In order to characterize the Engle Basin's present day and paleohydrology, we sequentially solved a series of two-dimensional transient, groundwater flow, heat, and solute/isotope transport equations. The heat, solute, and isotope transport equations were solved using a finite element implementation of the Lagrangian-based modified method of characteristics (MMOC). The groundwater flow equation was also solved using standard finite element methods.

Groundwater Flow

We solved for variable-density groundwater flow using the following stream function based groundwater equation:

$$\nabla_x \times \left[\mu_f \frac{k}{|k|} \nabla_x \psi \right] = -g \frac{\partial \rho_r}{\partial x} \qquad \text{(A1)}$$

where ∇_x is the gradient operator in the x- and z-directions, k is the permeability tensor, |k| is the magnitude of k, Ψ is the stream function, ρr is the relative density, μ_f is the water viscosity. The right-hand-side of equation (A1) accounts for variable-density fluid flow. Density-gradients in our model are primarily due to lateral and vertical salinity variations.

Relative density (ρr) and relative viscosity (μr) used in equations (A1) and (A3) are given by

$$\rho_r = \frac{\rho_f - \rho_0}{\rho_0} \qquad \text{(A2)}$$

$$\mu_r = \frac{\mu_0}{\mu_f} \qquad \text{(A3)}$$

where ρ_w is the density of water, ρ_f is the density of groundwater, ρ_0 is the water density at standard conditions (10 °C, 0.0ppt Salinity, and 0.0 MPa), μ_0 is the viscosity of water at standard conditions (10 °C, 0 ppt total dissolved solids concentration, and atmospheric pressure) and μ_f is the viscosity of water.
The Darcy flux is related to stream functions through the Cauchy-Reimann equations:

$$\frac{\partial \psi}{\partial z} = q_x \qquad \text{(A4)}$$

$$-\frac{\partial \psi}{\partial x} = q_z \qquad \text{(A5)}$$

Solute Transport

Transport of solute through porous media is controlled by advection, Fickian diffusion, and hydrodynamic dispersion (Freeze and Cherry, 1979). For relatively low flow velocities (<10^{-5} m/yr), solute transport is dominated by diffusion; dispersive transport and advective transport are more important when fluid velocities are higher. We used the following equation to represent advective/dispersive solute transport

$$\phi \frac{\partial C}{\partial t} = \nabla_x \left[\phi \mathbf{D} \nabla_x C \right] - \vec{q} \ \nabla_x C \qquad \text{(A7)}$$

where **D** is the hydraulic dispersion-diffusion tensor, $\vec{q}$ is the groundwater flux, ϕ is porosity, and *C* is species concentration (total dissolved solids concentration reported as solute mass fraction denoting kilograms of solute per kilograms of solution). Equation A7 neglects the effects of solute diffusion into low permeable blocks and rapid advective transport through fractures. Equation (A7) also neglects fluid-rock geochemical reactions at depth. Computed salinity units were converted parts per thousands (ppt) in this report. The tensor **D** has the four components, $\mathbf{D}_{xx}$, $\mathbf{D}_{zz}$, $\mathbf{D}_{zx}$, *and* $\mathbf{D}_{xz}$, defined by

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D_d$$
$$D_{zz} = \alpha_T \frac{v_x^2}{|v|} + \alpha_L \frac{v_z^2}{|v|} + D_d \qquad \text{(A8)}$$
$$D_{zx} = D_{xz} = (\alpha_L - \alpha_T)\frac{v_x v_z}{|v|}$$

where v_x and v_z are components of seepage velocity in the x- and z-directions ($v_x = q_x/f$ and $v_z = q_z/f$), D_d is the solute diffusion coefficient, and |v| is

$$|v| = \sqrt{v_x^2 + v_x^2} \qquad \text{(A9)}$$

Heat Transport

Temperature can affect fluid density and permafrost distribution in our model. FEMOC solves a conductive and convective-dispersive heat-transfer equation:

$$\left[c_f\rho_f\phi + c_s\rho_s(1-\phi)\right]\frac{\partial T}{\partial t} = \nabla_x\left[\lambda\nabla_x T\right] - \vec{q}\,\rho_f c_f \nabla_x T \qquad \text{(A11)}$$

where λ is the thermal dispersion-conduction tensor, ϕ is porosity, T is temperature, c_s and cf are the specific heat capacities of the solid and liquid phases, respectively, and ρ_s is the density of the solid phase. The tensor λ has the form:

$$\lambda_{xx} = \rho_f c_f \alpha_L \frac{q_x^2}{|q|} + \rho_f c_f \alpha_T \frac{q_z^2}{|q|} + \lambda_f\phi + (1-\phi)\lambda_s$$
$$\lambda_{zz} = \rho_f c_f \alpha_T \frac{q_x^2}{|q|} + \rho_f c_f \alpha_L \frac{q_z^2}{|q|} + \lambda_f\phi + (1-\phi)\lambda_s \qquad \text{(A12)}$$
$$\lambda_{zx} = \lambda_{xz} = (\alpha_L - \alpha_T)\frac{q_x q_z}{|q|}$$

where λ_{xx}, λ_{zz}, λ_{zx}, and λ_{xz} are the tensor components, α_L and α_T are the transverse and longitudinal thermal dispersivities, q_x and q_z are the Darcy fluxes in the x- and z- directions. λ_f and λ_s are the thermal conductivities of the fluid and solid phases, respectively, which are assumed to be isotropic and scalar quantities. q is the absolute value of the Darcy flux, which is given by

$$|q| = \sqrt{q_x^2 + q_x^2} \qquad \text{(A13)}$$

Equations of State

Thermodynamic equations of state are used to compute the density and viscosity of groundwater at elevated temperature, pressure, and salinity conditions. FEMOC uses the polynomial expressions of Batzle and Wange (1992). These polynomial expressions are valid for temperatures between 10 and 150 °C and salinities between 0 and 6*m* NaCl. Fluid density is more sensitive to temperature and salinity than fluid pressure.

Groundwater Residence Time

Goode (1996) was the first to develop an advection-dispersion based groundwater transport equation to quantify groundwater residence times:

$$\frac{\partial A}{\partial t} = \nabla_x \cdot \left[D\nabla_x A\right] - q\nabla_x A + 1 \qquad \text{(A14)}$$

where A is groundwater age (in years).