Mathematical Modeling Lecture 1

Conservation of volume

Zan Ahmad

Fall 2024

Compartment volume and boundary flux

$V(t)$ is stored volume. $Q_{\text{in}}(t)$ and $Q_{\text{out}}(t)$ are volume per time.

Compartment volume and boundary flux

$V(t)$ is stored volume. $Q_{\text{in}}(t)$ and $Q_{\text{out}}(t)$ are volume per time.

Question: determine $V(t)$ from $V(0)$ and the two inputs.

Pressure and particle identity are not yet state variables.

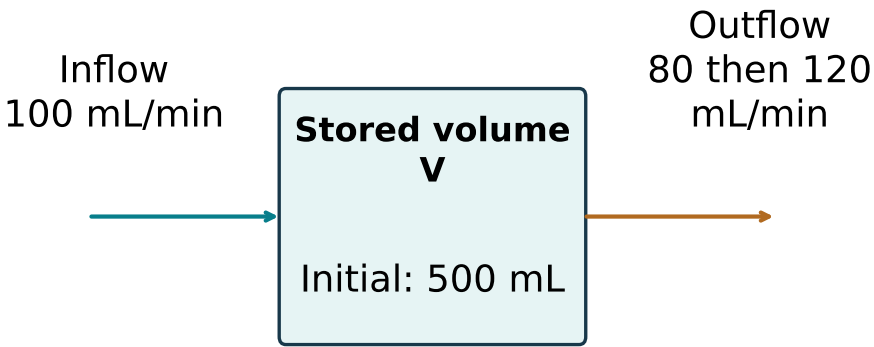
A closed route, several possible compartments

Right heart $\rightarrow$ lungs $\rightarrow$ left heart $\rightarrow$ systemic tissues $\rightarrow$ right heart.

A closed route, several possible compartments

Right heart $\rightarrow$ lungs $\rightarrow$ left heart $\rightarrow$ systemic tissues $\rightarrow$ right heart.
A compartment groups vessels by the question being asked; it is not an extra anatomical chamber. Artery and vein refer to direction relative to the heart.

The reservoir boundary



One bench reservoir; incompressible fluid

The reservoir boundary

Assume incompressible fluid and no unrecorded transfer. The arrows prescribe rates.

The reservoir boundary

Assume incompressible fluid and no unrecorded transfer. The arrows prescribe rates.

$$[V] = \mathrm{mL}, \qquad [Q] = \mathrm{mL/min}.$$

What additional relation would be needed to calculate the flows themselves?

Add small transferred amounts

On a short piece, $\Delta A_{\text{in}} \approx Q_{\text{in}}(t_k)\Delta t_k$.

Add small transferred amounts

On a short piece, $\Delta A_{\text{in}} \approx Q_{\text{in}}(t_k)\Delta t_k$.

$$A_{\text{in}}(t_0, t_1) = \lim \sum_k Q_{\text{in}}(t_k)\Delta t_k = \int_{t_0}^{t_1} Q_{\text{in}}(s)\, ds.$$

The integral adds volume, not flow.

Conservation before differentiation

$$\boxed{V(t_1) - V(t_0) = \int_{t_0}^{t_1} (Q_{\text{in}} - Q_{\text{out}})\, ds.}$$

Conservation before differentiation

$$\boxed{V(t_1) - V(t_0) = \int_{t_0}^{t_1} (Q_{\text{in}} - Q_{\text{out}})\, ds.}$$

$$V(t_0) = V_0$$

An initial value fixes which member of the solution family describes the experiment.

The local equation

$$\frac{V(t+h)-V(t)}{h} = \frac{1}{h}\int_t^{t+h} (Q_{\text{in}} - Q_{\text{out}})\, ds.$$

The local equation

$$\frac{V(t+h)-V(t)}{h} = \frac{1}{h}\int_t^{t+h} (Q_{\text{in}} - Q_{\text{out}})\, ds.$$

At a continuity point of the input, let $h \to 0$:

$$\boxed{\dot{V} = Q_{\text{in}} - Q_{\text{out}}.}$$

Unit conversion is part of the calculation

$$(100\ \text{mL/min})(30\ \text{s})\frac{1\ \text{min}}{60\ \text{s}} = 50\ \text{mL}.$$

Unit conversion is part of the calculation

$$(100\ \text{mL/min})(30\ \text{s})\frac{1\ \text{min}}{60\ \text{s}} = 50\ \text{mL}.$$

A volume divided by a flow has units of time, but its interpretation still depends on the flow law.

