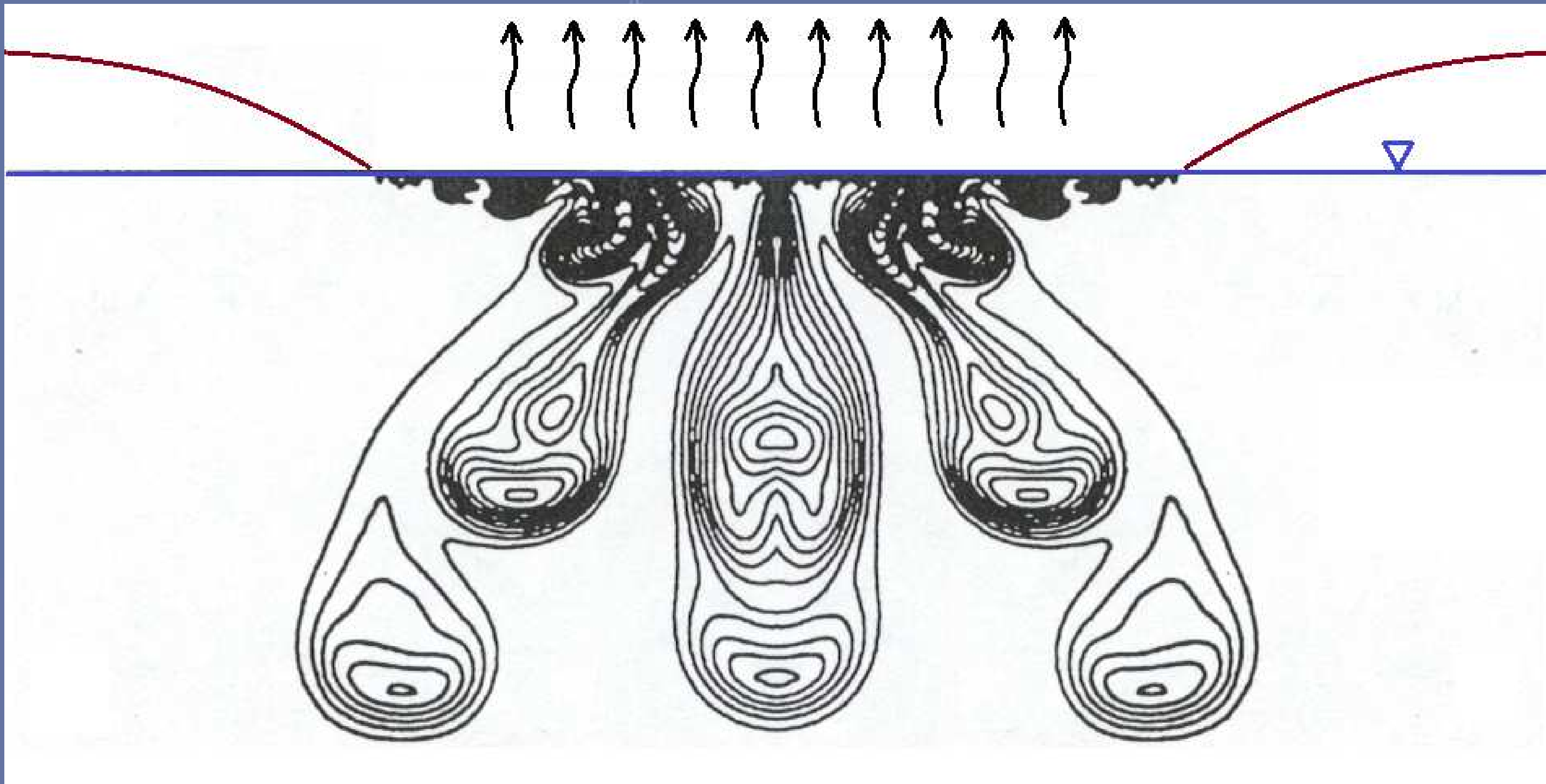
SEAWAT and the Salt-lake Benchmark Test

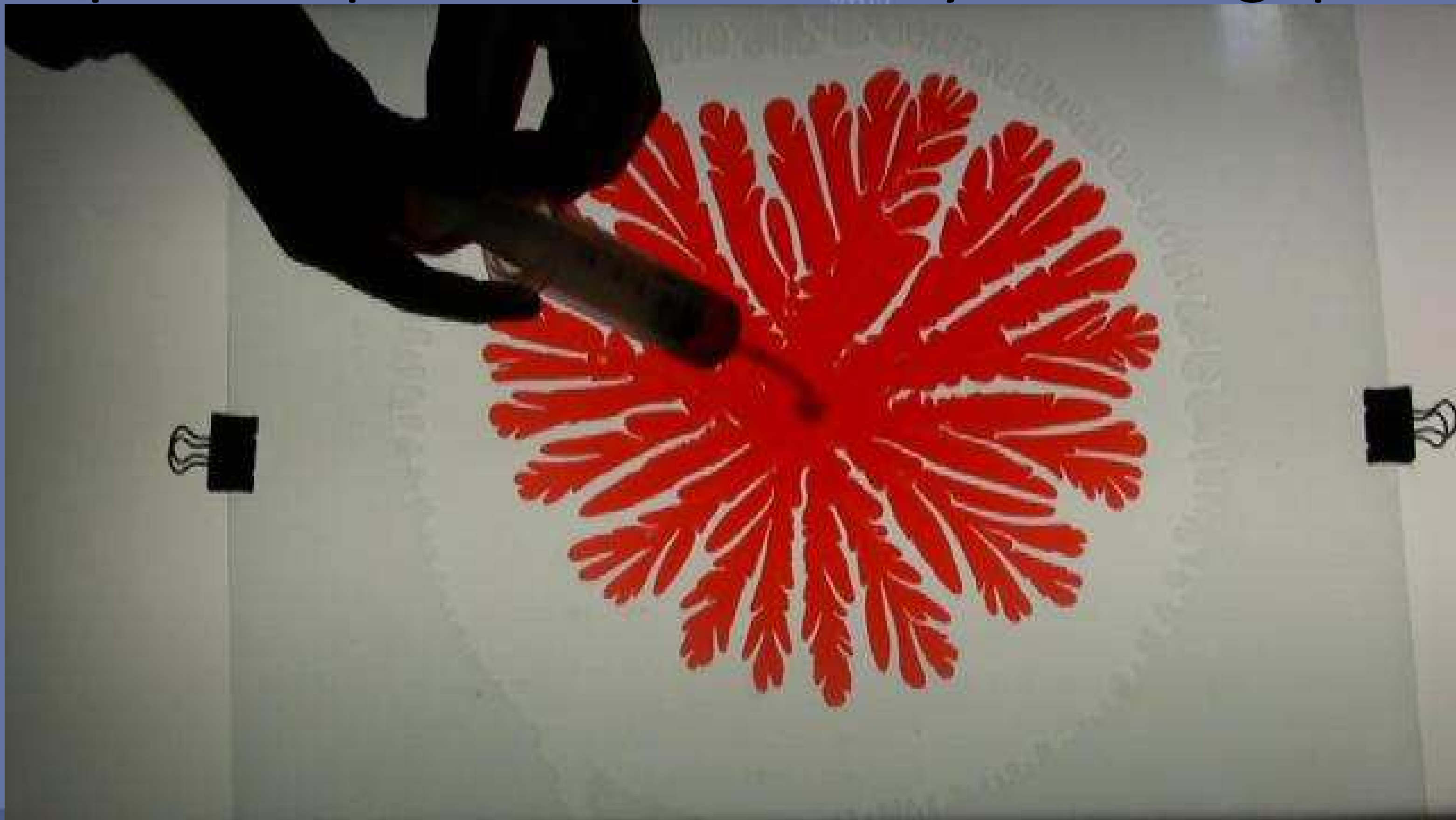
by David Garces

What is the Salt-Lake problem and why is relevant?



Hele-Shaw Cell

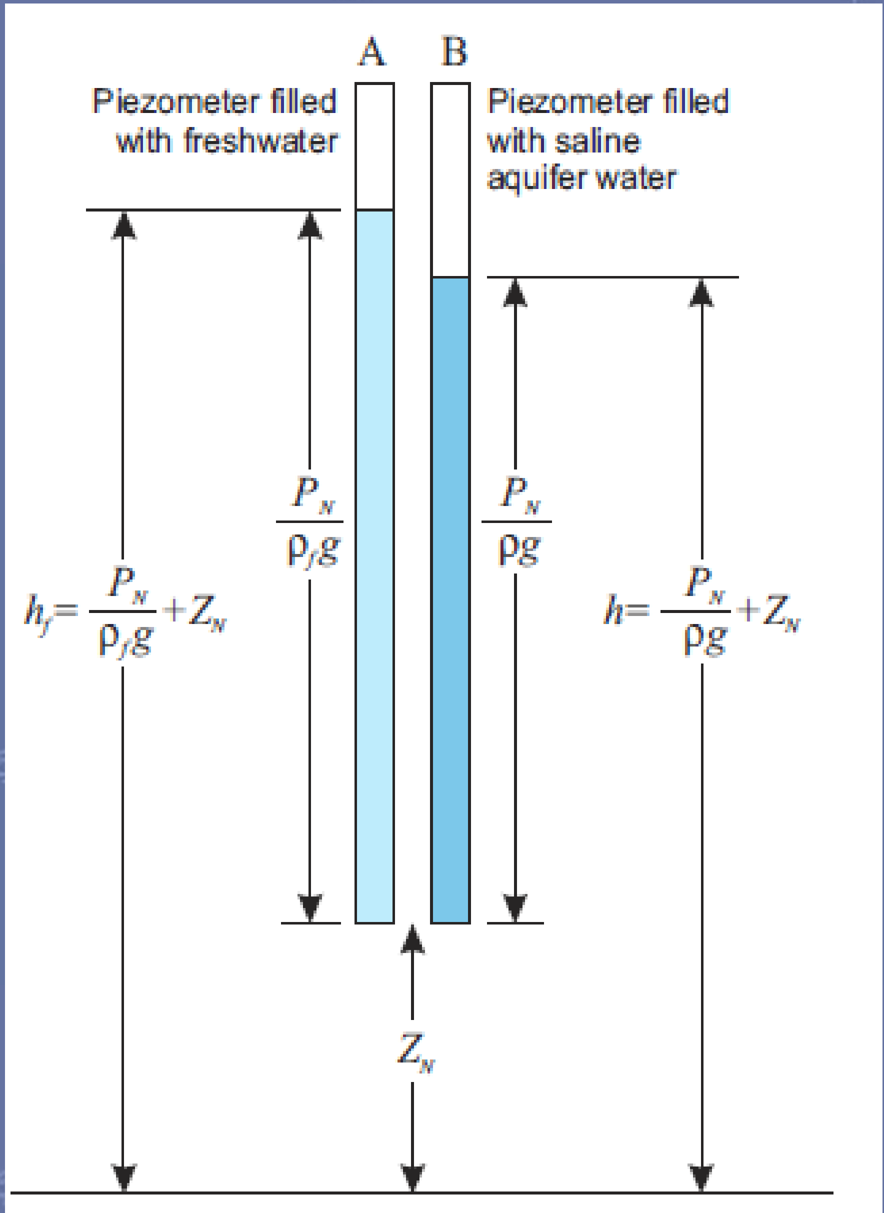
A Hele-Shaw cell is a physical analogue for flow through saturated porous media. It consists of two parallel plates separated by a small gap.



