Mathematical Modeling Lecture 8

Osmotic water transport and cell volume

Lecture notes

An impermeant amount determines concentration through volume, and concentration determines water flow. This feedback produces a nonlinear volume equation. We derive its equilibrium, timescale, implicit solution, and numerical restrictions while separating osmotic equilibration from active cell-volume regulation.

1 Amount, volume, and particle concentration

Slides for this section

Let n be the fixed amount of impermeant solute inside a membrane-bounded compartment and let $V(t) > 0$ be its water volume. The inside particle concentration is

$$c_{\text{in}}(t) = \frac{n}{V(t)}.$$

Solute amount is conserved; concentration need not be. In the companion, n is measured in femtomoles and V in picoliters. The unit conversion is

$$\frac{1\,\text{fmol}}{1\,\text{pL}} = \frac{10^{-15}\,\text{mol}}{10^{-12}\,\text{L}} = 10^{-3}\,\text{mol/L} = 1\,\text{mM}.$$

Concentration here counts independently moving osmotic particles. A concentration of a dissolved compound is not automatically the concentration of its particles after dissociation. The simple model contains one impermeant solute, a well-mixed interior, and a large exterior reservoir whose concentration c_{out} stays fixed. No solute exchange, active pump, or membrane deformation law is included.

2 Osmotic pressure and a water-flow law

Slides for this section

For an ideal dilute solution, osmotic pressure is $\Pi = \mathcal{R}Tc$ when c is molar particle concentration in units consistent with the gas constant $\mathcal{R}$. With inward volume flow positive, a linear membrane law is

$$J_{\text{in}} = L_p A_m \left[(\Pi_{\text{in}} - \Pi_{\text{out}}) - (P_{\text{in}} - P_{\text{out}})\right].$$

Here L_p is a hydraulic permeability and A_m is membrane area. A greater internal osmotic pressure draws water in; a greater internal hydrostatic pressure opposes entry. This sign convention follows the direction of water flow, not solute flow.

Assume equal hydrostatic pressures and a constant effective coefficient. Absorb membrane geometry, temperature, and unit conversions into L to obtain

$$J_{\text{in}} = L(c_{\text{in}} - c_{\text{out}}), \qquad [L] = \text{pL}/(\text{s}\,\text{mM}).$$

Conservation of water volume then closes the model:

$$\boxed{\dot{V} = L\left(\frac{n}{V} - c_{\text{out}}\right).}$$

The companion uses $L = 0.002\,\text{pL}/(\text{s}\,\text{mM})$. Constant L is an effective modeling assumption even while volume changes; the computation does not update permeability from a changing spherical area.

3 Equilibrium, direction of motion, and stability

Slides for this section

For $L > 0$, $n > 0$, and $c_{\text{out}} > 0$, the unique equilibrium is

$$V_* = \frac{n}{c_{\text{out}}}.$$

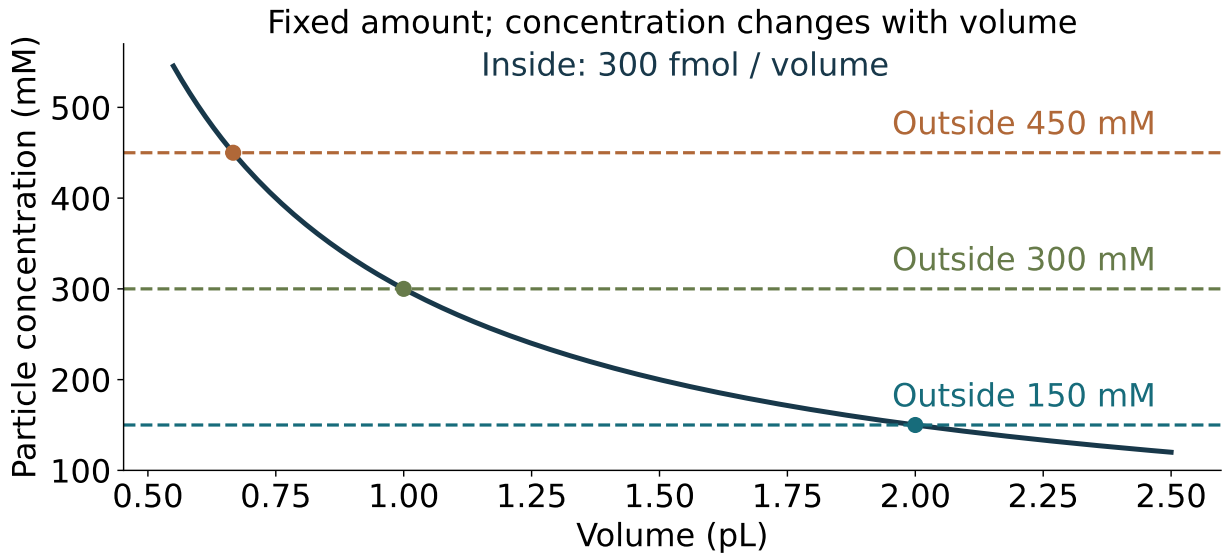
If $V < V_*$, the interior is more concentrated and $\dot{V} > 0$. If $V > V_*$, $\dot{V} < 0$. Thus trajectories move toward V_* and cannot cross it in finite time under the exact autonomous ODE: crossing would contradict uniqueness at the positive equilibrium.

