Scilab case study project on

Interactive GUI-Based Implementation of Gentamicin Elution Kinetics from Antibiotic-Loaded PMMA Bone Cement using Scilab

Chirag Veerwani

Biomedical Engineering / Drug Release Kinetics

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Abstract

This case study implements an interactive Scilab based graphical user interface (GUI) to model and visualize the kinetics of gentamicin elution from antibiotic loaded poly(methyl methacrylate) (ALBC) bone cement over a 28 day elution period, based on the experimental findings of the reference paper mentioned below. Seven cement formulations are considered: a commercial control cement, three MEPAR (microencapsulated paraffin) loaded variants and three DDM (1-dodecyl mercaptan) loaded variants. For each formulation, four widely used kinetic release models are implemented: the KorsmeyerPeppas power law, the LindnerLippold modified power law, the Frutos et al. combined diffusion-dissolution model, and the Hesaraki et al. exponential model using the best fit coefficients as reported in the paper. The GUI allows the user to select any cement group and any kinetic release model interactively, rendering the corresponding M_t/M_∞ verses time curve alongside digitized experimental data. This helps the user to easily compare and choose the kinetic model according to their preferences. Additional features include overlay of all seven groups for cross-group comparison and a bar chart with error bars for gentamicin diffusion coefficient. The study demonstrates that neither MEPAR nor DDM addition significantly alters the gentamicin diffusion of the diffusion mechanism as reported in the paper. This case study performs a partial replication of Lewis and Li (2019), focusing on visualization and comparison of the reported kinetic models and diffusion coefficients using Scilab. The original diffusion-coefficient computation, nonlinear fitting procedures, statistical analyses, and experimental measurements were not reproduced.

1. Introduction

Antibiotic-loaded poly(methyl methacrylate) bone cement (ALBC) is widely used in total joint arthroplasty (TJA) to anchor joint replacement components and reduce the risk of peri-prosthetic joint infection (PJI). Gentamicin, an antibiotic, is embedded in the PMMA matrix during preparation and elutes into the surrounding fluid after implantation.

One known problem with ALBC is the high maximum exothermic temperature (Tmax) produced during cement polymerization, which has been postulated to cause thermal necrosis of peri-prosthetic tissue. To reduce Tmax, additives such as microencapsulated paraffin (MEPAR) added to the cement powder, and 1-dodecyl mercaptan (DDM) added to the cement liquid, have been investigated. Lewis and Li (2019) studied seven such formulations and computed the gentamicin diffusion coefficient (Dgent) and fit four kinetic release models to the elution data for each group.

This case study replicates some of those results in Scilab through an interactive GUI. The user can select any of the seven cement groups and any of the four models, and the GUI plots the corresponding M_t/M_∞ versus time curve alongside normalized experimental scatter data. The project also provides a cross-group elution overlay and a Dgent bar chart with error bars, making it straightforward to compare both the models and the cement formulations side by side.

This case study performs a partial replication of Lewis and Li (2019), focusing on visualization and comparison of the reported kinetic models and diffusion coefficients using Scilab. The original diffusion-coefficient computation, nonlinear fitting procedures, statistical analyses, and experimental measurements were not reproduced.

2. Problem Statement

When making antibiotic-loaded bone cement (ALBC), engineers often add things like paraffin (MEPAR) or sulfur chemicals (DDM) to lower the high heat produced when the cement sets. While these additives help protect patient tissue from heat damage, it is crucial to know if they disrupt how the antibiotic (gentamicin) escapes from the cement into the body.

A major study by Lewis and Li (2019) collected raw data on this process and calculated mathematical values for four different drug-release equations. However, their findings were left as static tables of numbers and individual equations. Without a way to look at everything at once, it is difficult to see how these mathematical formulas actually hold up when compared directly against the real-world data points. To solve this, this project creates an interactive Scilab program with a graphical user interface (*GUI*). The tool is built to let you choose any cement type and match it up against any of the four formulas instantly on a single graph.

By giving users a direct visual comparison, this tool makes it easy to see that while the additives do not change the underlying physical diffusion mechanism, the standard mathematical equations have clear limitations when trying to precisely predict real-world release behavior.

