

Solute Transport Module for Groundwater Quality Modeling in IWFM

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Overview

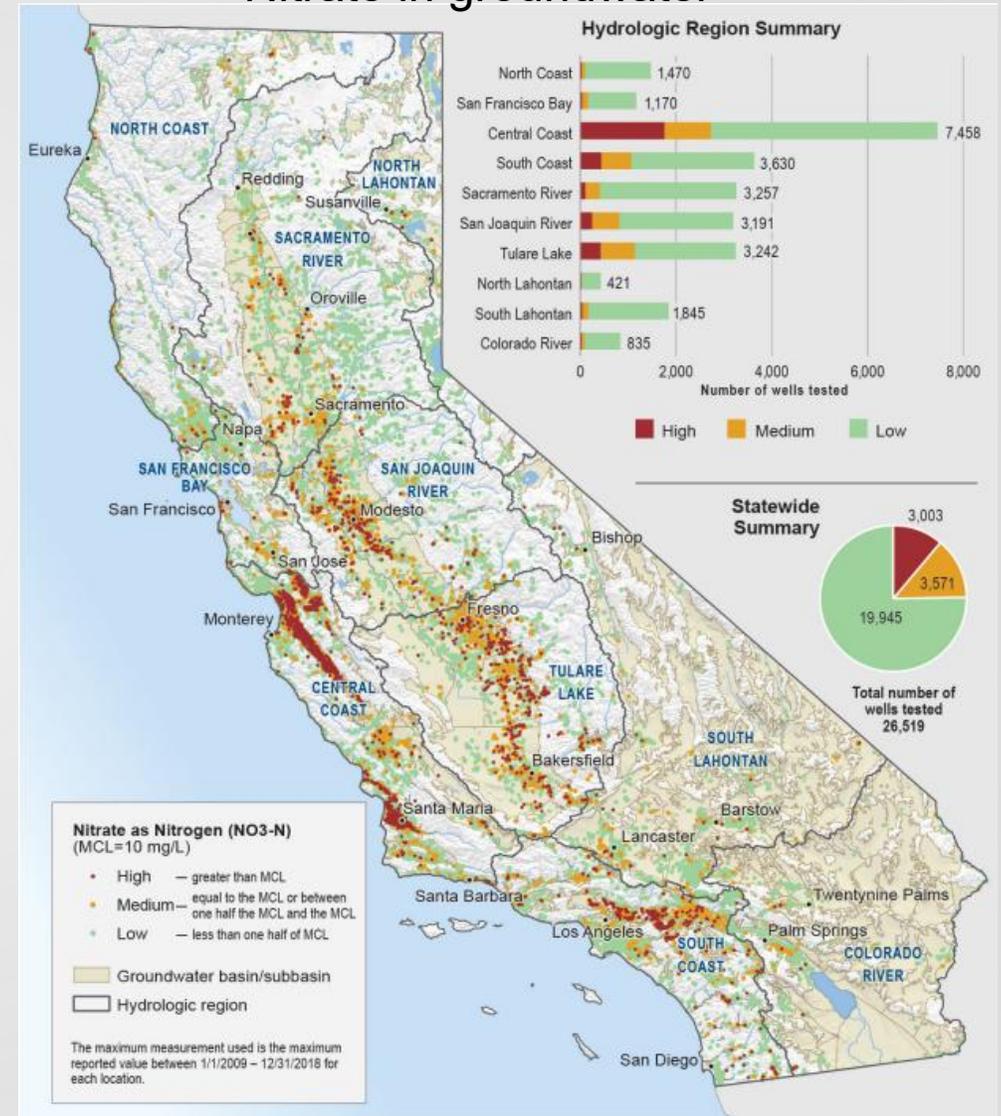
- Why solute transport modeling
- Governing processes and equation
- Numerical implementation of the solute transport model
- Coupling the solute transport model with **Integrated Water Flow Model (IWFM)** and core functionality
- Application to a real-world problem
- Next steps