First constant-flow interval

$$V_0 = 500, \quad Q_{\text{in}} = 100, \quad Q_{\text{out}} = 80.$$

First constant-flow interval

$$V_0 = 500, \quad Q_{\text{in}} = 100, \quad Q_{\text{out}} = 80.$$

$$V(t) = 500 + (100 - 80)t, \qquad V(3) = 560 \text{ mL}.$$

Entry is 300 mL; storage gain is only 60 mL.

Switch the rate, preserve the state

At $t = 3$, change the outflow to $120\ \mathrm{mL/min}$.

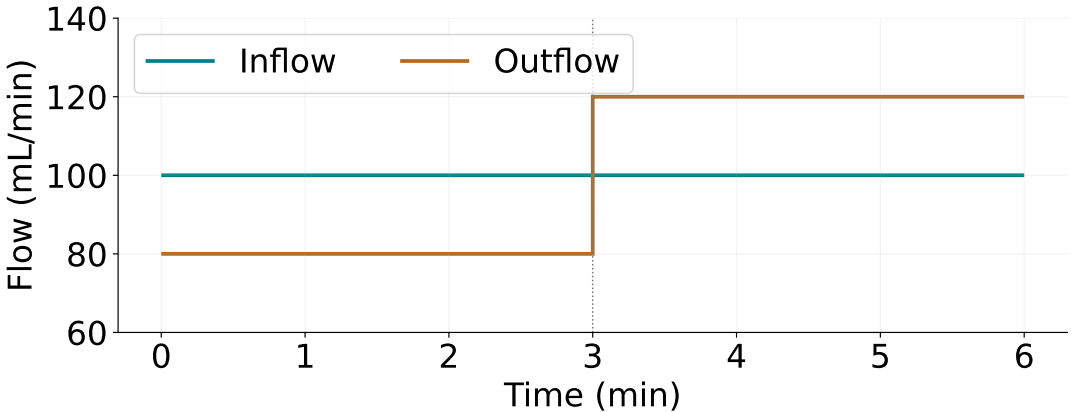
Switch the rate, preserve the state

At $t = 3$, change the outflow to $120\ \mathrm{mL/min}$.

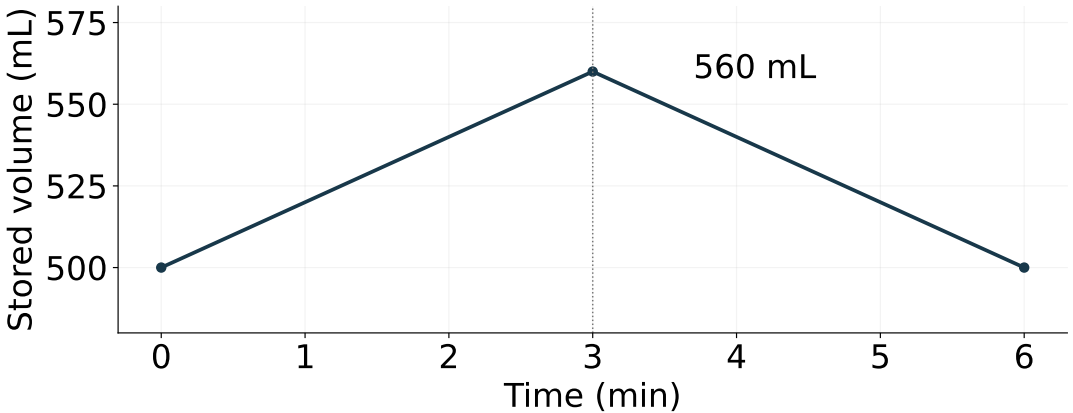
$$V(t) = 560 - 20(t-3), \qquad 3 \le t \le 6.$$

$$V(3^-) = V(3^+) = 560, \qquad V(6) = 500.$$

Prescribed inflow and outflow



The resulting stored volume



Piecewise-linear storage

$$\dot{V} = +20 \quad (t < 3), \qquad \dot{V} = -20 \quad (t > 3).$$

Piecewise-linear storage

$$\dot{V} = +20 \quad (t < 3), \qquad \dot{V} = -20 \quad (t > 3).$$

A finite rate jump changes slope. A finite volume jump would require an impulsive transfer.