SEAWAT

SEAWAT simulates three-dimensional, variable-density, transient ground-water flow in porous media. The source code for SEAWAT was developed by combining MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations

MODFLOW was modified to conserve fluid mass rather than fluid volume and uses equivalent freshwater head as the principal dependent variable



EXPLANATION

h_f	Equivalent freshwater head [L]
h	Head [L]
P_N	Pressure [$ML^{-1}T^{-2}$]
ρ_f	Density of freshwater [ML^{-3}]
ρ	Density of saline aquifer water [ML^{-3}]
g	Acceleration due to gravity [LT^{-2}]
Z_N	Elevation [L]

“Two points having equal pressures and the same elevation but different water densities, different values of h will be recorded”

$$\frac{\partial}{\partial \alpha}\left(\rho K_{f\alpha}\left[\frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right]\right) + \frac{\partial}{\partial \beta}\left(\rho K_{f\beta}\left[\frac{\partial h_f}{\partial \beta} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \beta}\right]\right) + \frac{\partial}{\partial \gamma}\left(\rho K_{f\gamma}\left[\frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right]\right) = \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} - \bar{\rho} q_s.$$

A new partial differential equation is also needed to describe solute transport in the aquifer

$$\rho = \rho_f + EC$$

$$\frac{\partial \rho}{\partial C} = E$$

fluid density is assumed to be solely a function of the concentration of dissolved constituents and they are related by the equation of state

Sounds simple but at some point we have to deal with this:

$$\hat{\rho}_{i+1/2,j,k}\frac{K_{\alpha,i+1/2,j,k}}{\Delta\alpha_{i+1/2,j,k}}A_{j,k}\left[h_{f,i+1,j,k}-h_{f,i,j,k}+\frac{\rho_{i+1/2,j,k}-\rho_f}{\rho_f}(Z_{i+1,j,k}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i-1/2,j,k}\frac{K_{\alpha,i-1/2,j,k}}{\Delta\alpha_{i-1/2,j,k}}A_{j,k}\left[h_{f,i,j,k}-h_{f,i-1,j,k}+\frac{\rho_{i-1/2,j,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i-1,j,k})\right]$$

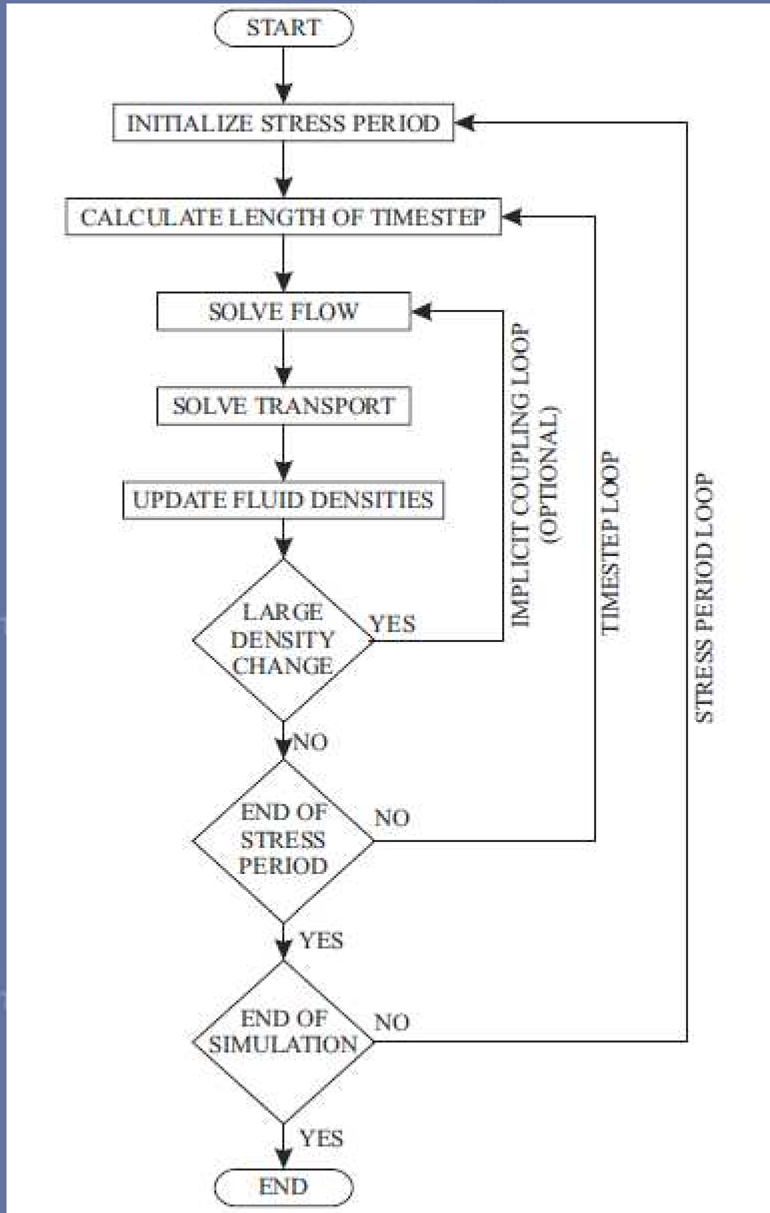
$$+\hat{\rho}_{i,j+1/2,k}\frac{K_{\beta,i,j+1/2,k}}{\Delta\beta_{i,j+1/2,k}}A_{i,k}\left[h_{f,i,j+1,k}-h_{f,i,j,k}+\frac{\rho_{i,j+1/2,k}-\rho_f}{\rho_f}(Z_{i,j+1,k}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i,j-1/2,k}\frac{K_{\beta,i,j-1/2,k}}{\Delta\beta_{i,j-1/2,k}}A_{i,k}\left[h_{f,i,j,k}-h_{f,i,j-1,k}+\frac{\rho_{i,j-1/2,k}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j-1,k})\right]$$

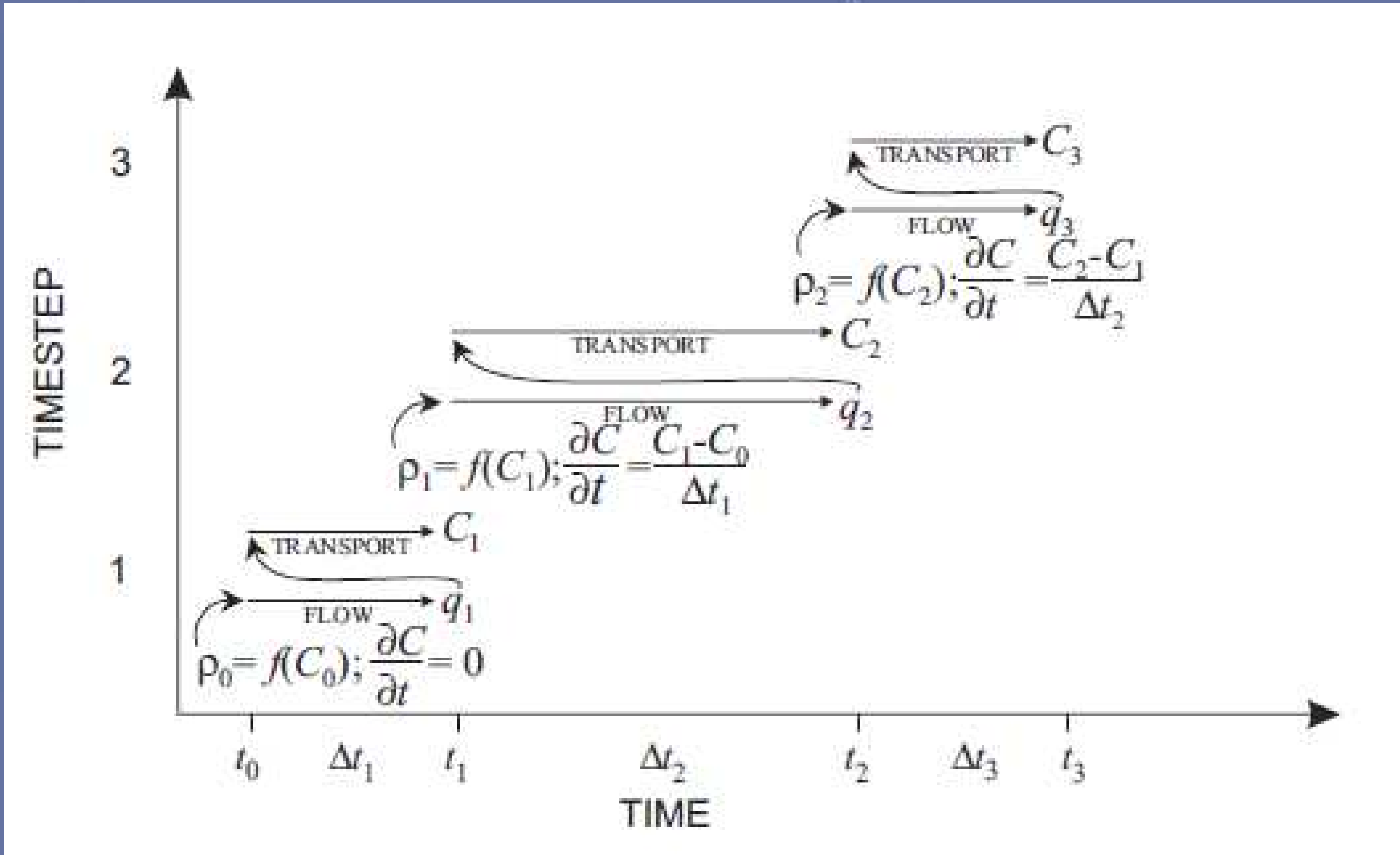
$$+\hat{\rho}_{i,j,k+1/2}\frac{K_{\gamma,i,j,k+1/2}}{\Delta\gamma_{i,j,k+1/2}}A_{i,j}\left[h_{f,i,j,k+1}-h_{f,i,j,k}+\frac{\rho_{i,j,k+1/2}-\rho_f}{\rho_f}(Z_{i,j,k+1}-Z_{i,j,k})\right]$$