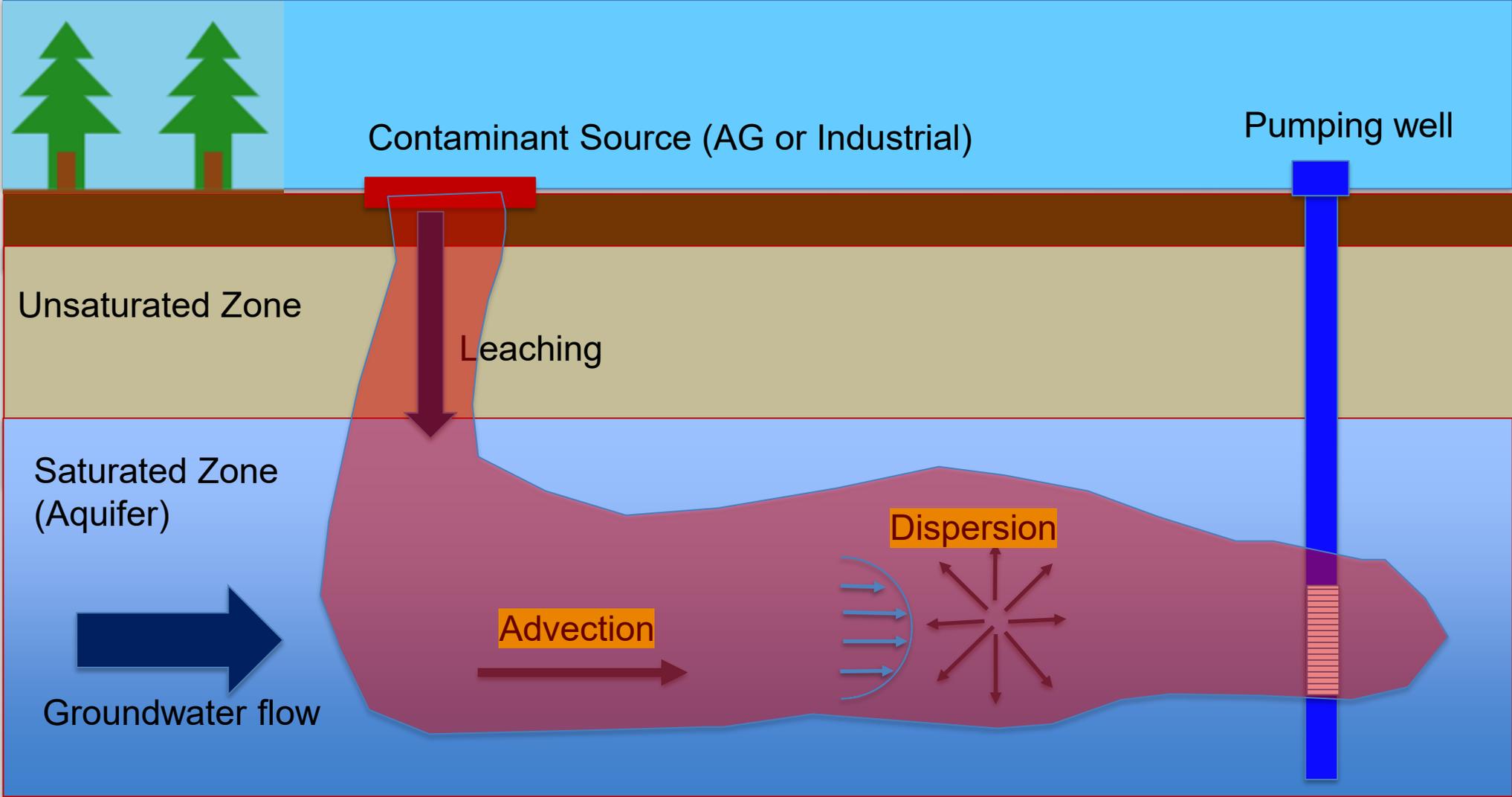
Why groundwater solute transport modeling?

- **Water quality degradation** is one of the sustainability indicators established by the **Sustainable Groundwater Management Act (SGMA)**
 - **Groundwater Sustainability Agencies (GSAs)** need to establish minimum thresholds for point and nonpoint source pollutants in their basins
 - GSAs need plan of actions to improve degraded water quality
- Identifying and managing water quality degradation issues requires numerical tools that can simulate solute transport through groundwater
- IWFM currently simulates only flow; cannot simulate solute transport

Nitrate in groundwater



Governing Processes



Dispersion=Mechanical dispersion + Molecular diffusion



Governing Equation: Advection-Dispersion

$$\theta \frac{\partial C^k}{\partial t} + \frac{\partial}{\partial x_i} (\theta v_i C^k) = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial C^k}{\partial x_j} \right) + q_s C_s^k$$

Diagram annotations:

- A blue arrow points from the box labeled "Advection" to the term $\frac{\partial}{\partial x_i} (\theta v_i C^k)$.
- A blue arrow points from the box labeled "Dispersion" to the term $\frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial C^k}{\partial x_j} \right)$.
- A blue arrow points from the box labeled "Source/Sink" to the term $q_s C_s^k$.

- θ = porosity of the aquifer (-),
- C^k = dissolved concentration of solute k [M/L^3],
- t = time [T],
- D_{ij} = dispersion coefficient tensor [L^2/T]-both hydrodynamics and molecular diffusions ,
- v_i = linear pore water velocity [L/T],
- q_s = volumetric flow rate per unit volume representing sources or sinks [$1/T$],
- C_s^k = source or sink concentration of solute k [M/L^3]