3. Basic concepts related to the topic

3.1 Gentamicin Elution

Elution is a process where a trapped drug gets out of a solid material by a surrounding liquid. For these bone cements, gentamicin powder is stirred directly into the cement mix before it hardens. Once, the cement hardens, the drug is locked inside a tight plastic matrix. When body fluids or lab fluids touch the cement, the liquid creeps into the tiny microscopic pores, dissolves the gentamicin molecules, and lets them slowly seep out via simple diffusion.

3.2 Diffusion Coefficient (Dgent)

Dgent is a measure of how fast or slow a substance can move through a solid material. Dgent is computed from Mt / M∞ versus time data using the governing equation for diffusion out of a long cylinder (Equation 1 of the paper). M∞ is the equilibrium release, defined as the value at which the Mt versus t curve flattens. Dgent was computed in the original paper using Wolfram Mathematica; this case study uses the tabulated values from Table 4 of the paper directly.

3.3 The four Kinetic Release Models

All four equations model the dimensionless ratio Mt / M∞ as a function of time t in days. The models and rheir coefficients stored in the code are:
Equation 2 (Korsmeyer-Peppas): *Mt/M∞ = k1 · t^n1* Coefficients: [k1, n1] Equation 3 (Lindner-Lippold): *Mt/M∞ = b + k2 · t^n2* Coefficients: [b, k2, n2].
Equation 4 (Frutos et al.): *Mt/M∞ = A + B·(1 − exp(−n3·t)) + C·t^0.5* Coefficients: [A, B, C, n3].

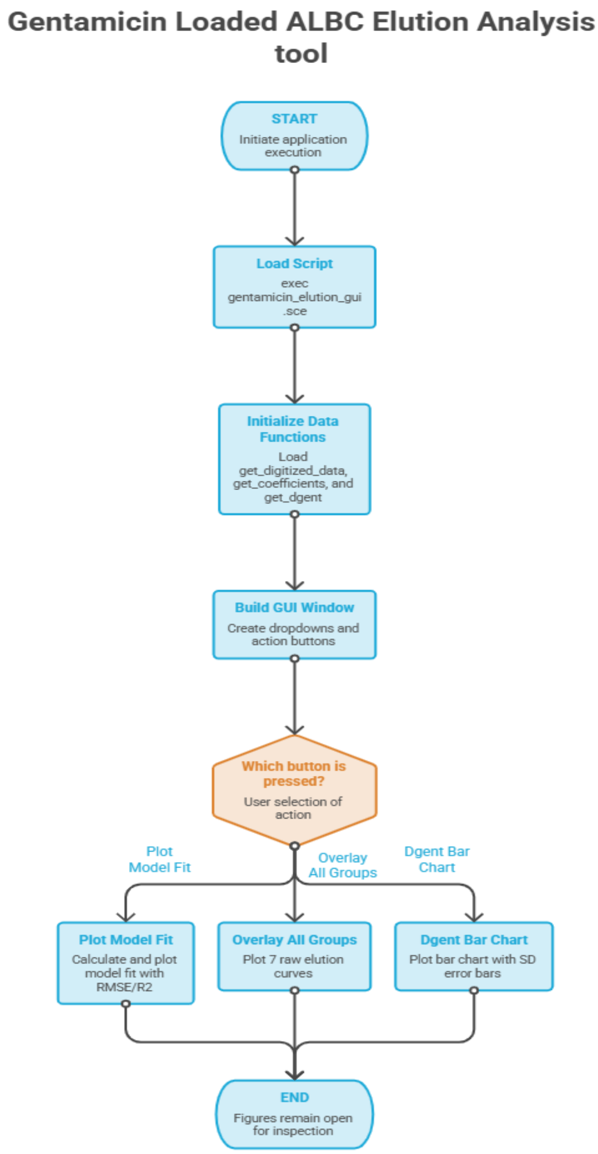
Equation 5 (Hesaraki et al.): $Mt/M\infty = k3\cdot(1 - \exp(-(t/\tau)\cdot d))$ Coefficients: [k3, τ, d].

Table: Physical Meanings of coefficients in Equations (2) – (5).

