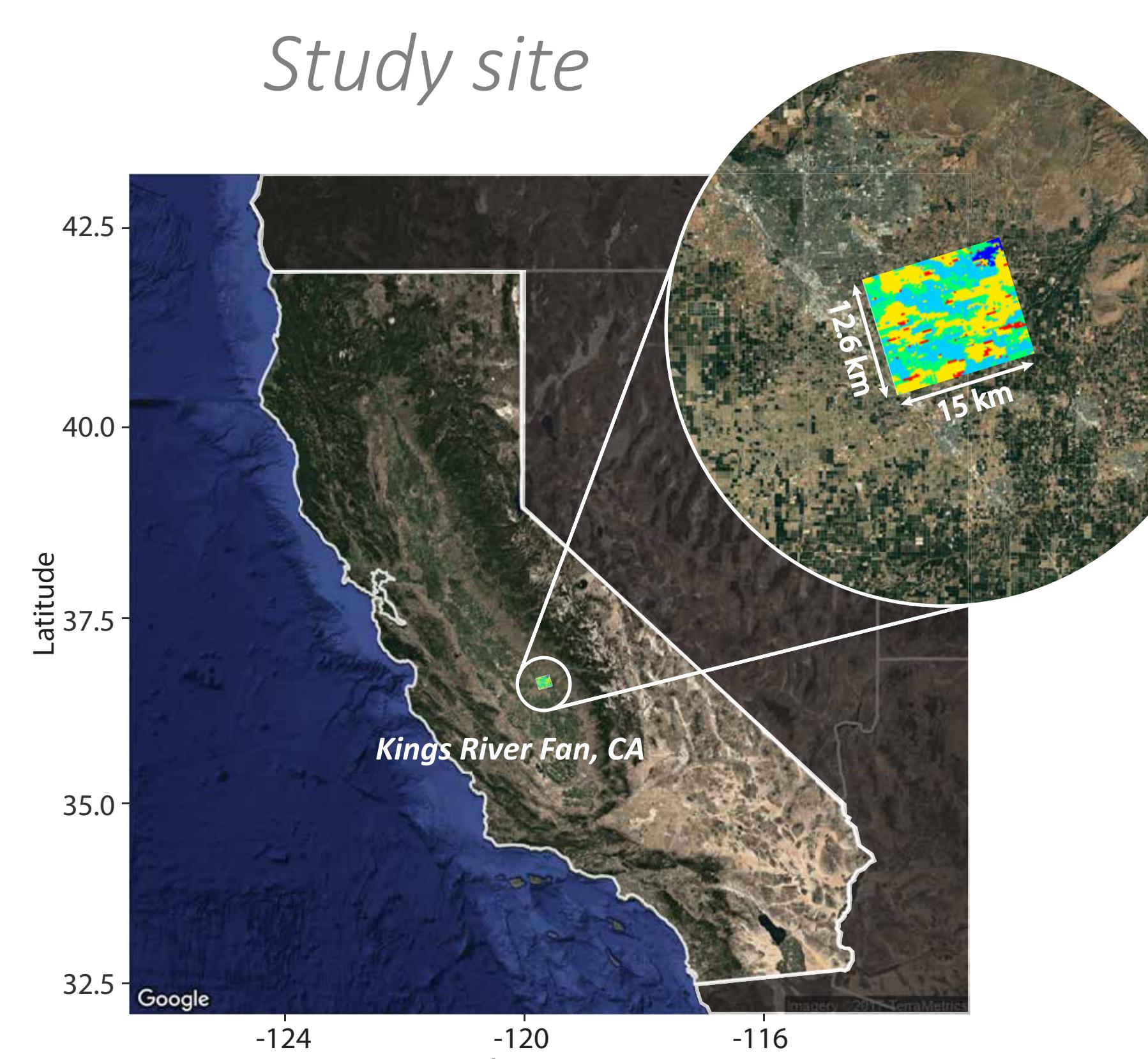
Partial closure of basin: groundwater pumping causes reduction or elimination of baseflow to streams. Pumped groundwater returns to the basin via irrigation return flow. Dissolved solids begin to accumulate in groundwater.