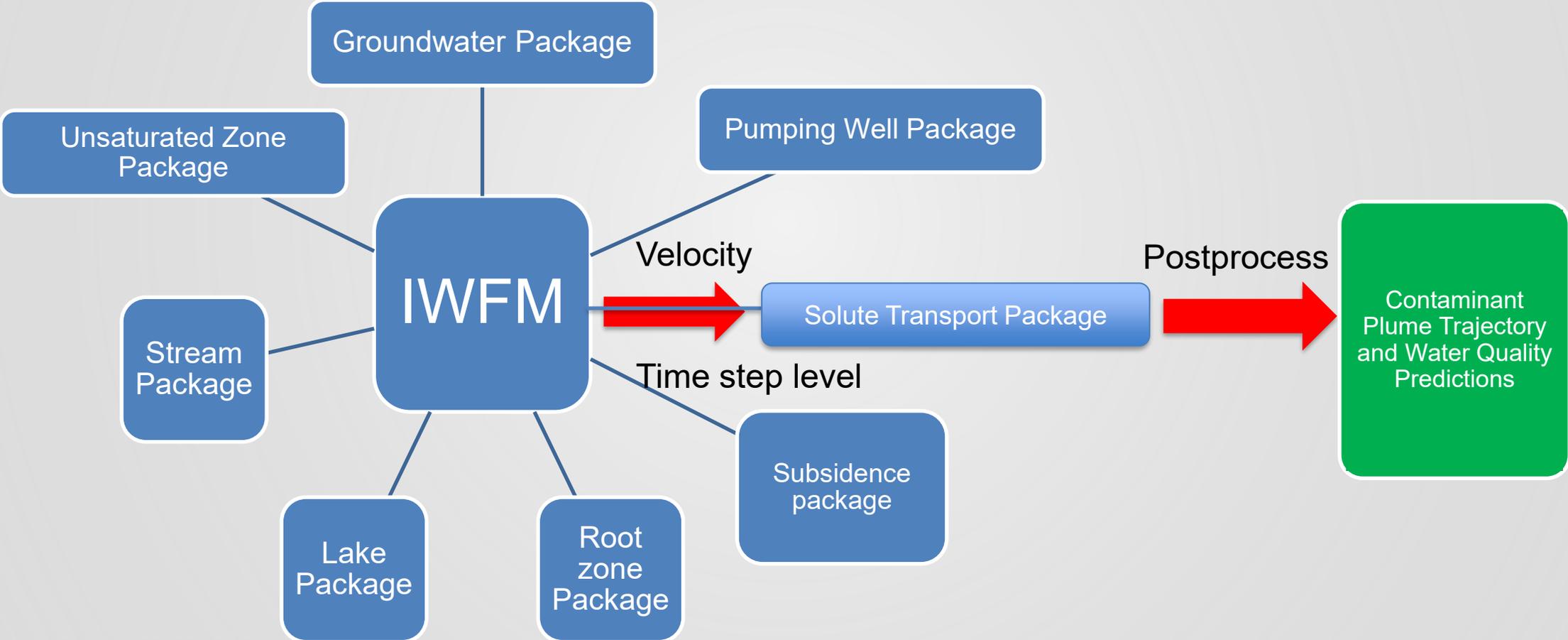


Numerical Implementation-Lagrangian Parcel Model

- Free of numerical dispersion, oscillations and good mass balance
- Easy to implement: No need to solve system of equations
- Limitation: Valid only for diluted conditions
 - Aquifer Storage Recovery (ASR), Managed Aquifer Recharge (MAR)
 - Not good for seawater intrusion simulations
- Solute mass is represented by a large number of parcels (LP) that have time dependent coordinates
- Parcels are introduced into groundwater at spill sites corresponding to each spill rate and are displaced due to advection and dispersion
- Parcels are removed when they approach sinks such as pumping wells based on user specified radius of influence
- We have developed and validated a 3D groundwater solute transport model against analytical and field data using LP method: In preparation for journal publication



Coupling the Groundwater Solute Transport Model with IWFM



Solute Transport Model Core Functionality

- Particle tracking (forward and backward)
 - Simulate only advection (no dispersion)
 - Identify plume paths, source areas (capture zones) for pumping wells
 - Only locations no concentrations
- Solute transport
 - Simulate both advection and dispersion (more accurate)
 - Can simulate both spatial extents and concentrations of contaminant plumes
 - Estimate and predict water quality in pumping wells
 - Multi-species solute transport capability



Solute Transport Module Input Data

- Input parameters
 - Longitudinal dispersivity-horizontal
 - Transverse dispersivity-horizontal and vertical
 - Porosity
- Transport domain data (part of the flow domain)
 - Concentration grid dimension-horizontal (dx and dy)
 - Lower left and upper right corner of the transport domain
- Source Data
 - Spill locations
 - Concentration of the contaminant
 - Spill rates & durations