$$-\hat{\rho}_{i,j,k-1/2}\frac{K_{\gamma,i,j,k-1/2}}{\Delta\gamma_{i,j,k-1/2}}A_{i,j}\left[h_{f,i,j,k}-h_{f,i,j,k-1}+\frac{\rho_{i,j,k-1/2}-\rho_f}{\rho_f}(Z_{i,j,k}-Z_{i,j,k-1})\right]$$

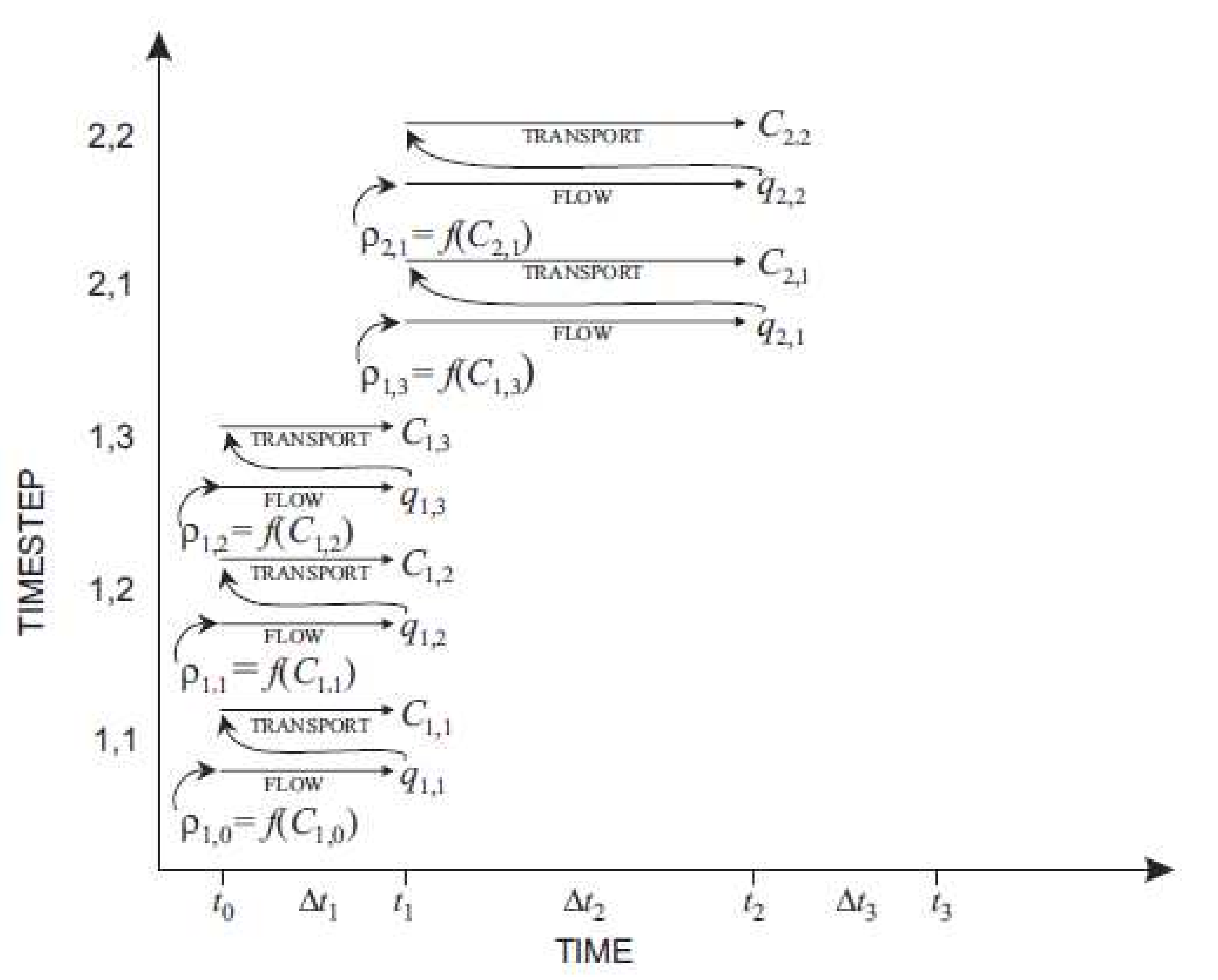
$$=\left(\rho_{i,j,k}S_{f,i,j,k}\frac{h^{n+1}_{f,i,j,k}-h^{n}_{f,i,j,k}}{t_{n+1}-t_n}+\theta E\frac{\partial C}{\partial t}\right)V_{i,j,k}-(\bar{\rho}Q_s)_{i,j,k},$$


START
INITIALIZE STRESS PERIOD
CALCULATE LENGTH OF TIMESTEP
SOLVE FLOW
SOLVE TRANSPORT
UPDATE FLUID DENSITIES
LARGE DENSITY CHANGE
YES
NO
END OF STRESS PERIOD
NO
YES
END OF SIMULATION
NO
YES
END
IMPLICIT COUPLING LOOP (OPTIONAL)
TIMESTEP LOOP
STRESS PERIOD LOOP