Coefficient	**Physical Meaning**
k1; k2	Each is related to the characteristics of the macromolecular network of the cement matrix and the gentamicin.
n1; n2; C; d	Each denotes that the mechanism of release of the gentamicin from the cement matrix is a diffusion process.
b; A	Each is a term that characterizes the initial burst of the gentamicin from the cement.
B; n3	Each term is associated with a Noyes-Whitney dissolution process of the gentamicin within the cement matrix.
k3	A term whose value is related to the initial loading of the gentamicin in the cement.
τ	A time constant related to the mechanism of release of the gentamicin from the cement.

4. Flowchart

(on the next page)



5. Software/Hardware used

Operating System: Windows 11

Scilab Version: 2026.0.1

Required Toolboxes: None. All functions used are part of Scilab core.

Hardware: Standard laptop. No GPU or specialized hardware required.

Data Source: Experimental data digitized from Figure 1 of Lewis and Li (2019) using WebPlotDigitizer (free, browser-based).

6. Procedure of execution

Step 1: Open Scilab and set the working directory to the folder containing gentamicin_elution_gui.sce. Execute the Script:

exec('gentamicin_elution.sce')

Step 2: A GUI window will open giving a brief introduction about the tool, click on the Launch button to move ahead to the dashboard.

Step 3: A GUI window titled 'Gentamicin Elution from ALBC Analysis' opens with two dropdowns (Cement Formulation, Mathematical Model) and three buttons.

Step 4: Select a cement group from the first dropdown and a kinetic model from the second. Click 'Plot Red Curve Fit Over Experimental Points'. Figure 1 opens showing the model curve (red) overlaid on normalized experimental points. The equation formula and the coefficients are also displayed in the plot.

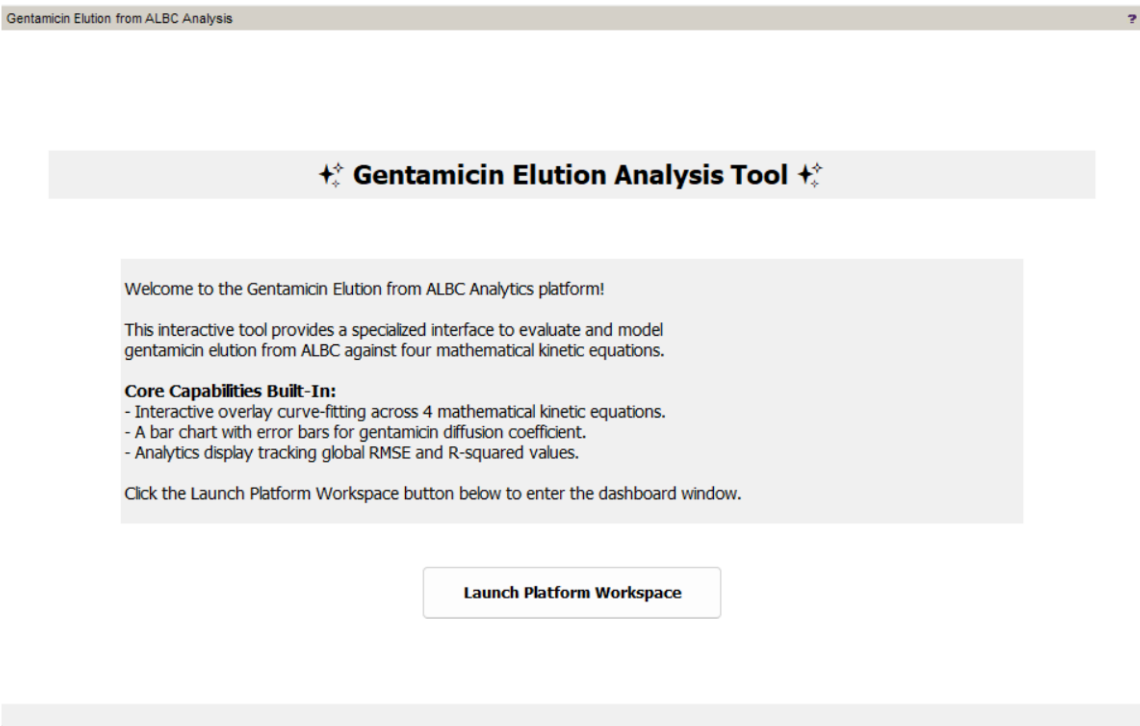
Step 5: Compare the red curves for the same group by keeping the cement group fixed and switching to a different model.