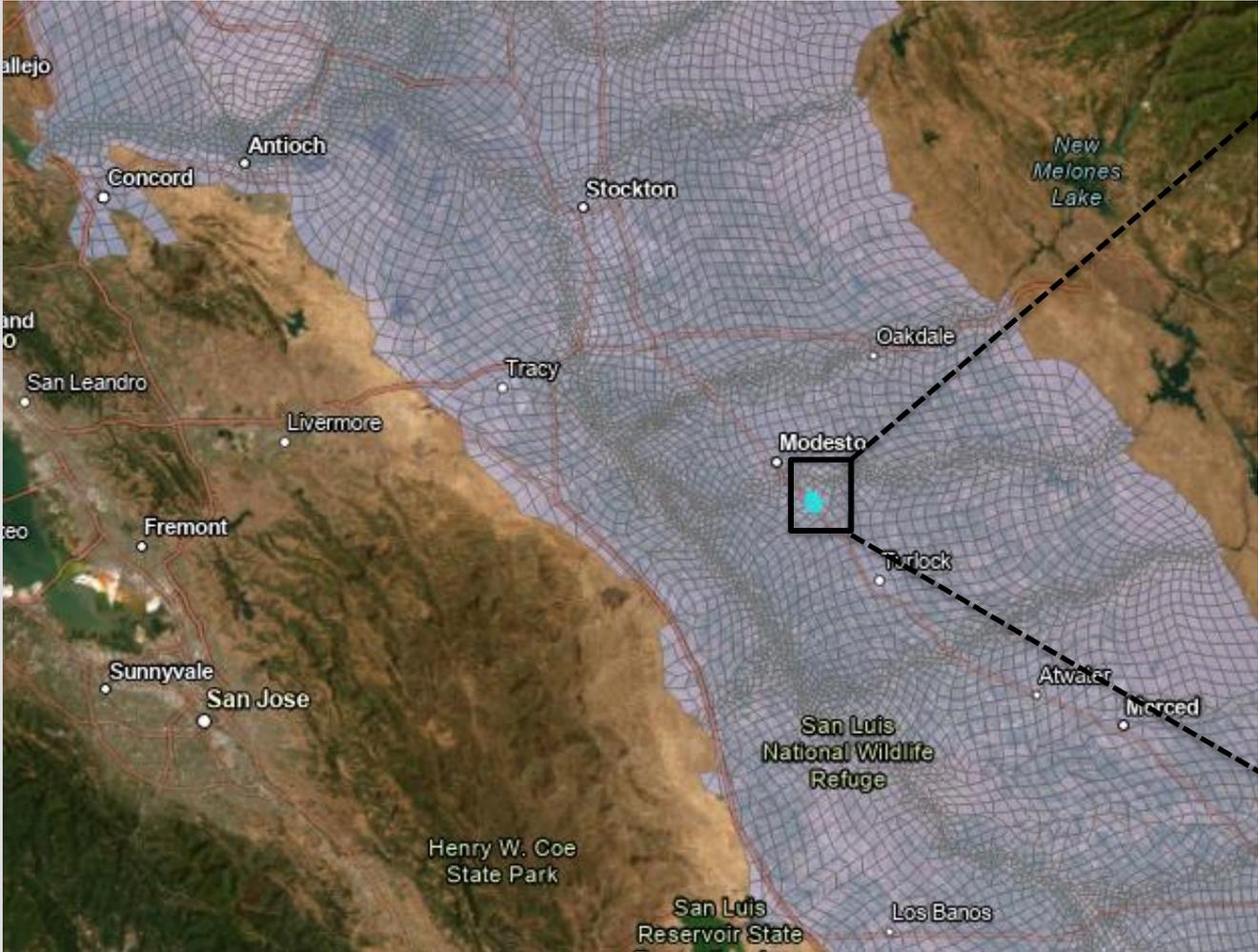
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C2VSimFG_SoluteTransport.dat X
C*****
C                               Solute Transport Data Specifications
C
C  DX      ; Concentration Grid size in the X direction
C  DY      ; Concentration Grid size in the X direction
C  DT      ; Transport time steps (unit same as flow model)
C  NT_SKIP ; Output skip timesteps (unit same as flow model)
C  T_Sim   ; Transport simulation duration (unit same as flow model)
C  NUM_PARCELS; Number of Lagrangian parcels used
C  LWRLEFT ; Lower left coordinates of the transport domain
C  UPRRIGHT ; Upper right coordinates of the transport domain
C  Src_Type ; Source Type (1=Instantaneous source; 2=Continous source)
C  Num_Sources; Number of contaminant sources
C-----
C                               VALUE                               DESCRIPTION
C-----
C                               36                               /Longitudinal Dispersivity (ft)
C                               0.1                             /Ratio of Horizontal Transverse to Longi
C                               0.1                             /Ratio of Vertical Transverse to Longit
C                               0.3                             /Porosity
C-----
C                               DOMAIN DATA
C-----
C                               250.0                             / DX [L]
C                               250.0                             / DY [L]
C                               1                               / DT [T]
C                               12                              / NT_SKIP [T]
C                               574                             / T_Sim [T] -similar to flow model units
C                               1000000                         / NUM_PARCELS
C                               2227861.0 13645742.0 -6921.6 / LWRLEFT
C                               2270442.0 13670964.0 3280.00 / UPRRIGHT
C-----
C                               SOURCE DATA
C-----
C                               2                               / Src_Type
C                               12                              / Num_Sources
C                               2237294.69 13650301.83 -50.0 17921 10.0 30500.0 0 203 / X_SRC, Y_SRC,
C                               2237016.66 13650136.33 -50.0 17921 10.0 30500.0 0 203 / X_SRC, Y_SRC,
C                               2236665.80 13649944.36 -50.0 17921 10.0 30500.0 0 203 / X_SRC, Y_SRC,
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C                               2234004.59 13648355.57 -50.0 17921 10.0 30500.0 203 371 / X_SRC, Y_SRC,
C                               2233673.60 13648123.88 -50.0 17921 10.0 30500.0 203 371 / X_SRC, Y_SRC
    
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Scenario: Water quality in pumping well in city of Ceres