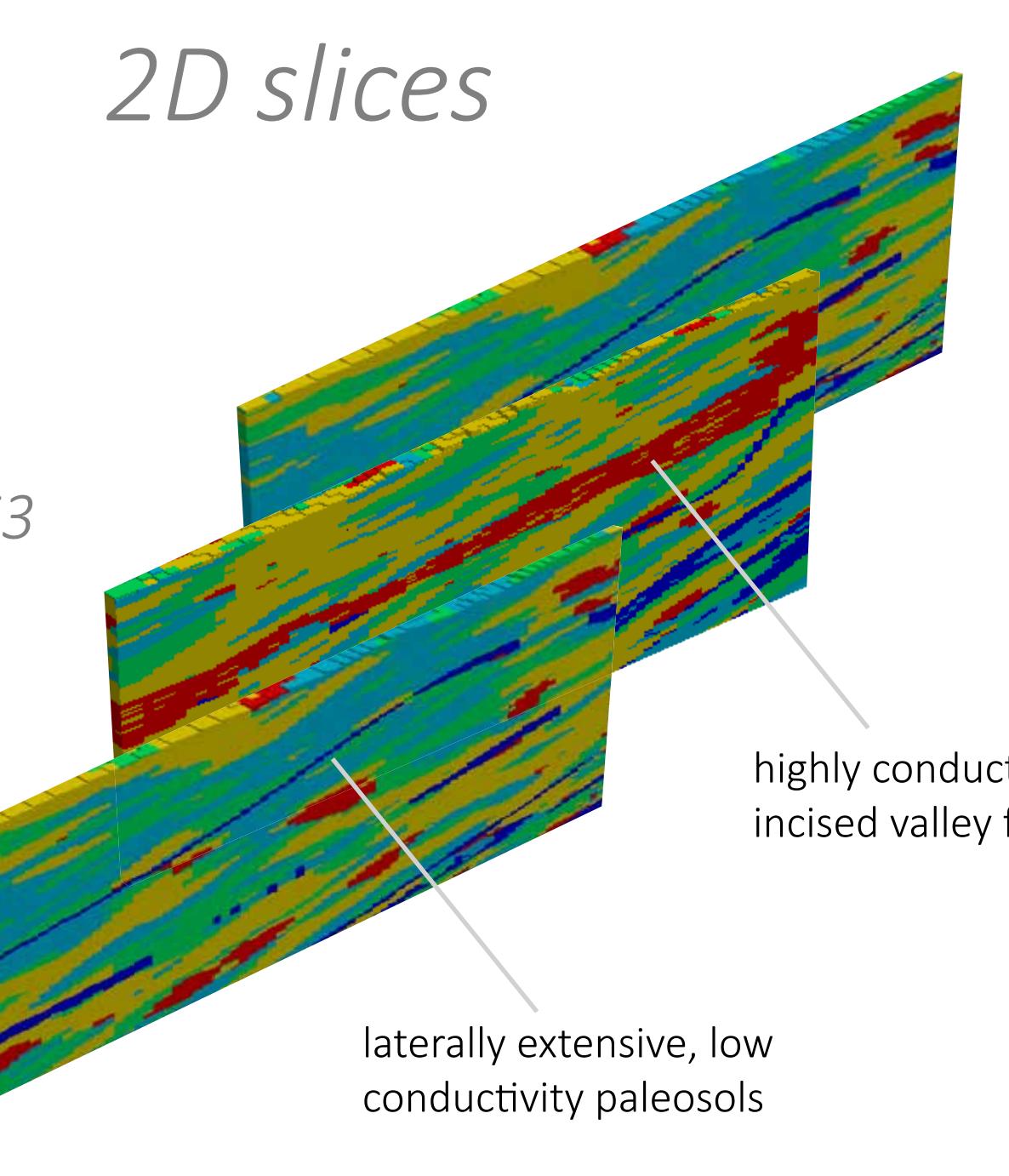
Closed basin: falling groundwater levels cause subsurface interflow to drain adjacent basins. Streams lose to groundwater. Water primarily exits via evapotranspiration, which further concentrates dissolved solids in groundwater.

Legend: low TDS (blue), high TDS (red), groundwater well (orange), water budget terms (green), agriculture (green).