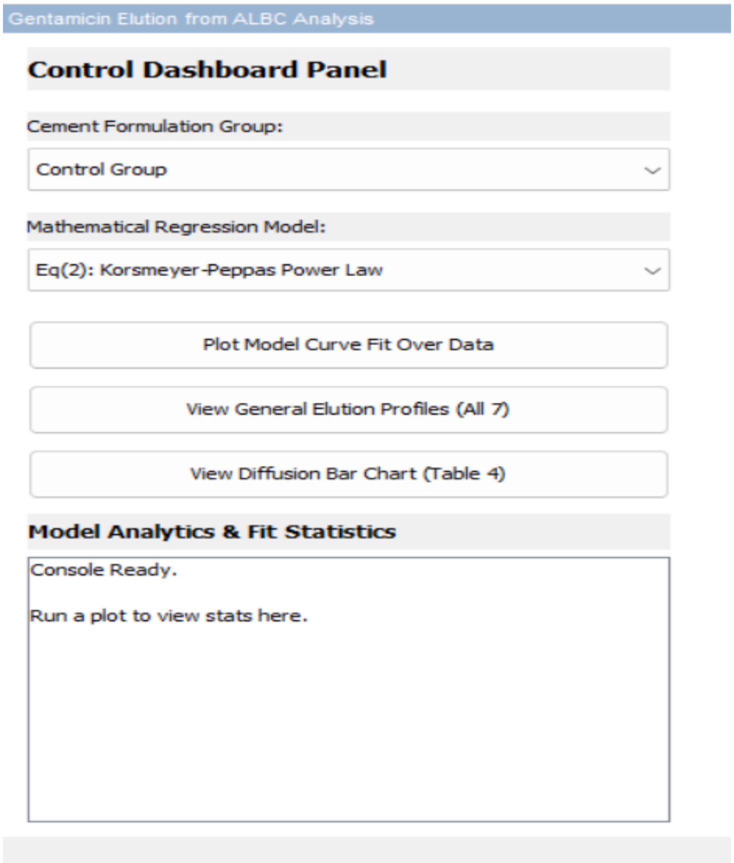
Step 6: Overlay all groups: Click 'View General Elution Profiles (All Groups)'. Figure 2 opens with raw elution curves for all seven cement groups on one axis, replicating Figure 1 of the paper.

Step 7: View Dgent by clicking 'View Diffusion Coefficients Bar Chart (Table 4)'. Figure 3 opens with a bar chart of Dgent mean values representing the population standard deviation for each group.