C2VSimFG 1.5



Solute transport model domain



Scenario: Water quality in pumping well in city of Ceres

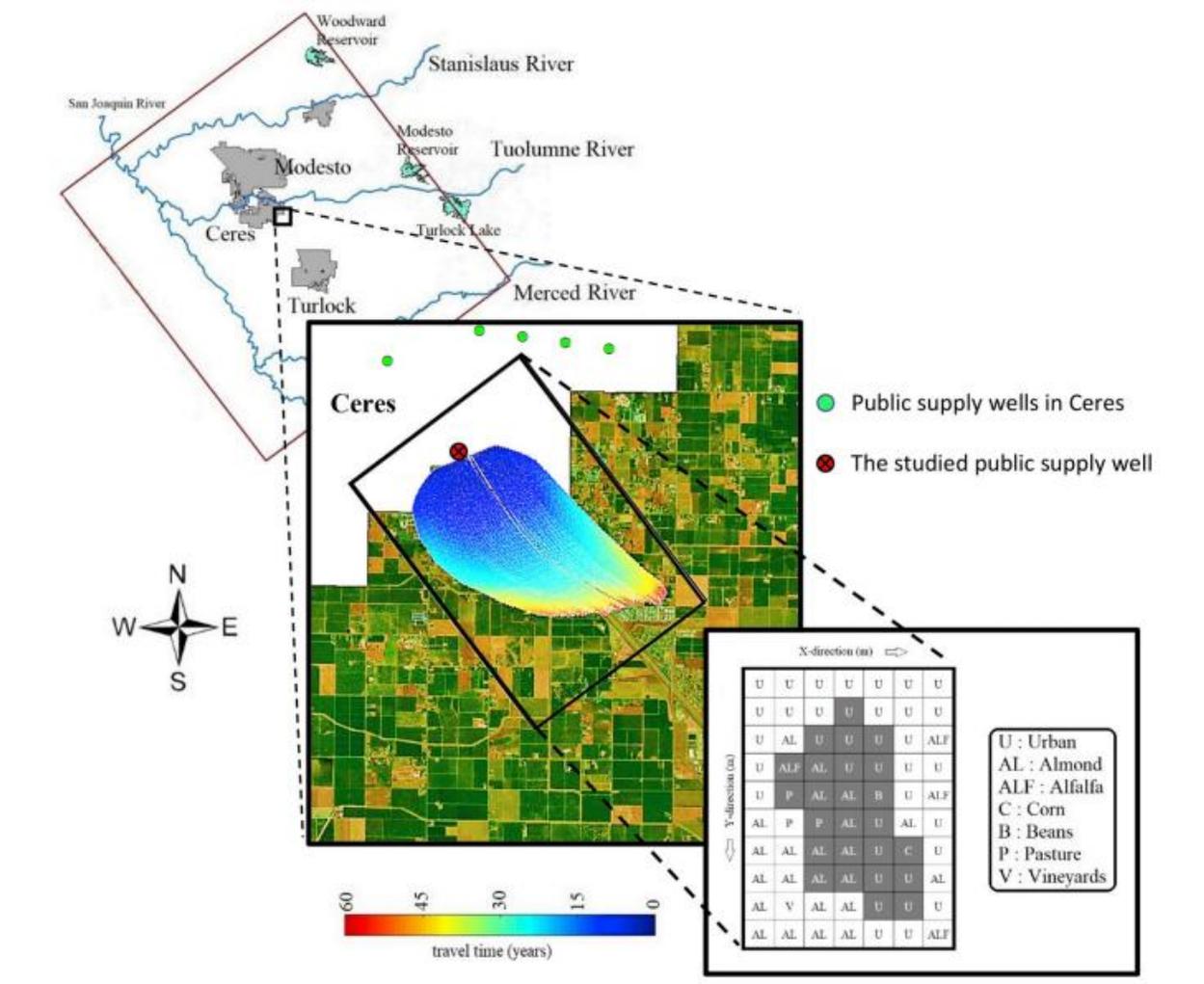


Table 3

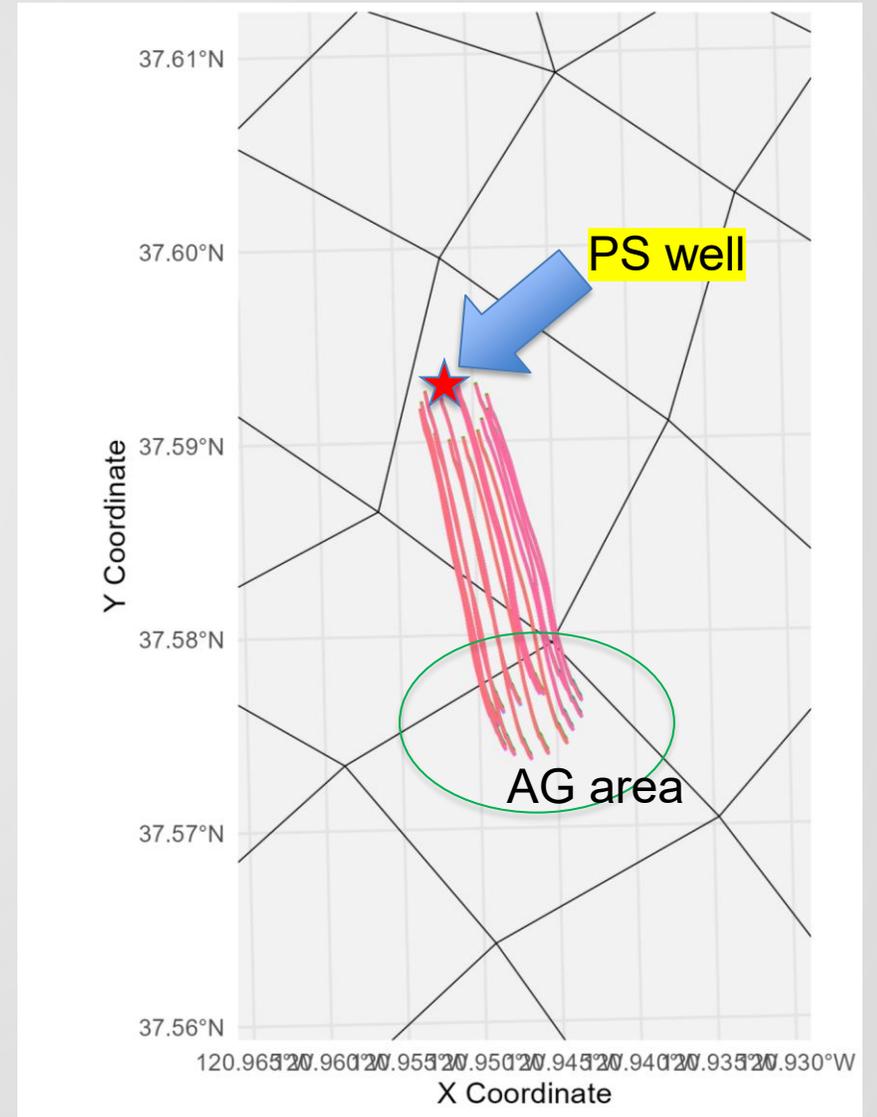
Estimated nitrate mass load for simulation period of 1960–2004 (Modified from Harter et al., 2017).

