Molecular Concentration Gradient Design — MATLAB Simulation Codes

This repository contains all MATLAB scripts used to generate the main figures in the manuscript:

"Molecular Concentration Gradient Design using Closed-Form Solutions for Concentration Field Steady-State."

Each script computes analytical and/or numerical steady-state concentration profiles of reaction–diffusion systems and automatically generates the corresponding figure shown in the paper.

Overview

All scripts are self-contained and require no external data files.

They calculate concentration fields generated by localized sources under reaction–diffusion dynamics and plot the steady-state solutions in 1D, 2D, and 3D geometries.

Each MATLAB file produces one figure identical to those in the manuscript.

Figure	File name	Description
Fig. 2a	fig2a.m	Calculates and plots the 1D steady-state concentration profile. Compares analytical and numerical solutions.
Fig. 2b	fig2b.m	2D steady-state concentration field using Bessel function–based analytical solution and numerical verification.
Fig. 2c	fig2c.m	3D spherical steady-state concentration profile with analytical and numerical comparison.
Fig. 2d	fig2d.m	Semi-logarithmic plot of 1D dimensionless concentration profile showing exponential decay.
Fig. 2e	fig2e.m	Semi-logarithmic plot of 2D profiles showing nonlinear transition near the source boundary.
Fig. 2f	fig2f.m	Semi-logarithmic plot of 3D profiles highlighting dimension-dependent decay behavior.
Fig. 3a	fig3a.m	Calculates surface concentration ($C'_{surface}$) as a function of dimensionless parameter ($R' = R(k/D)^{0.5}$).
Fig. 3b	fig3b.m	Computes the half-width at half-maximum (HWHM) vs. (R') to quantify gradient steepness across dimensions.

Requirements

- MATLAB R2021a or later
- Built-in MATLAB functions only (no toolboxes required)

How to Run

Clone or download this repository.

Open MATLAB and set the repository folder as the working directory.

Run any figure script in the Command Window

Each script:

- Computes the analytical (and if applicable, numerical) solution.
- Plots the figure automatically.
- Saves the resulting figure in the current directory.

Output

Running all scripts will generate:

- Figure 2 (a–f): Validation of closed-form analytical solutions and visualization of exponential decay in 1D–3D systems.
- Figure 3 (a–b): Dimensional scaling relationships between surface concentration, gradient width, and the dimensionless parameter