With $n = 300\,\text{fmol}$ and $V_0 = 1\,\text{pL}$, the initial concentration is 300 mM. Exterior concentrations of 150, 300, and 450 mM give equilibria 2, 1, and 2/3 pL, respectively. The first case swells, the second stays constant, and the third shrinks. These calculations do not assess viability or membrane rupture.

Let $V = V_* + \eta$ with small η. Taylor expansion gives

$$\dot{\eta} = -\frac{Ln}{V_*^2}\eta + O(\eta^2), \qquad \tau = \frac{V_*^2}{Ln} = \frac{n}{Lc_{\text{out}}^2}.$$

This is the local relaxation timescale. At the three exterior concentrations, τ is about 6.667, 1.667, and 0.741 seconds. The exact nonlinear solution is not generally a single exponential away from equilibrium.



For 300 fmol of impermeant solute, c_in = 300/V. Fixed external concentrations 150, 300 and 450 mM intersect at volumes 2, 1 and 2/3 pL under equal hydrostatic pressures.

4 Dimensionless dynamics and an implicit exact solution

Slides for this section

Set $v = V/V_*$ and $\theta = t/\tau$, with the positive quantities defined above. Then

$$\frac{\mathrm{d}v}{\mathrm{d}\theta} = \frac{1}{v} - 1 = \frac{1-v}{v}.$$

All constant-parameter cases share this dimensionless equation. For a nonequilibrium initial value $v_0 > 0$, separate variables on its side of $v = 1$:

$$\theta = \int_{v_0}^{v} \frac{z}{1-z}\,\mathrm{d}z = v_0 - v + \log\left|\frac{1-v_0}{1-v}\right|.$$

The logarithm diverges as $v \to 1$, expressing asymptotic approach. If $v_0 = 1$, use the constant solution instead; inserting it in the logarithmic expression would create an undefined ratio. This relation provides a reference for checking a numerical solution without introducing a second time-stepping method.

A useful dissipation function is

$$\Phi(v) = v - 1 - \log v \geq 0 \quad (v > 0).$$

Its derivative is

$$\frac{\mathrm{d}\Phi}{\mathrm{d}\theta} = \left(1 - \frac{1}{v}\right)\left(\frac{1}{v} - 1\right) = -\left(1 - \frac{1}{v}\right)^2 \leq 0.$$

Thus the dynamics decrease a nonnegative function whose unique minimum is equilibrium. This mathematical stability statement depends on the stated fixed-reservoir model.

5 A volume update and its concentration consequence

Slides for this section

Explicit Euler holds the starting flow fixed over a time interval h:

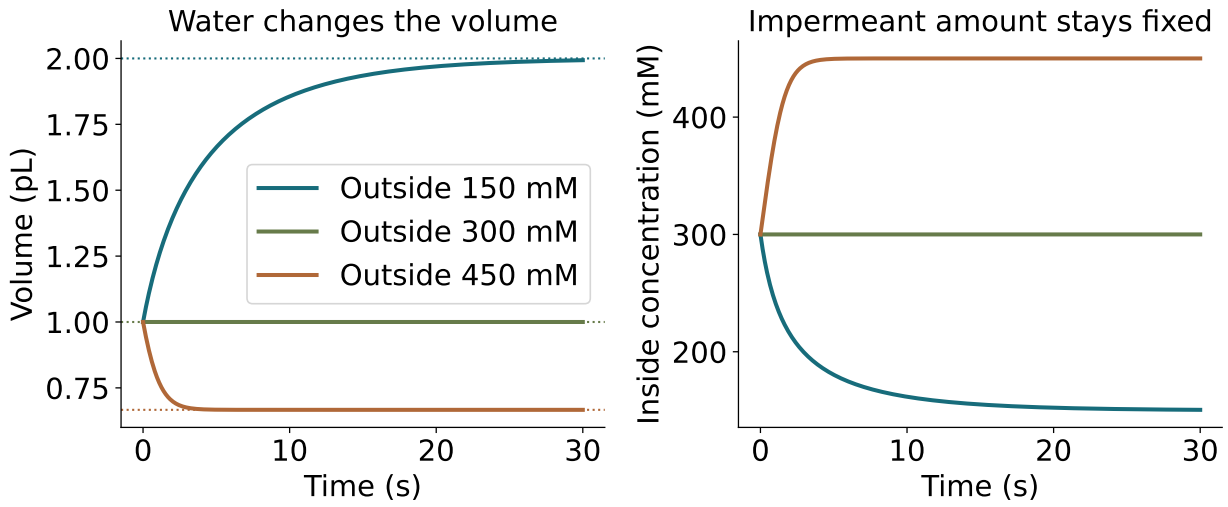
$$V_{n+1} = V_n + hL(n/V_n - c_{\mathrm{out}}), \qquad c_{n+1} = n/V_{n+1}.$$