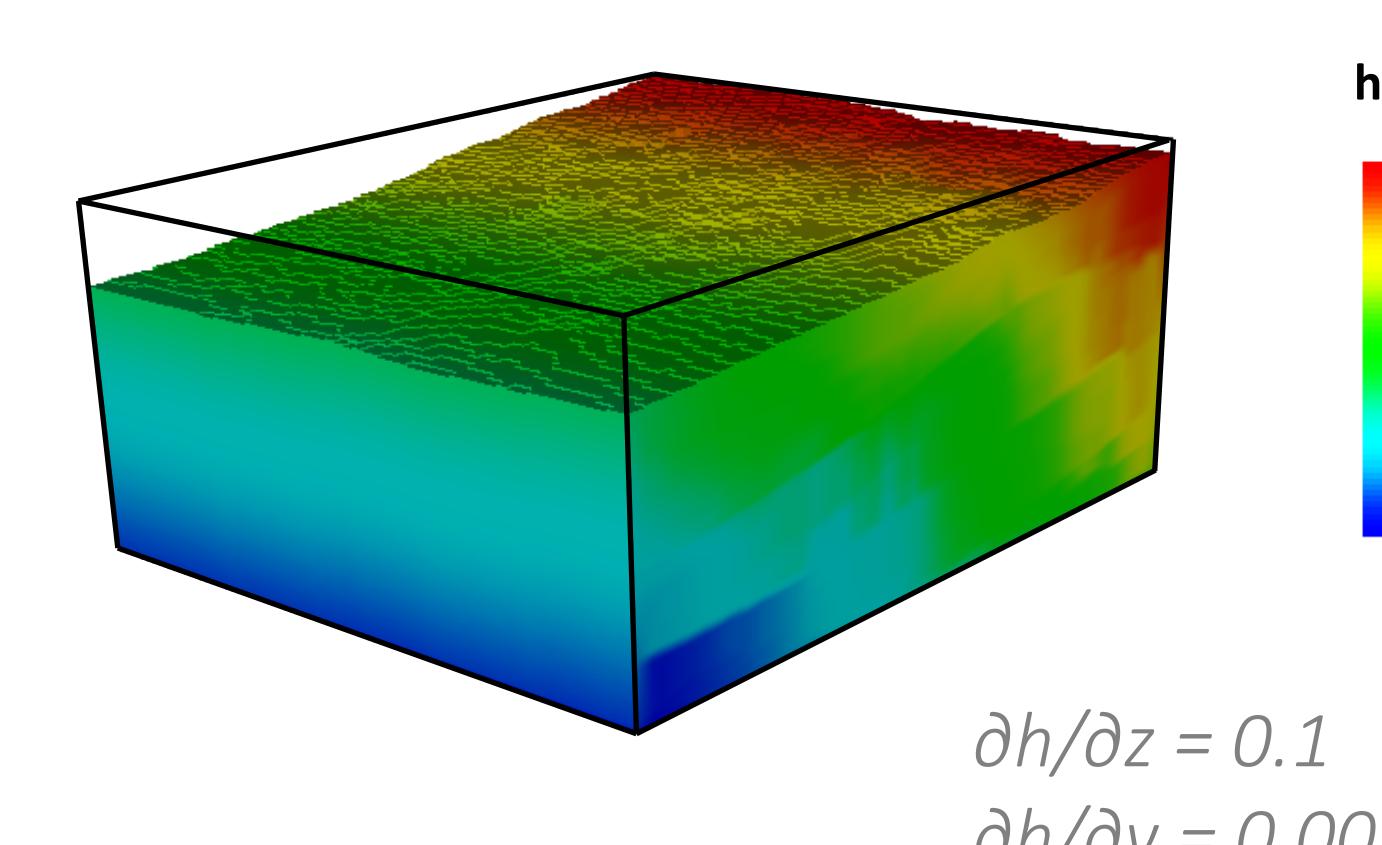
Geostatistical Transition Probability Model