Land use type	Nitrate load as N (kg/ha/yr)		
	Years 1960–1975	Years 1975–1990	Years 1990–2004
Fallow	0	0	0
Grain	73.3	48.8	89.3
Rice	7.9	20.3	39.1
Field crops	62.6	75.8	79.3
Cotton	27	54.1	115
Corn	60.7	63.6	153.2
Pasture	0	0	0
Alfalfa	30	30	30
Truck crops	82.7	133.4	185.7
Artichoke	50	50	50
Asparagus	109.8	144.7	143.6
Christmas tree	30	30	30
Strawberry	140.8	150.2	182.6
Almonds	29	48.9	136.9
Citrus tree	122.6	138.9	141
Vineyards	40.7	46.2	22.9
Natural vegetation	15	15	15
Urban	20	20	20

Fig. 4. Selected public supply well in the city of Ceres and its source area delineation.

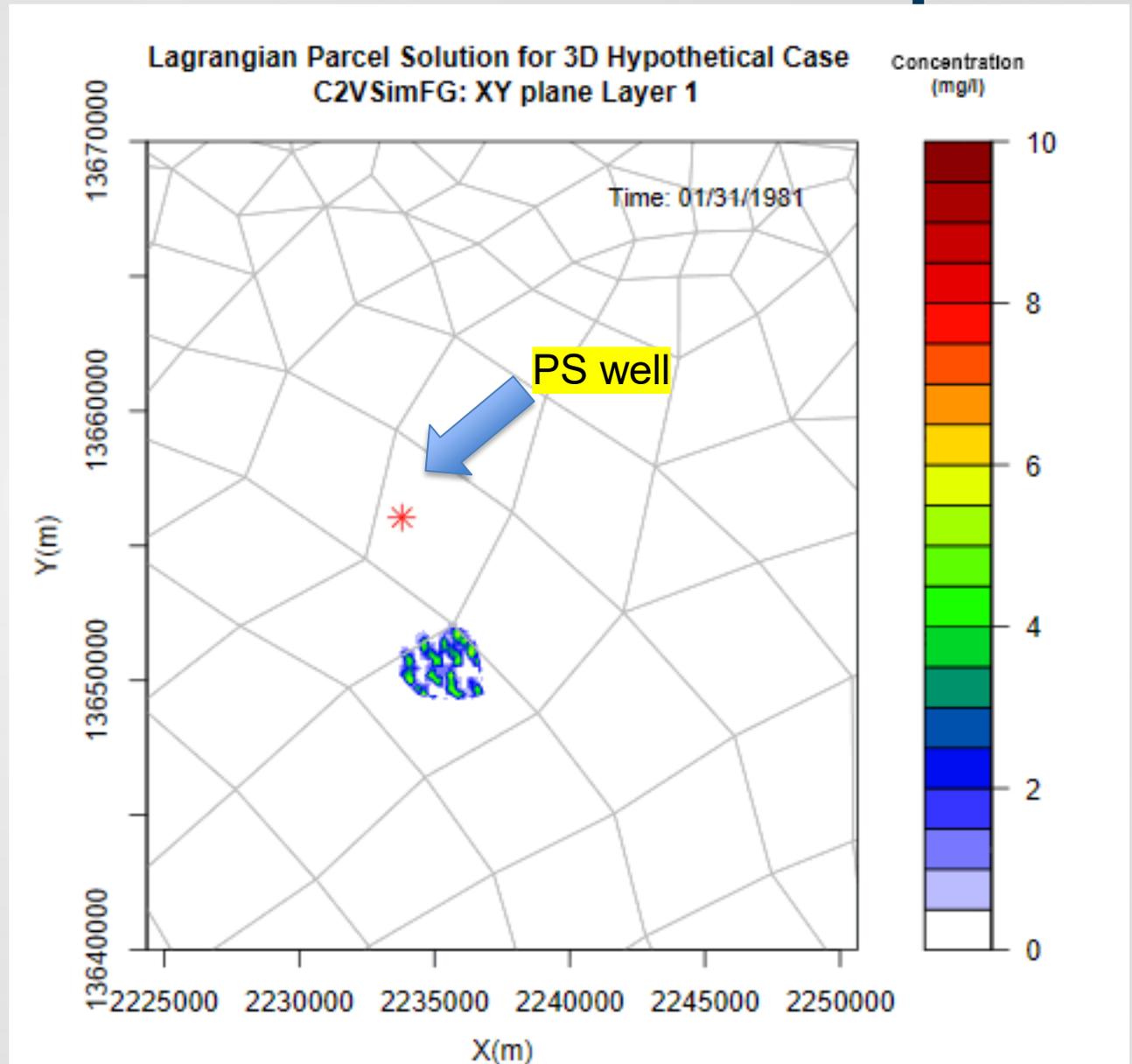
Contaminant source identification: Backward Particle Tracking

- Velocity data saved from a C2VSimFGV1.5 model run from 1973-2021
- Particles are introduced around the public supply well
- Velocity data is provided in reverse order with opposite sign during each stress period
- Contaminant source can be determined by using path lines, which indicate the groundwater flow directions