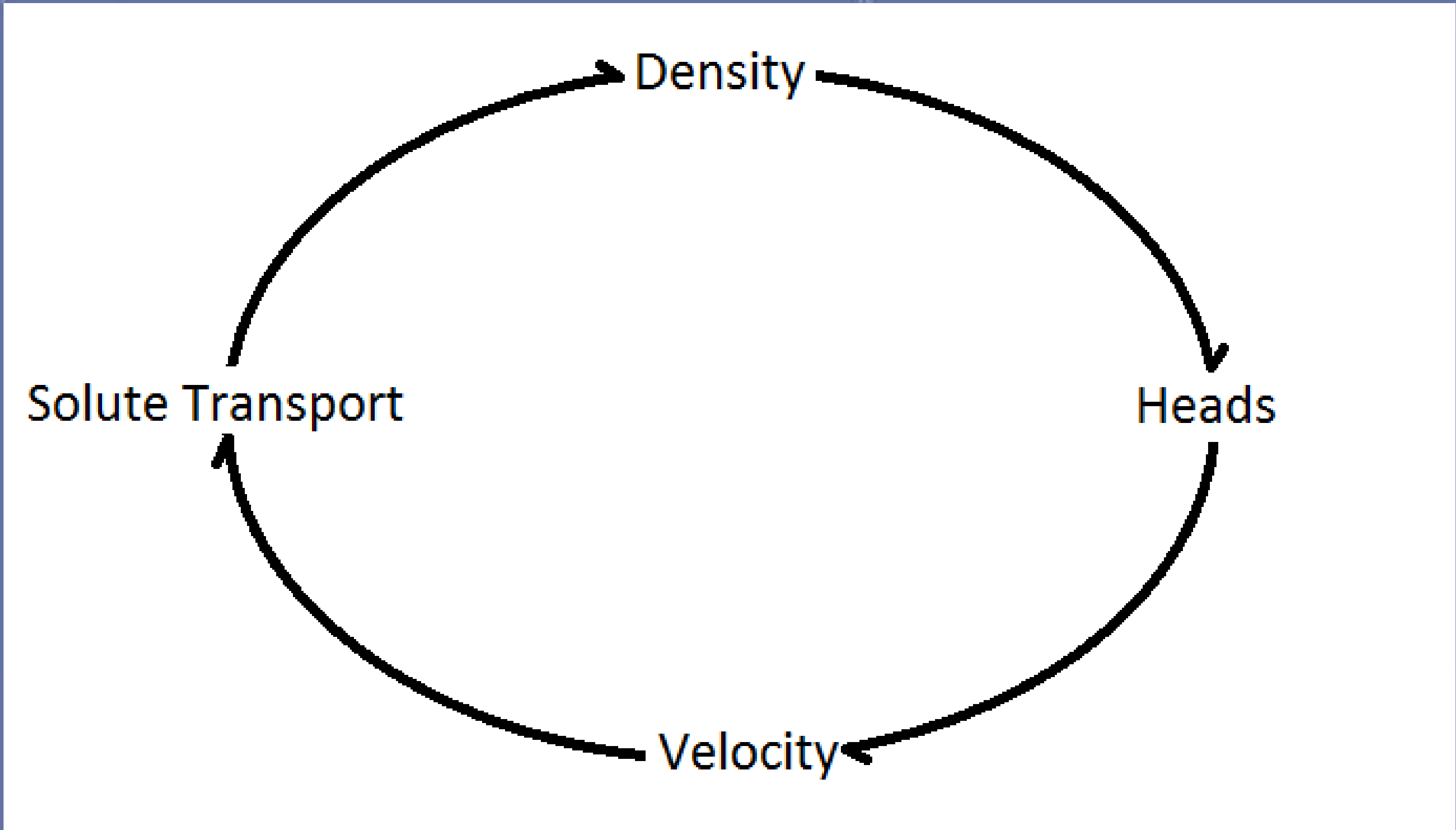
Explicit Coupling



Implicit Coupling



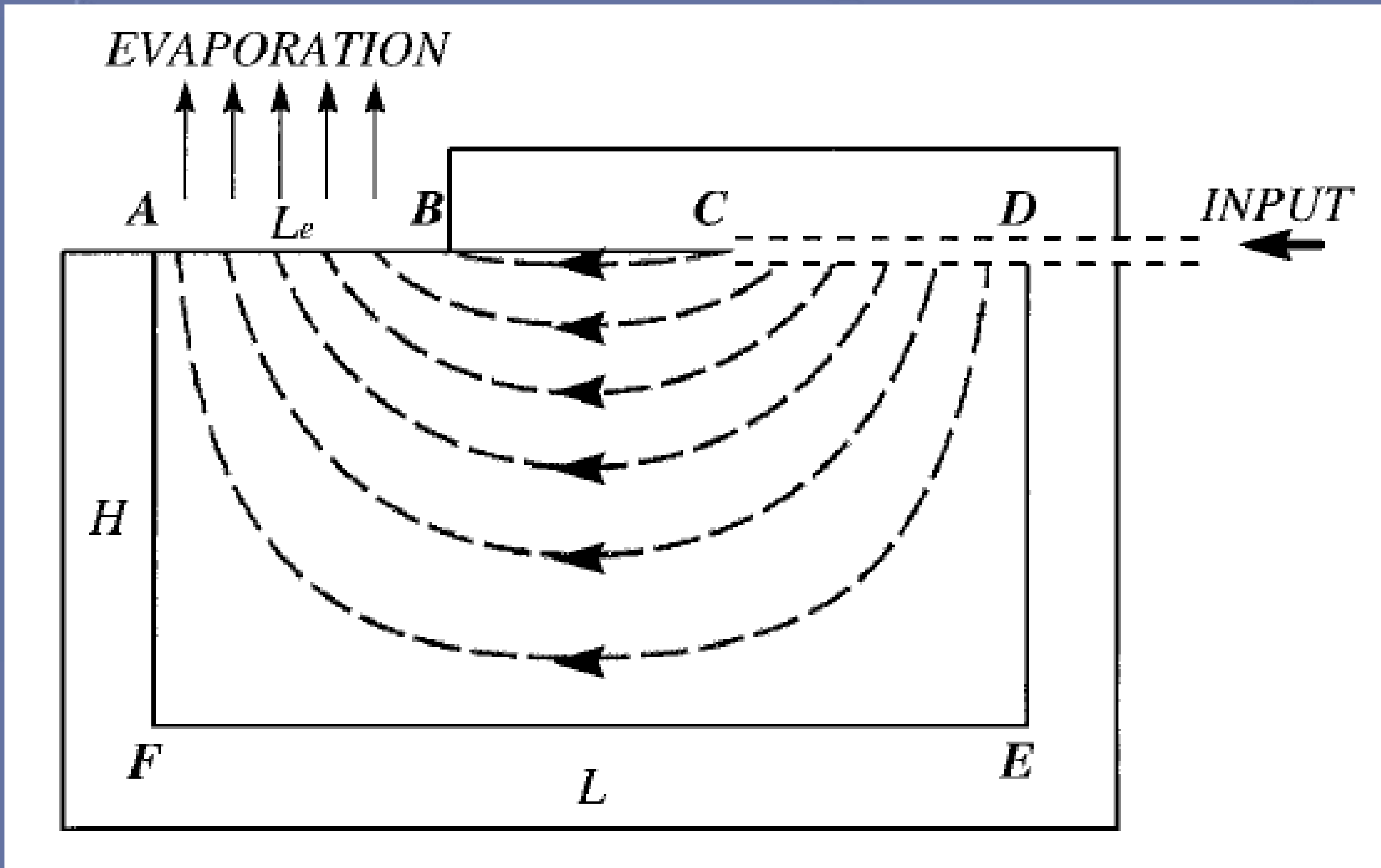
Why coupling flow and transport?



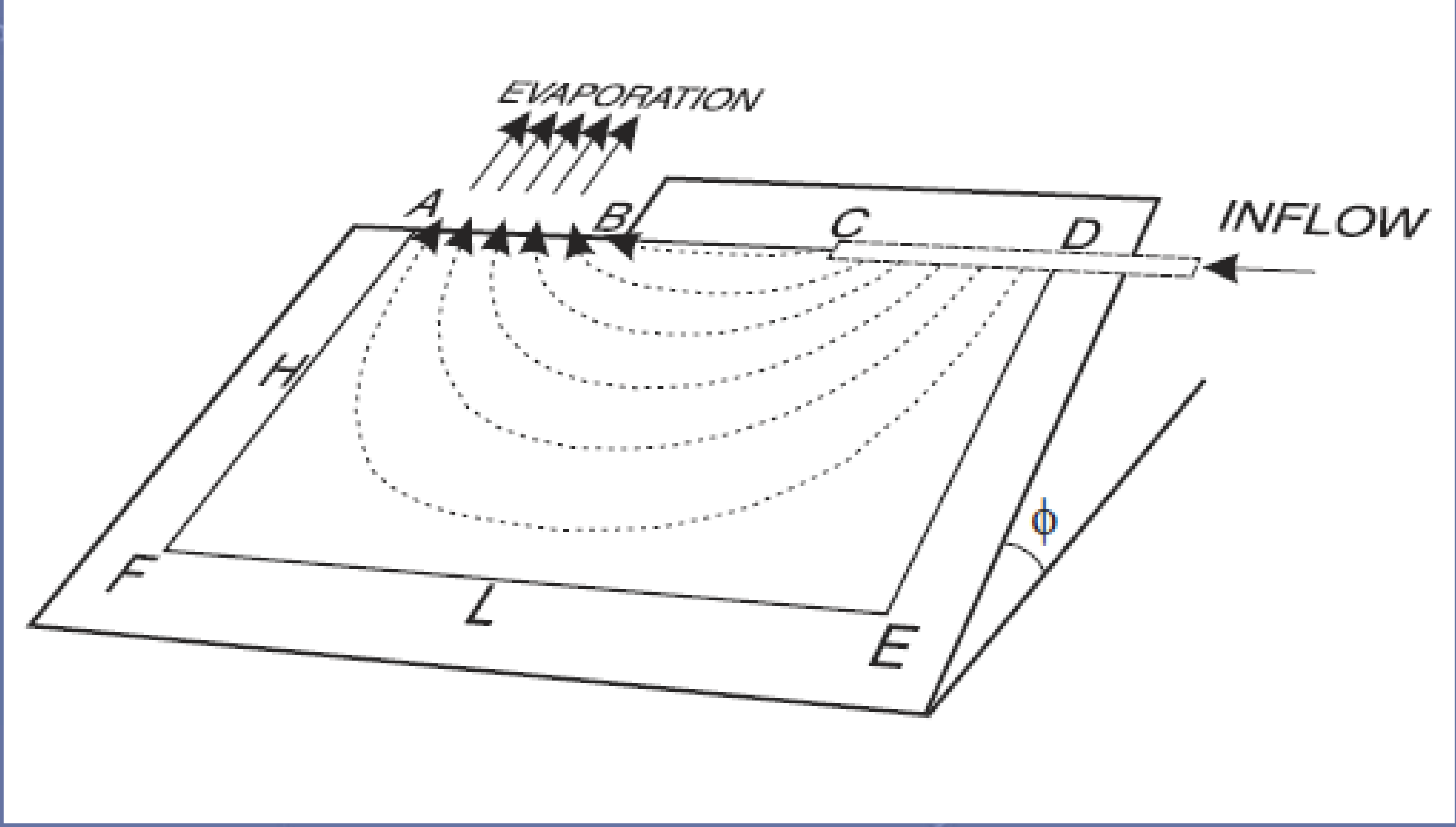
Uses:

- Saltwater Intrusion
- Aquifer Storage and Recovery (ASR)
- Brine Disposal

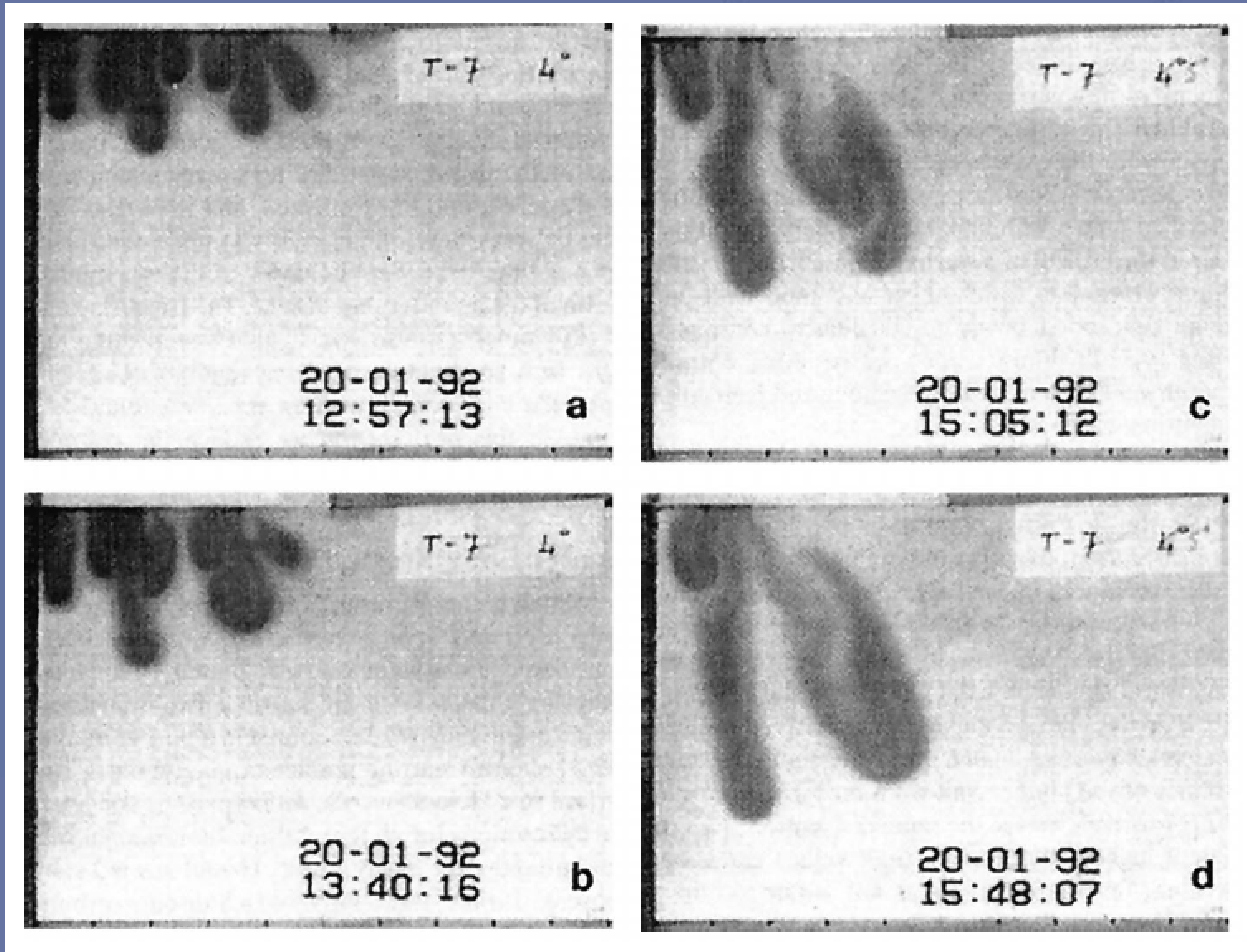
The Hele-Shaw Cell Experiment

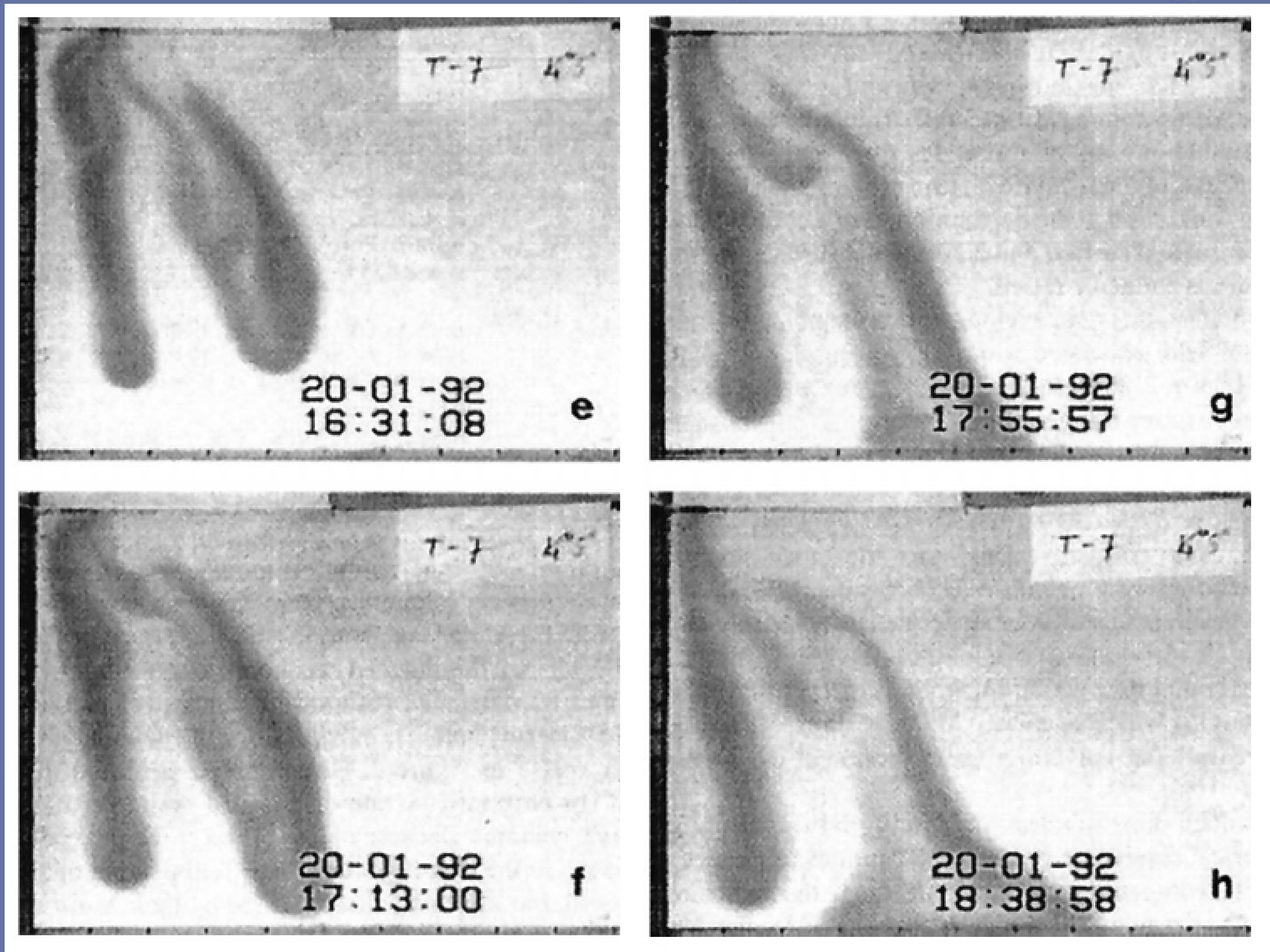


The Hele-Shaw cells experiment

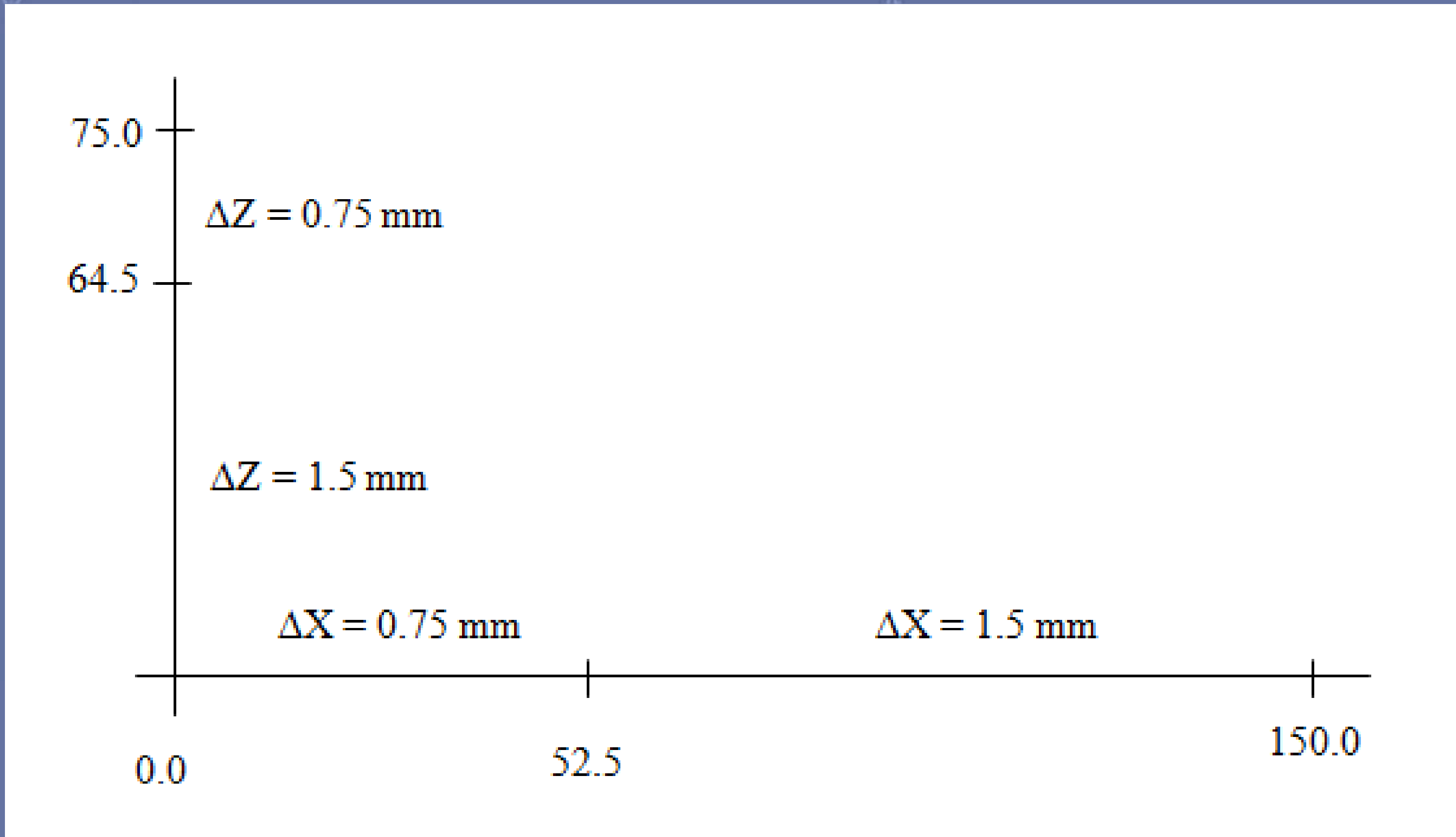


Experiment height	H	75 mm
Experiment length	L	150 mm
Evaporation length	L_e	50 mm
Plate spacing	b_{gap}	0.2 mm
Equivalent freshwater hydraulic conductivity	$K_f = \frac{b_{gap}^2 \rho_f g \cdot \sin\phi}{12\mu}$	3.05 mm/s
Porosity	θ	1
Inflow fluid density	ρ_{in}	1.0646 g/cm^3
Saturated fluid density	ρ_{sat}	1.0814 g/cm^3
Diffusion coefficient	D_m	9×10^{-4} mm/s
Cell angle to the horizontal	ϕ	5 degrees
Initial evaporation rate		1.03×10^{-3} mm/s
Recharge rate		1.03×10^{-3} mm/s
Inflow fluid concentration	C_{in}	84 g/L
Saturated fluid concentration	C_{sat}	110 g/L
Fluid dynamic viscosity	m	1.1×10^{-3} kg/m·s
Density change per concentration change	$\delta\rho/\delta C$ or *DENSESLP**	0.646
Water compressibility	β_w	4.5×10^{-10} kPa^{-1}
Equivalent freshwater specific storage	$S_f = \rho_f g \theta \beta_w \sin\phi$	3.8×10^{-10} mm^{-1}
Longitudinal dispersivity	α_L	9×10^{-7} mm
Transverse dispersivity	α_T	9×10^{-7} mm
Acceleration due to gravity	$g \sin \phi$	855 mm/s^2