For $V_n = 1\,\mathrm{pL}$, $n = 300\,\mathrm{fmol}$, and $c_{\mathrm{out}} = 150\,\mathrm{mM}$, the initial inflow is $0.002(300 - 150) = 0.3\,\mathrm{pL/s}$. A 0.2-second step gives $V_{n+1} = 1.06\,\mathrm{pL}$ and $c_{n+1} = 300/1.06 \simeq 283.019\,\mathrm{mM}$. It would be inconsistent to retain the old concentration after changing volume.

For shrinking states with $n/V_n < c_{\mathrm{out}}$, positivity requires

$$h < \frac{V_n}{L(c_{\mathrm{out}} - n/V_n)}.$$

Near equilibrium, Euler has perturbation multiplier $1 - h/\tau$; $0 < h/\tau < 2$ gives local linear stability, while $h/\tau \leq 1$ avoids local alternating overshoots. These are distinct from global accuracy. A step can produce a nonphysical overshoot even though the exact ODE is monotone. The supplied trajectories use $h = 0.05$ seconds and reject inadmissible volumes; they do not silently clip them.



Synthetic explicit-Euler trajectories at step 0.05 s and L = 0.002 pL/(s mM). All start at 1 pL with 300 fmol trapped solute. Dotted lines show volume equilibria; survival and rupture are not modeled.

6 Limiting cases and extension to volume regulation

Slides for this section

If $L = 0$, no water moves and $V(t) = V_0$. If $c_{\text{out}} = 0$ with $L, n > 0$, there is no finite equilibrium. The equation becomes $V\dot{V} = Ln$, giving

$$V(t) = \sqrt{V_0^2 + 2Lnt}.$$

This limiting solution is a useful independent numerical test. The model still does not predict a rupture threshold. Its unbounded growth simply records the absence of a balancing mechanism.

The source discussion of animal-cell volume regulation includes permeant ions and active transport. Our single-impermeant-solute experiment isolates the osmotic contribution and is not a reproduction of that full regulation model. Adding permeant species requires equations for their amounts as well as water volume; adding mechanical pressure requires a constitutive relation between pressure and geometry.

For the current companion, verify $n = c_{\text{in}}V$, the equilibrium case, the sign of motion, and convergence under smaller steps. Compare $V(t)$ and $c(t)$ as coupled observables. A constant product checks bookkeeping; the implicit exact relation checks the trajectory. Neither demonstrates that a real cell has the chosen permeability or fixed external environment.

Exercises

MM08-E1. Amount, concentration and one step

Use n = 240 fmol, V0 = 0.80 pL, c_out = 200 mM and L = 0.003 pL/(s mM).
a Compute initial inside concentration and inward-positive flow.

b Estimate V after 0.10 s with one explicit step; compute its concentration.

c Find equilibrium volume and explain what stays conserved during approach.

MM08-E2. Predict shrinking and separate timescale

Use n = 360 fmol, V0 = 1.20 pL, c_out = 450 mM and L = 0.002 pL/(s mM).
a Predict the initial direction and compute flow.

b Compute equilibrium volume. What changes if positive L doubles?

c What happens if L is instead exactly zero at the initial state?

MM08-E3. Check a conserved quantity

A simulated compartment has fixed trapped amount 300 fmol.
a Find inside concentration at volumes 0.75 pL and 1.50 pL.

b A log reports V = 1.50 pL and c_in = 250 mM. Is it consistent with the stated amount?

c Would constant total solute alone prove that a volume trajectory is accurate or biologically validated?

MM08-E4. Locate the model boundary

Consider using the demonstration to predict what happens to an actual cell in a changed external solution.
a Name two mechanisms missing from the water-only model and a quantity each could alter.

b Explain why the computed volume 2 pL does not establish that a cell survives.

c Propose an observation and a numerical check for testing a volume-response explanation.

References

Zan Ahmad, Fall 2024 HEART syllabus. PDF pages 1–2.

Hoppensteadt and Peskin, Modeling and Simulation in Medicine and the Life Sciences, second edition. Printed pages 109–115; PDF pages 122–128 in the supplied copy.