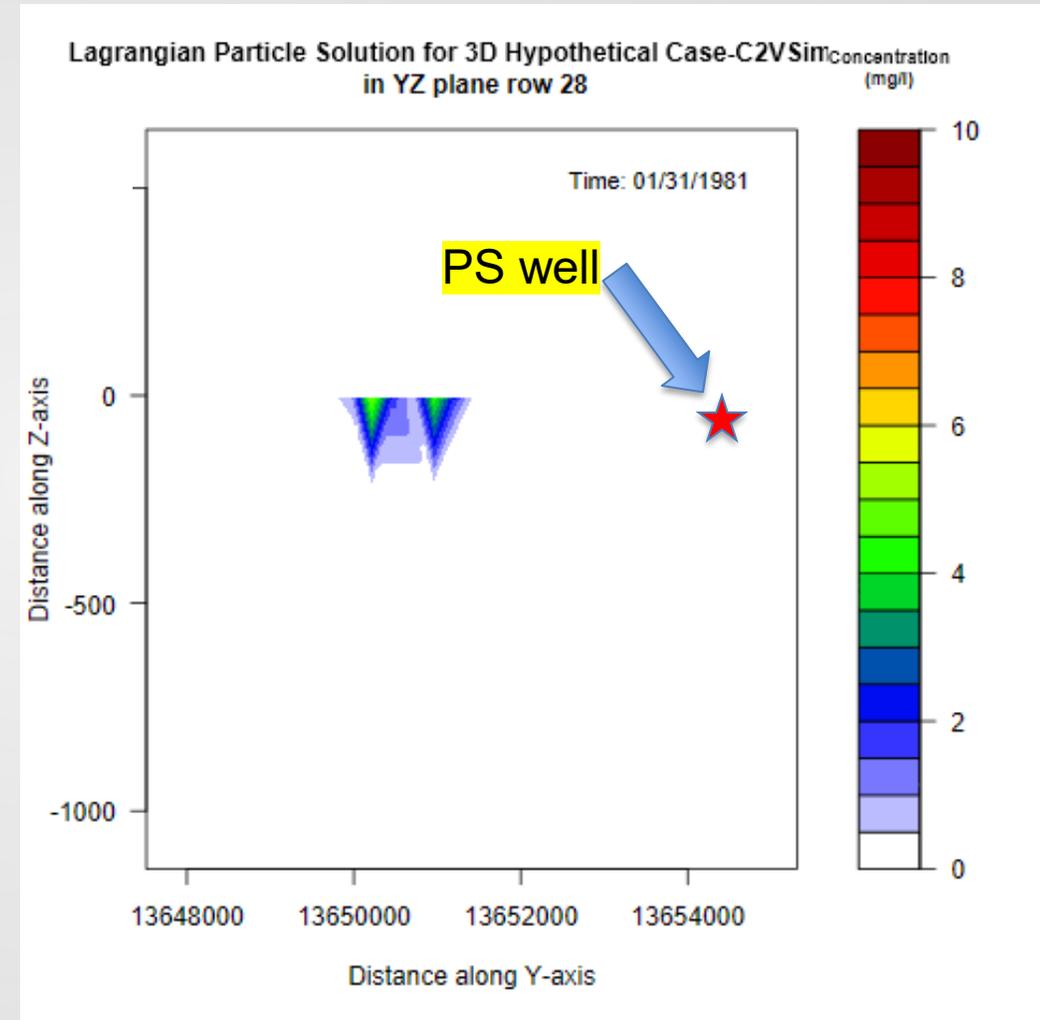
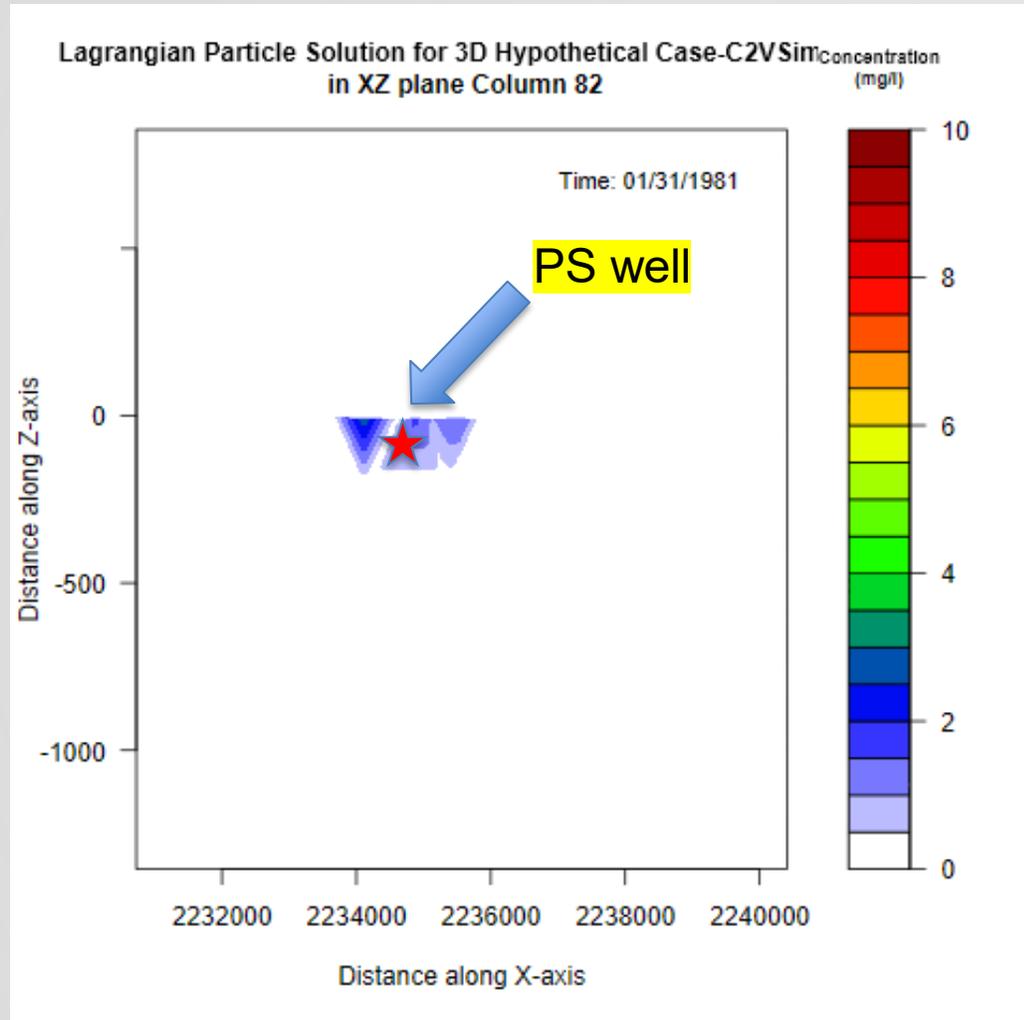