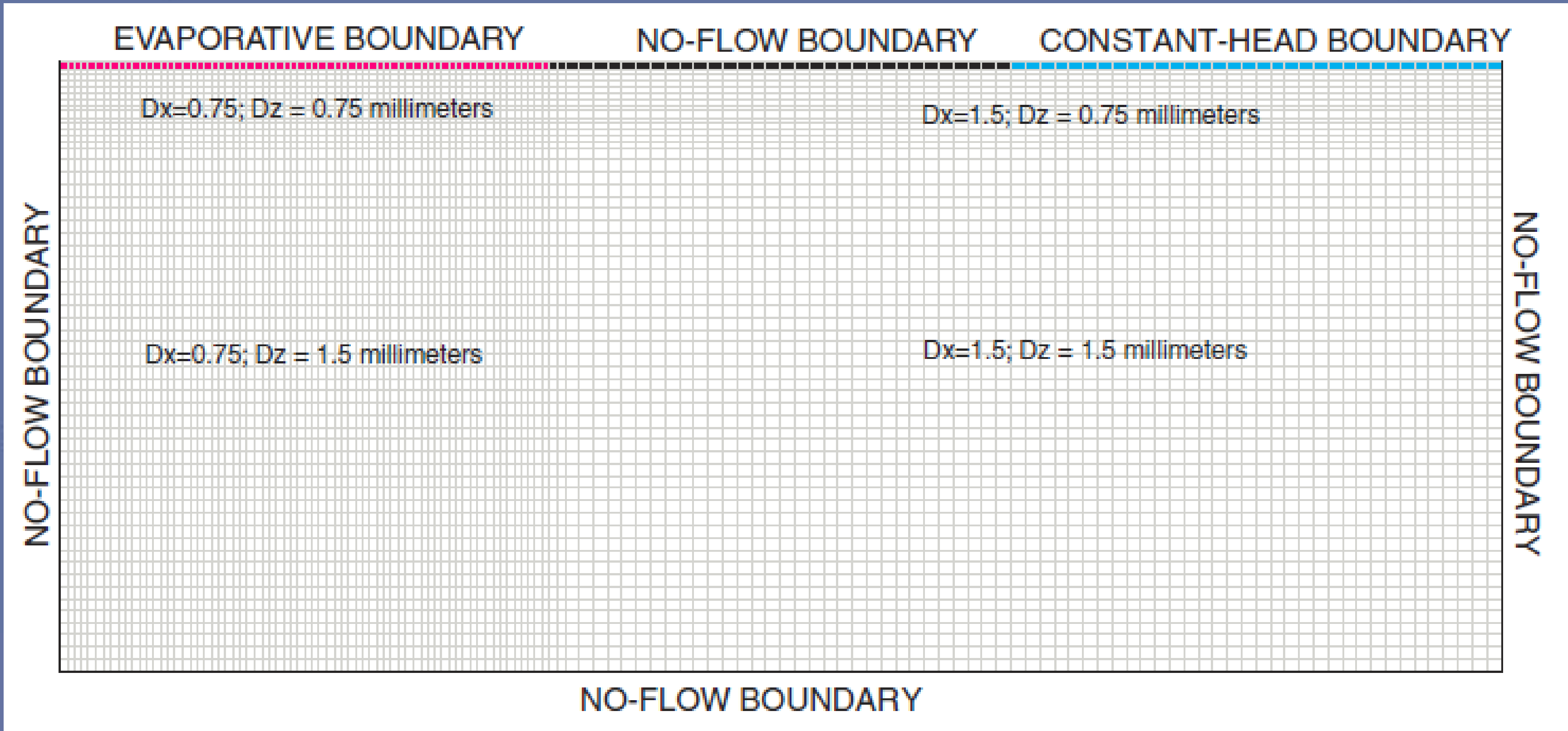

T-7 4°
20-01-92
12:57:13
a
T-7 4°5'
20-01-92
15:05:12
c
T-7 4°
20-01-92
13:40:16
b
T-7 4°5'
20-01-92
15:48:07
d


T-7
20-01-92
16:31:08
e
T-7
20-01-92
17:55:57
g
T-7
20-01-92
17:13:00
f
T-7
20-01-92
18:38:58
h

The SEAWAT Numerical Model



The SEAWAT numerical model



Changes to the original code

Modify the relationship between solute concentration and fluid density in the equation of state

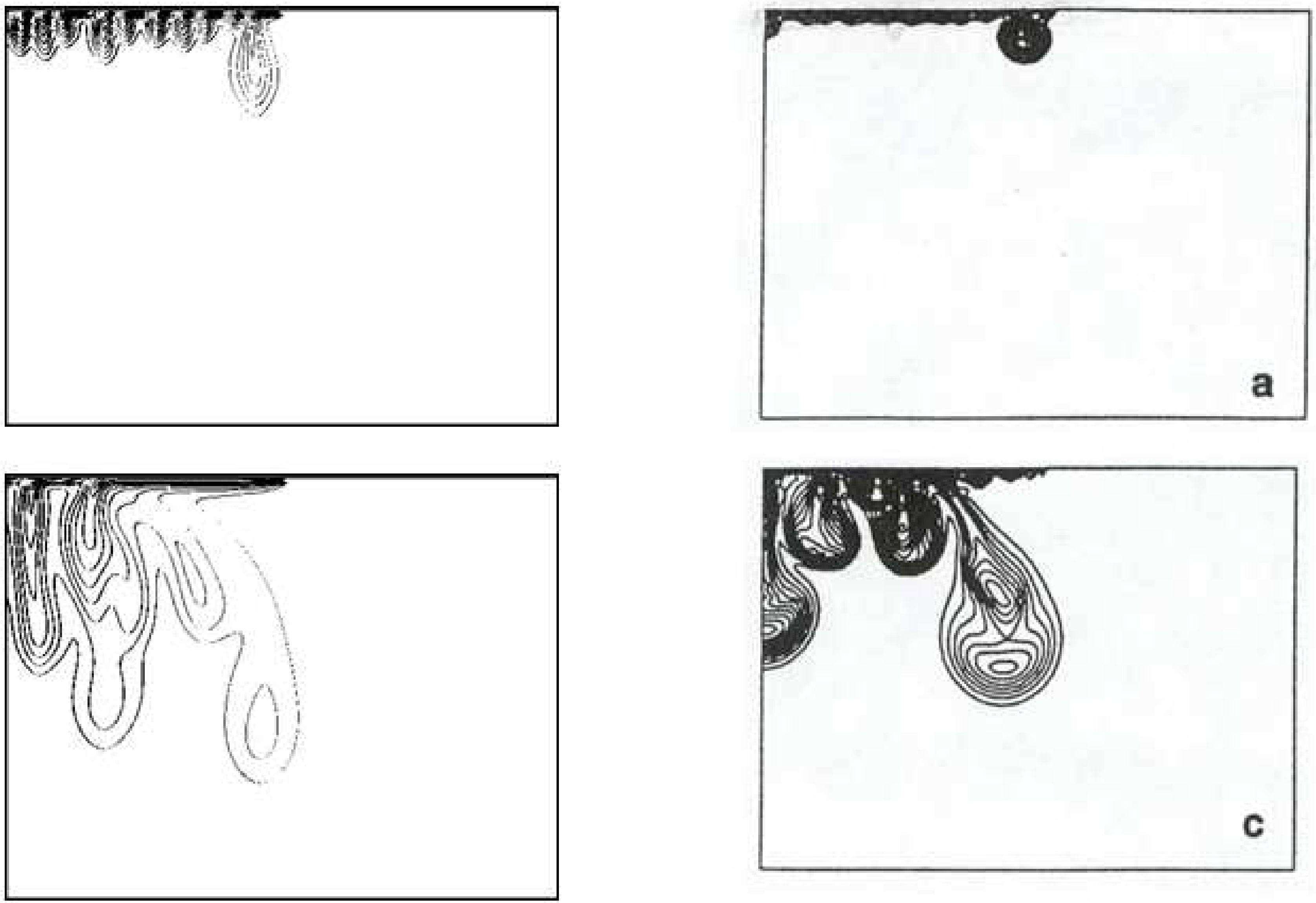
- $\rho = \rho_f + 0.714\ C$ *(Saltwater)*
- $\rho = \rho_f + 0.646\ C$ *(K_2SO_4)*