Check the entire experiment

$$A_{\text{in}} = 100(6) = 600, \qquad A_{\text{out}} = 80(3) + 120(3) = 600.$$

Check the entire experiment

$$A_{\text{in}} = 100(6) = 600, \qquad A_{\text{out}} = 80(3) + 120(3) = 600.$$

$$V_0 + A_{\text{in}} = V(6) + A_{\text{out}}.$$

The endpoint returns to its initial value despite nonzero throughput.

Steady storage permits throughput

$$\dot{V} = 0 \quad \Longleftrightarrow \quad Q_{\text{in}} = Q_{\text{out}}.$$

Steady storage permits throughput

$$\dot{V} = 0 \quad \Longleftrightarrow \quad Q_{\text{in}} = Q_{\text{out}}.$$

Both $(Q_{\text{in}}, Q_{\text{out}}) = (0, 0)$ and $(100, 100)$ satisfy it. Volume alone cannot identify replacement or mixing.

Enlarge the boundary

$$\dot{V}_1 = a - q, \qquad \dot{V}_2 = q - b.$$

Enlarge the boundary

$$\dot{V}_1 = a - q, \qquad \dot{V}_2 = q - b.$$

$$\boxed{\frac{d}{dt}(V_1 + V_2) = a - b.}$$

The same internal transfer must appear with opposite signs.

The network version of the same argument

An incidence column has one -1 and one $+1$.

$$\dot{\mathbf{V}} = B\mathbf{Q} + \mathbf{u}.$$

The network version of the same argument

An incidence column has one -1 and one $+1$.

$$\dot{\mathbf{V}} = B\mathbf{Q} + \mathbf{u}.$$

$$\mathbf{1}^T B = 0 \quad \Rightarrow \quad \frac{d}{dt}\sum_i V_i = \sum_i u_i.$$

Locate the first impossible continuation

If $r = Q_{\text{in}} - Q_{\text{out}} < 0$,

$$V(t_k + s) = V_k + rs.$$

Locate the first impossible continuation

If $r = Q_{\text{in}} - Q_{\text{out}} < 0$,

$$V(t_k + s) = V_k + rs.$$

$$\tau = V_k/(-r), \qquad 50/20 = 2.5 \text{ min}.$$

Stop or change the model at emptying; clipping hides a transfer.

An exact interval algorithm

For each constant-rate interval:

$$\Delta V_k = (Q_{\text{in},k} - Q_{\text{out},k})\Delta t_k, \quad V_{k+1} = V_k + \Delta V_k.$$

An exact interval algorithm

For each constant-rate interval:

$$\Delta V_k = (Q_{\mathrm{in},k} - Q_{\mathrm{out},k})\Delta t_k, \quad V_{k+1} = V_k + \Delta V_k.$$

Reject an inadmissible interval. Splitting an interval into two pieces must give the same endpoint.

A residual checks the account

$$\mathcal{R}_k = V_k - V_0 - \sum_{j<k} (Q_{\mathrm{in},j} - Q_{\mathrm{out},j}) \Delta t_j .$$

A residual checks the account

$$\mathcal{R}_k = V_k - V_0 - \sum_{j<k} (Q_{\mathrm{in},j} - Q_{\mathrm{out},j}) \Delta t_j.$$

$\mathcal{R}_k \approx 0$ checks implementation. It cannot reveal an omitted leak that is absent from both code and equations.

Model discrepancy

Predict $V(t)$ using independently measured flows.

Model discrepancy

Predict $V(t)$ using independently measured flows.

$$e(t) = V^{\mathrm{obs}}(t) - V^{\mathrm{pred}}(t).$$

Inspect the time pattern, the measurement uncertainty, and the first violated assumption.