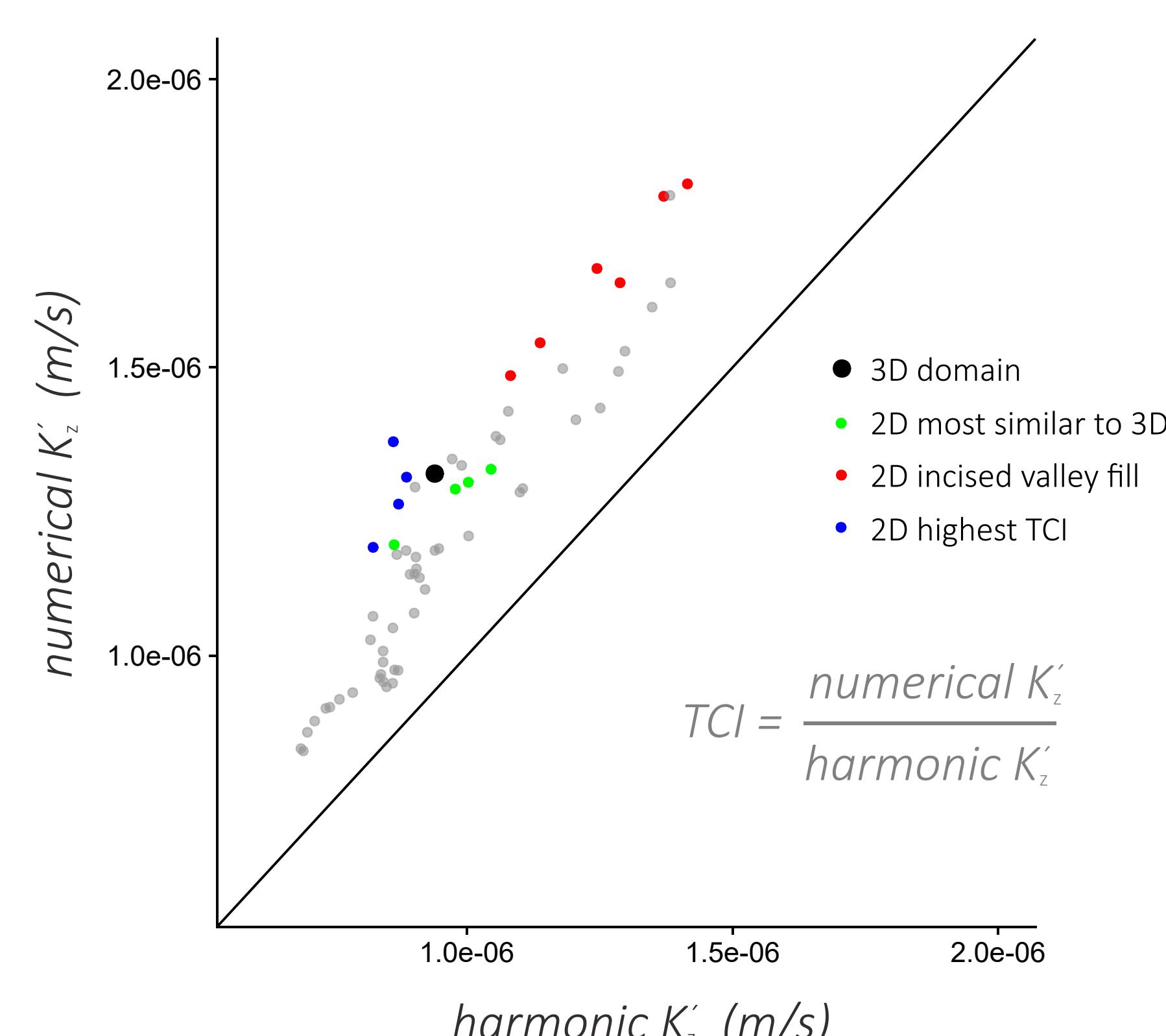
3D domain
70x vertical exaggeration
 K_z (m/s): 1 E-2, 1 E-3, 1 E-5, 1 E-6, 1 E-7



Steady State Flow Model



3D Transport Indicators



Discussion

Nonpoint source regional groundwater salinization threatens vulnerable populations worldwide.

These experiments suggest that 2D heterogeneous domains can mimic 3D non-Fickian transport.

Early arriving particles in a domain are explained by the presence of high-K facies, and high connectivity², but 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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- [1] Weissmann, G.S., S.A. Carle, and G.E. Fogg. 1999. "Three-dimensional hydrofacies modeling based on soil survey analysis and transition probability geostatistics." *Water Resources Research* 35 (6): 1761–70.
- [2] Bianci, M., & Pedretti, D. (2017). "Geological entropy and solute transport in heterogeneous porous media." *Water Resources Research*, 46(9), 4701–4708. <https://doi.org/10.1002/2016WR020195>