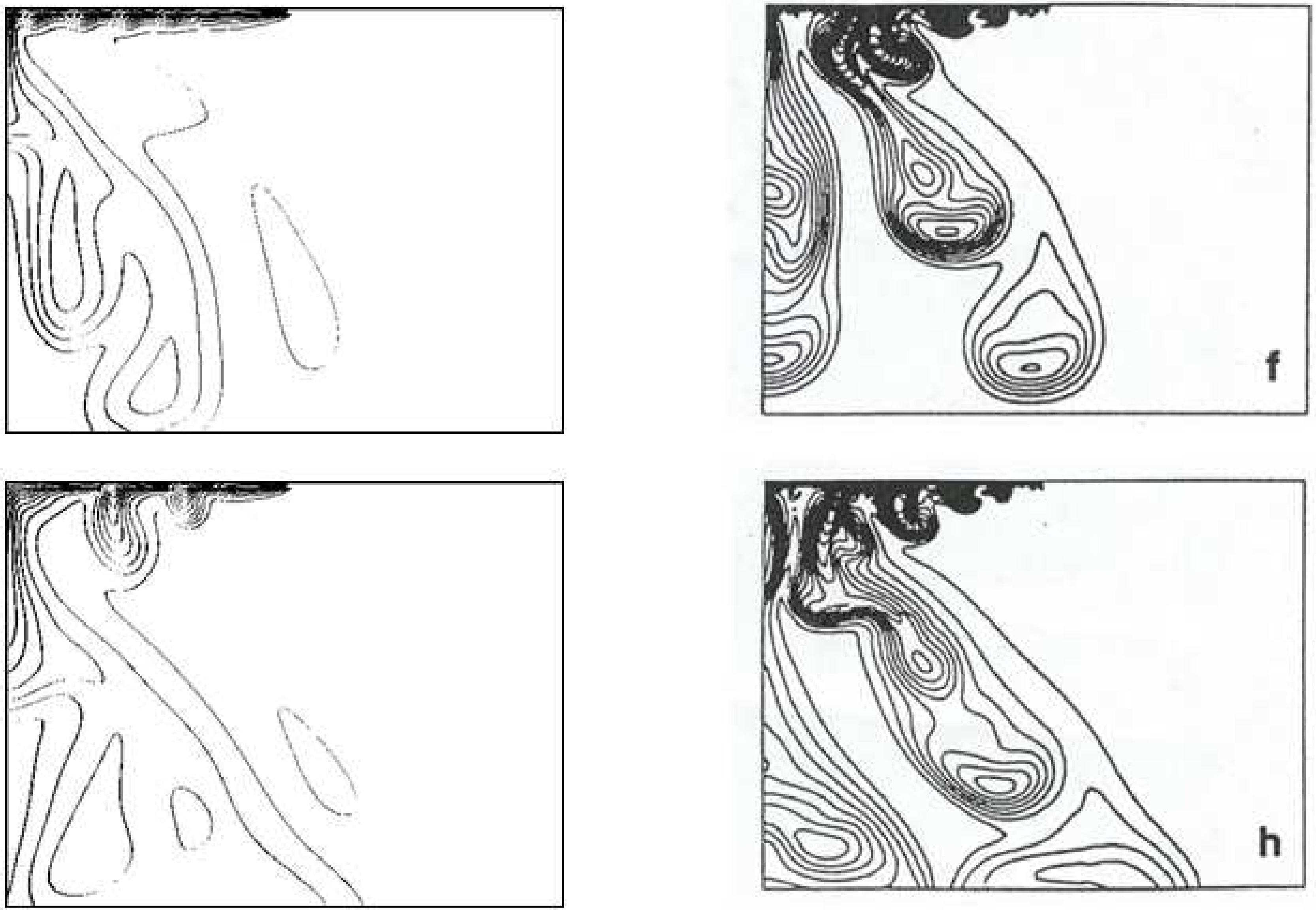
SEAWAT.FOR

```
        FUNCTION CALCDENS(CONCENTRATION)
C***********************************************************************
C   THIS FUNCTION CALCULATES FLUID DENSITY AS A FUNCTION OF CONCENTRATION
C***********************************************************************
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /DENSITY/PF, CONVERSION
      CALCDENS=PF+CONVERSION*CONCENTRATION
C--SEAWAT: THE FOLLOWING TWO LINES IMPLEMENT EQUATION OF STATE FOR
C--SEAWAT: THE HYDROCOIN TEST PROBLEM
C       RC=1./280.*CONCENTRATION
C       CALCDENS=(RC/1200.+(1-RC)/1000.)**-1
      RETURN
      END
```

A random subroutine that applies a “noise” to the concentration boundary that represents the salt lake. The perturbation of 0.5 % of the total salinity difference is necessary to create an instability that triggers

$$C(t) = C_{sat} + \frac{1}{100}(C_{sat} - C_{in}) \cdot (rand(0) - 0.5)$$


a
c


f
h

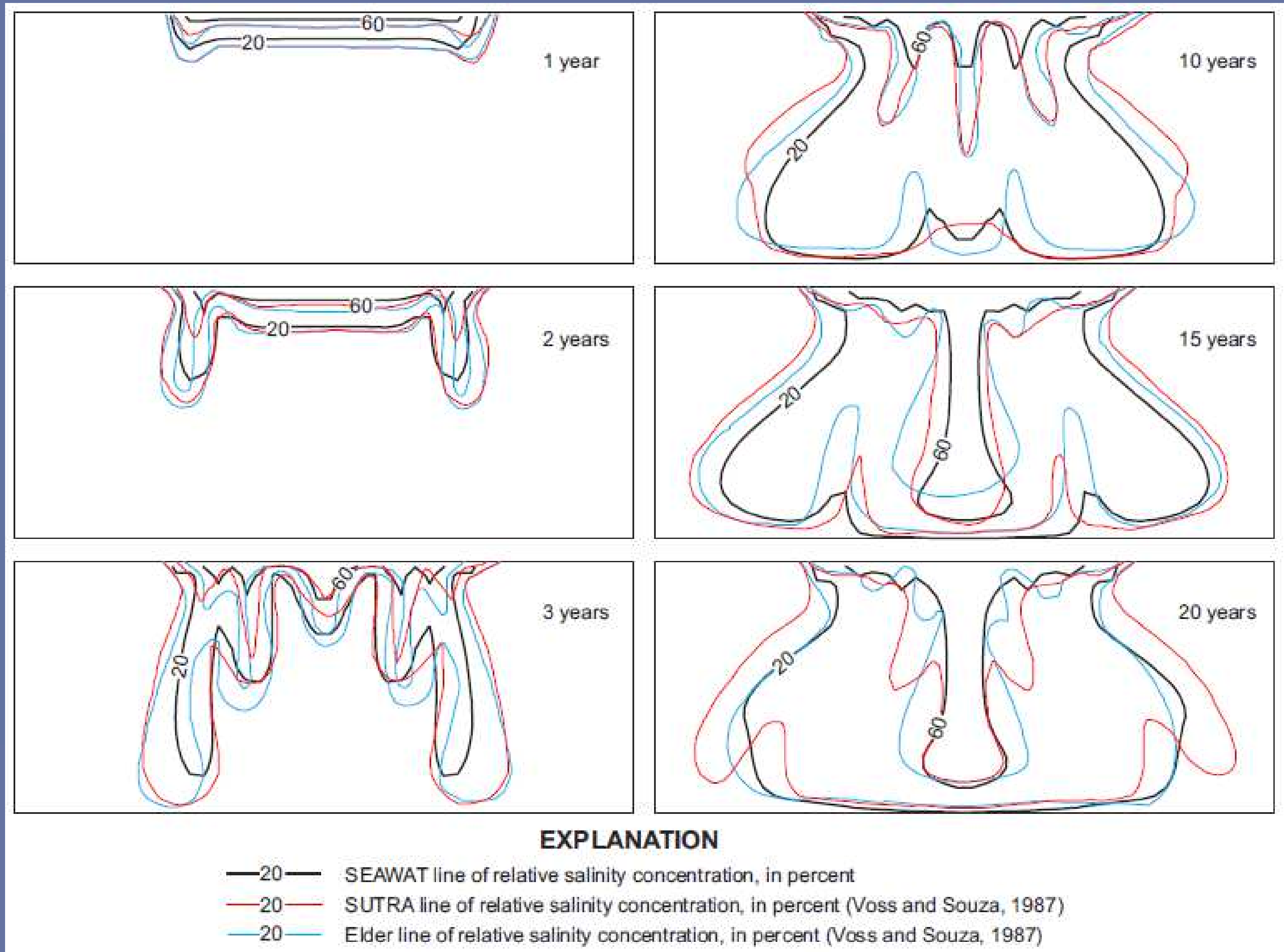
Time = 60

Simmons proposal of a new Benchmark test has been successful since it has been implemented by the USGS

Though more complete than the existing benchmark tests it does not replace them but complement them

Always keep in mind that it is a “qualitative” test and we are comparing flow patterns and not concentrations

