



PK-Sim: Clinical Pharmacokinetics Simulator

Documentation & User Guide

Release Date: September 2026

Platform: Universal (HTML5/JavaScript) - Client-Side Only

1. Introduction

PK-Sim is a comprehensive browser-based clinical pharmacokinetics simulator designed for pharmacy students and practitioners. Moving beyond static calculators, PK-Sim utilizes a dynamic rendering engine to generate instant concentration-time profiles, allowing users to explore the dynamics of drug absorption, distribution, metabolism, and excretion. It runs entirely on the client-side, ensuring fast performance, offline functionality, and complete privacy without server interactions.

Key Features:

- **Dynamic Interactive Visualizer:** Leverages the HTML5 Canvas API to render immediate concentration curves, featuring a 'Freeze Comparison' toggle and Therapeutic/Toxic band overlays.
- **Clinical Logic Database:** Includes a clinically normalized drug database focusing on Narrow Therapeutic Index (NTI) drugs, with automatic elimination rate adjustments based on estimated renal function.
- **Solver Tools & Predictor:** Features a Clinical Sampling Predictor based on analytical formulas and exact steady-state calculators for Therapeutic Drug Monitoring (TDM) and regimen planning.
- **Gamified Quiz Mode:** An interactive module challenging users to hit specific peak and trough targets by adjusting dosage variables on the fly.

2. Core Concepts & Mechanics

PK-Sim operates on exact analytical pharmacokinetic equations rather than simplified stepwise approximations. Understanding these mechanics is essential for accurate clinical forecasting.

The Patient-Specific Engine

The simulation continuously assesses patient demographics. Ideal Body Weight (IBW) is calculated using the Devine formula, and renal function is estimated via the Cockcroft-Gault equation for Creatinine Clearance (CrCl). These patient-specific metrics dynamically scale the population elimination rate constants (k_{pop}) specifically for renally cleared medications.



Exact Analytical Pharmacokinetics

The engine utilizes a One-Compartment Open Model with First-Order Elimination. Volume of Distribution (V_d) and Clearance (Cl) are treated as independent physiological variables. The system accurately calculates multiple IV Bolus, IV Infusion, and Multiple Oral dosing curves, utilizing a constant absorption rate (K_a) for oral formulations.

3. How to Use

Step 1: Patient Data Initialization

Enter the patient's Sex, Height, Weight, Age, and Serum Creatinine in the left-hand sidebar. The system instantly updates the IBW and CrCl in the adjacent summary box.

Step 2: Drug & Route Selection

Select a drug from the categorized dropdown (e.g., Narrow (Renal), Short $t_{1/2}$, Hepatic) or opt for 'Custom / Manual Mode' to input entirely custom physiological parameters. Define the Route of Administration (IV Bolus, IV Infusion, Oral). If IV Infusion is selected, define the precise infusion time.

Step 3: Dosing Regimen Tuning

Adjust the Dose amount, Dosing Interval (τ), and Number of Doses using the sliders or direct text input. Toggle the 'Include Loading Dose (2x)' checkbox to observe the immediate impact on the time to steady state.

Step 4: Analyze the Profile

Observe the generated curve on the Workspace canvas. Use the 'Semilog Plot' toggle to evaluate the linearity of the terminal elimination phase. Engage the 'Freeze Comparison' button to save a baseline graphical curve before modifying the regimen to view an overlay.

4. Core Tools & Modules

PK Solver Tools

- **Dose Planner:** Input a desired target peak and trough concentration. The solver calculates the required maintenance dose, loading dose, and practical dosing interval based on the current patient's V_d and K_{el} .
- **TDM Analysis (Two-Point):** Enter measured serum levels (Peak and Trough) along with their sampling times. The tool computes the patient's actual elimination rate (K_{el}) and Half-life, allowing you to instantly apply these parameters to the main simulator for individualized forecasting.

Clinical Sampling Predictor

An integrated analytical display that outputs the exact predicted plasma concentration at any specified sampling time post-dose. It dynamically renders the full mathematical



formula used in the calculation, providing educational transparency for the underlying math.

5. Troubleshooting

Issue	Possible Cause	Solution
Chart is not rendering or appears completely blank	Browser lacks HTML5 Canvas support or hardware acceleration is disabled.	Update to a modern web browser (Chrome, Edge, Safari). Ensure hardware acceleration is toggled on in settings.
Clearance (Cl) is not auto-adjusting when changing Serum Creatinine	Simulator is currently set to "Custom / Manual Mode".	In Manual Mode, renal function intentionally does not auto-adjust Clearance. Select a specific drug from the database to re-enable dynamic renal adjustments.
Semilog plot cuts off the bottom of the visible curve	Mathematical limitation of $\log(0)$ and low-level visual capping.	The system dynamically sets a Y-axis floor (minimum 0.001 mg/L) to prevent infinite log scaling errors. This is intended visual behavior.

6. Glossary of Clinical PK Terms

Vd (Volume of Distribution): A theoretical volume that would be necessary to contain the total amount of an administered drug at the same concentration that it is observed in the blood plasma.

Cl (Clearance): The volume of plasma from which a substance is completely removed per unit time, factoring both hepatic and renal pathways.

NTI (Narrow Therapeutic Index): Drugs where small differences in dose or blood concentration may lead to dose-dependent, serious therapeutic failures or adverse drug reactions (e.g., Digoxin, Vancomycin).

TDM (Therapeutic Drug Monitoring): The clinical practice of measuring specific drugs at designated intervals to maintain a constant, safe concentration in a patient's bloodstream.

Steady State (SS): The point at which the rate of drug administration equals the rate of drug elimination, typically achieved after 4 to 5 half-lives.



7. Technical Specifications

Architecture: Single-Page Application (SPA).

Language: HTML5, CSS3, Vanilla JavaScript (ES6).

Graphics Engine: Native HTML5 Canvas API.

Privacy & Data: 100% Client-Side processing utilizing browser memory and localStorage mechanisms. No patient details or simulation data are transmitted to external servers, ensuring strict privacy.

Pharmacokinetic Logic: Dr. Shery Jacob, Professor, College of Pharmacy, Gulf Medical University.

VIBE coding: Dr. Muhammad AlShorbagy, Dean, College of Pharmacy, Gulf Medical University.

Distribution: Hosted and distributed via the Acabuild AI LabHub on ToolabX, serving as an open-access academic tool for educators and students.