Simulated nitrogen plume evolution-horizontal plane

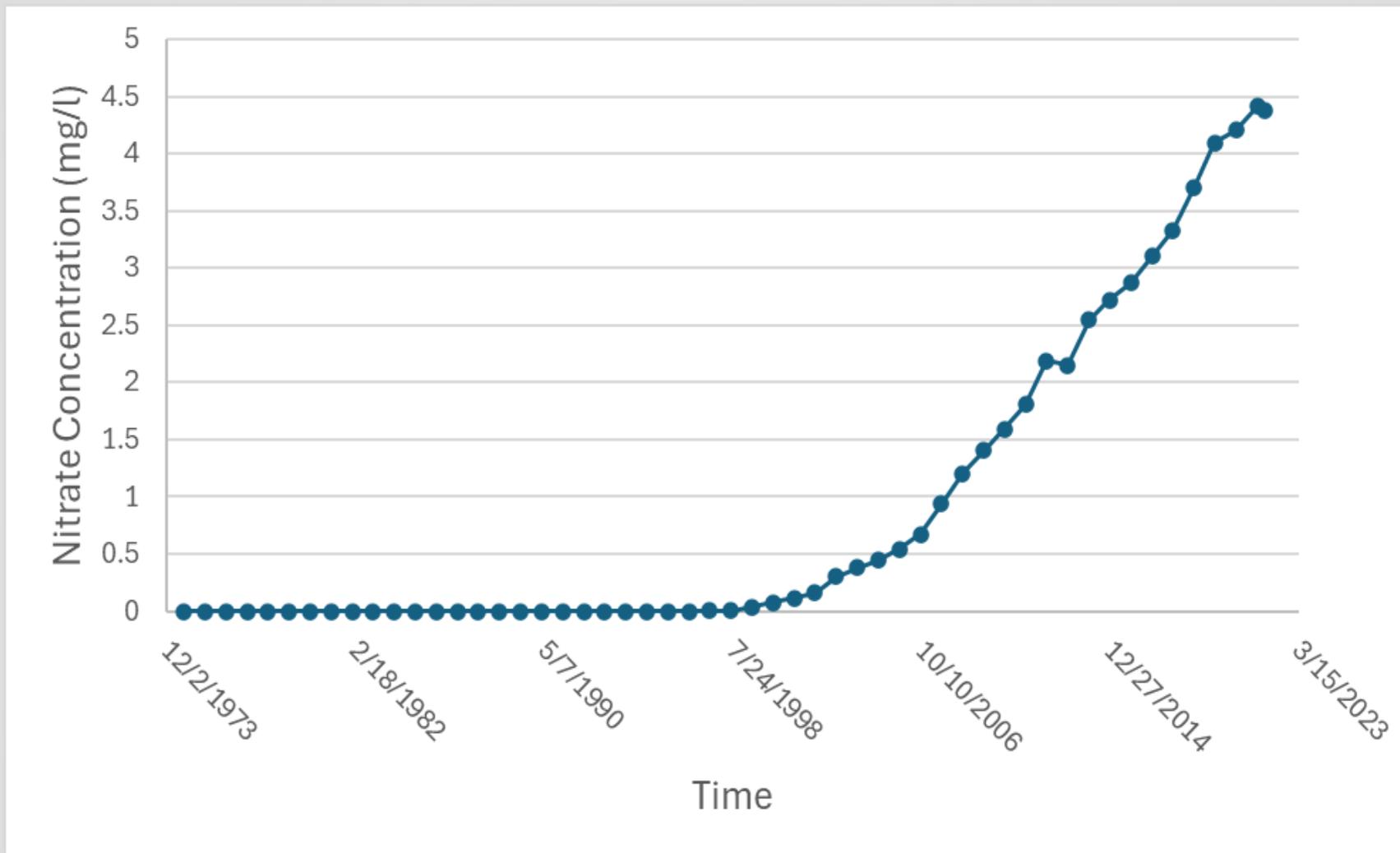
- 48-year simulation
- Introduced one million Lagrangian parcels at source locations to represent nitrate loading
- Concentration grid size 250 ft x 250 ft
- About 10-15 minutes additional runtime for solute transport simulation (C2VSimFG run time - 2.5 hr)



Simulated nitrogen plume evolution-vertical plane



Simulated concentration at the PS well



Next steps

- Public release
 - End of summer 2025
- Seawater intrusion modeling
 - Density dependent flow model is required
 - Currently IWFM is not a density dependent model
 - IWFM needs to be substantially updated
 - Currently working on Discontinuous Galerkin Finite Element solute transport model
 - Hybrid version of Finite Element and Finite Volume methods
 - No numerical dispersion and no oscillations, good mass balance
 - Complex implementation and increased runtime



Summary

- New solute transport module was added to IWFM
- Potential applications and uses of the solute transport module
 - Water quality management
 - Contaminant source identification: Reverse particle tracking to identify pollution origins
 - Recharge project evaluations: ASR, AgMAR
 - Regulatory compliance forecasting: Predictive modeling for water quality standards
 - Contaminated site remediation assessment
 - Environmental Impact Assessment: Industrial releases
 - Long-term trend assessment
 - Multi-decadal water quality projections under different climate scenarios



Thank You !