The Elder problem



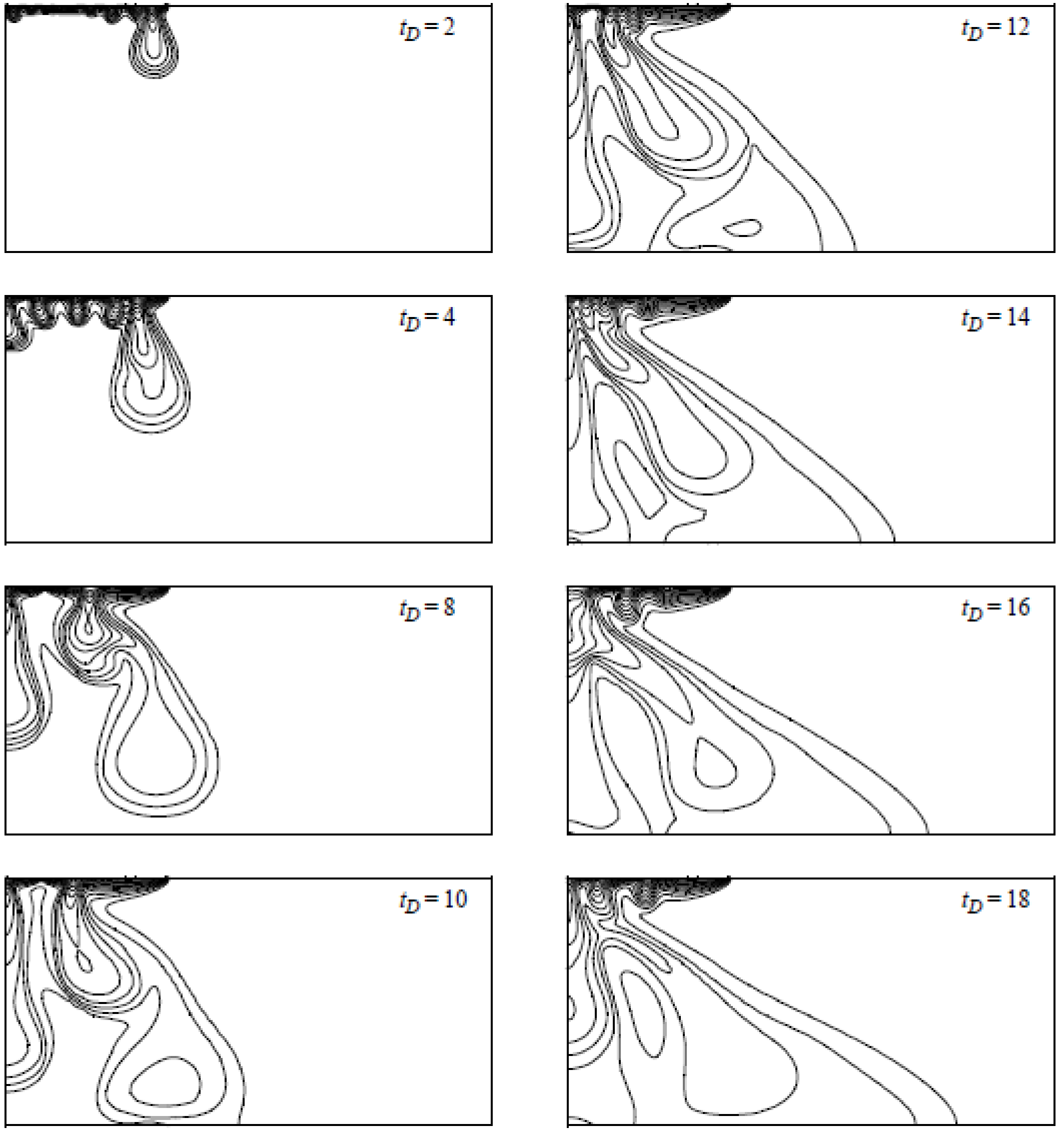


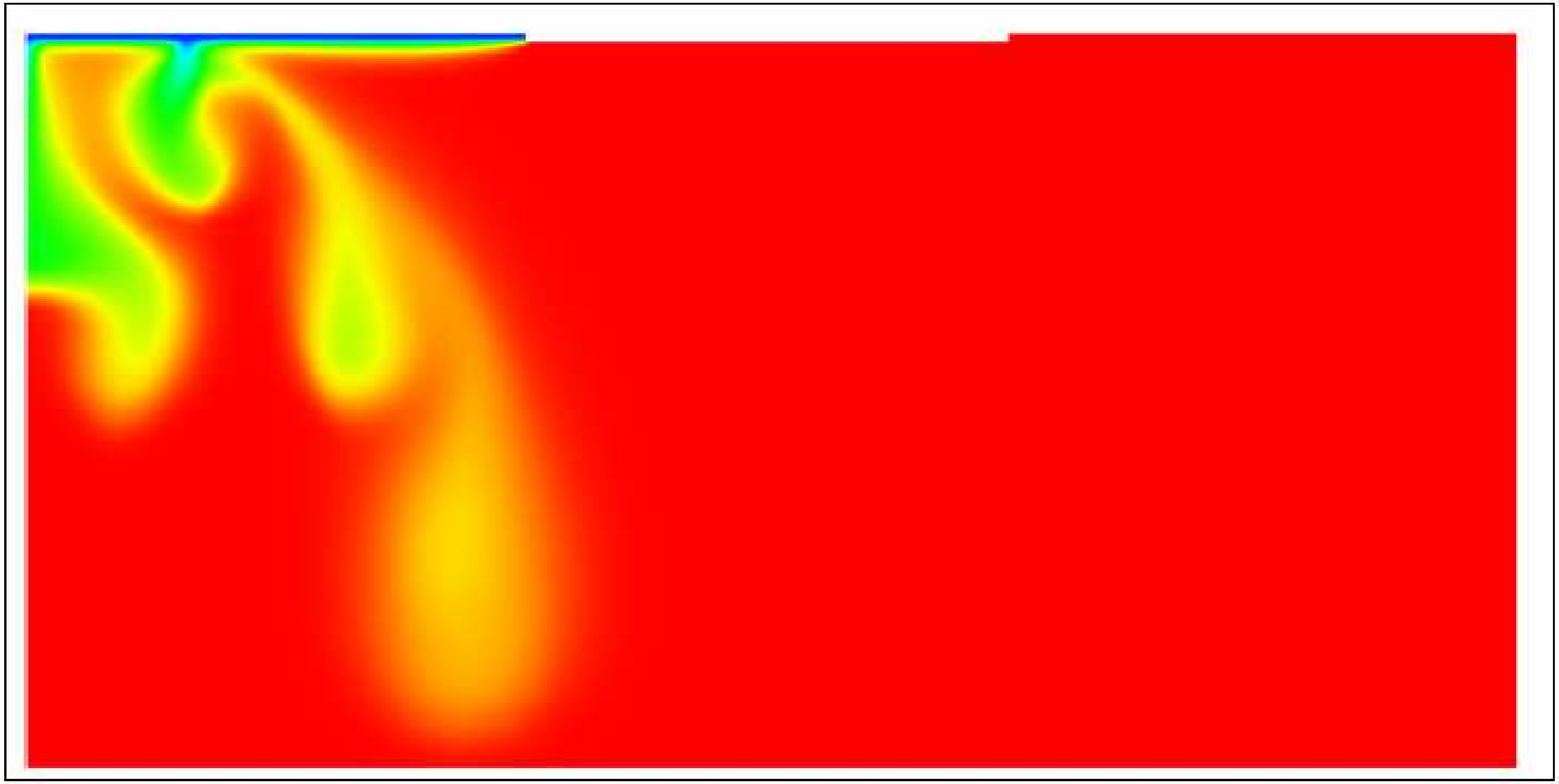
Figure 1.26 Salinities for different dimensionless times t_D. One unit in dimensionless times is equivalent to 21.4 minutes real time. Contour interval is $2 \cdot 10^{-3}$. FEFLOW simulations on a coarse mesh (4733 quadrilateral elements), full upwinding and AB/TR time stepping. Total number of adaptive times steps is 290.

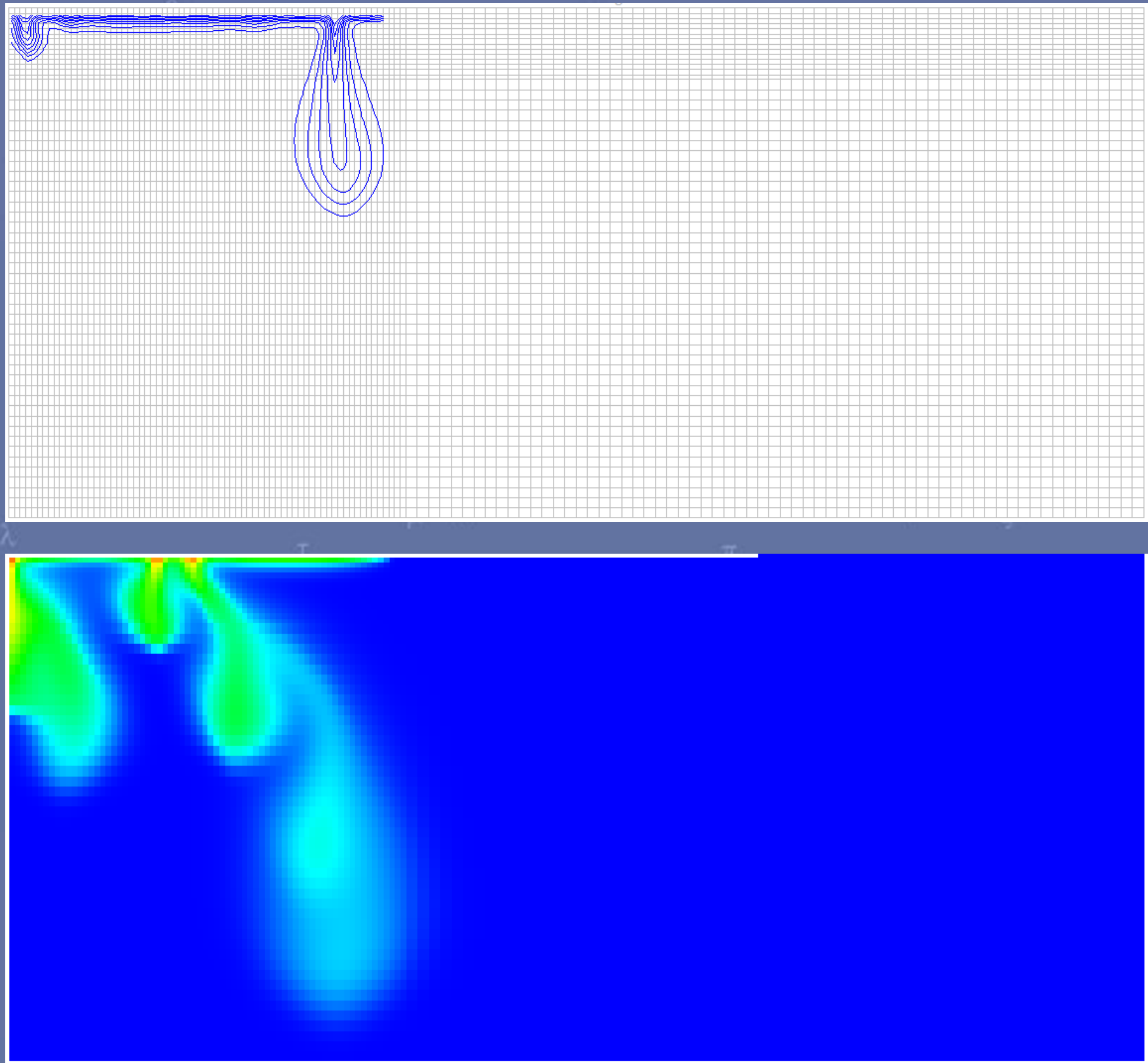
exist. The Elder problem thus appears rather simple, compared to the salt lake problem. As the numerical requirements for the Elder problem were already quite expensive, the salt lake problem indeed appears to be a challenge for numerical modelers. Fortunately, (in contrast to many prior benchmarks) experimental results are available here. The main difficulty can be expected in the extremely dynamic behavior of the convection process, where physical perturbations caused by laboratory-scale heterogeneities that trigger instabilities must be mimicked in a numerical simulation. Taking that into account we tend to conclude that the salt lake problem is at the moment essentially unsolved.

GMS 8.2 Tutorial

SEAWAT – Hele-Shaw Experiment

Simulate the Hele-Shaw Salt Lake experiment using SEAWAT in GMS





Acknowledgments

Weixing Guo

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