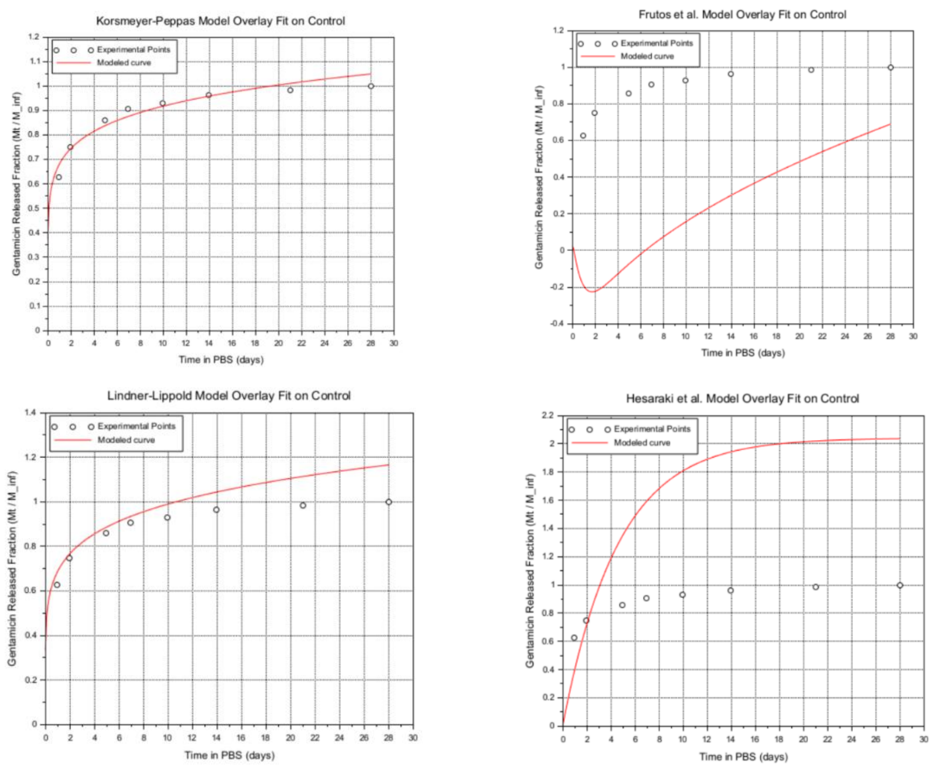
7. Result

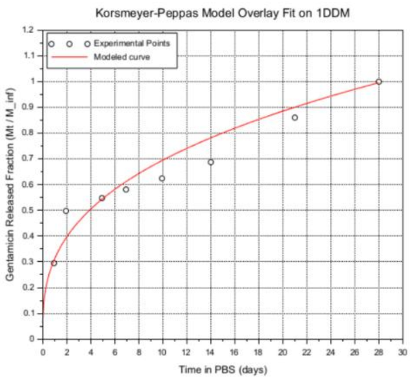
7.1 Application starting window and the dashboard

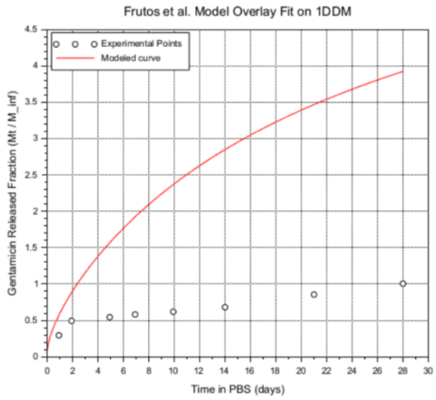


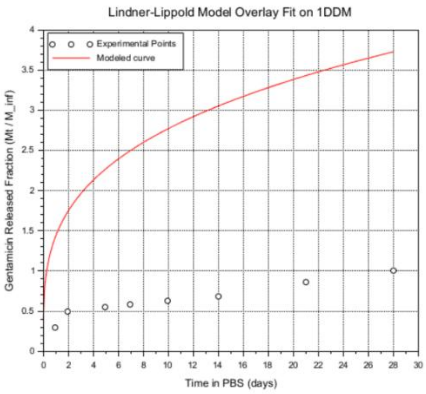


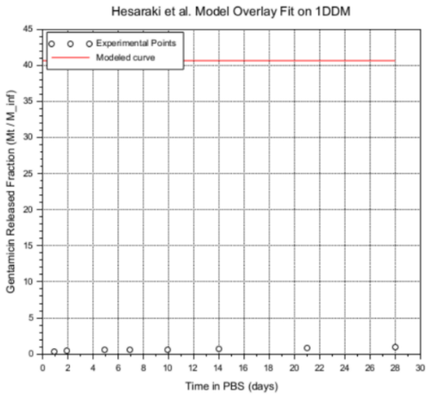
7.2 Model curves for each group against each of the four kinetic equations

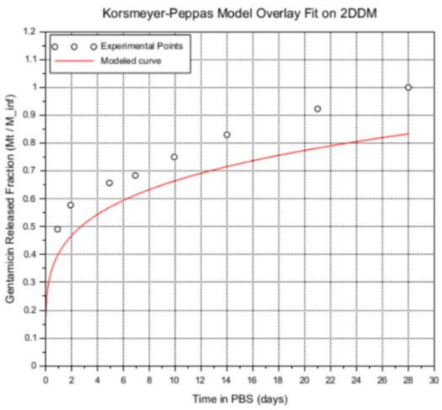



Korsmeyer-Peppas Model Overlay Fit on 1DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Frutos et al. Model Overlay Fit on 1DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Lindner-Lippold Model Overlay Fit on 1DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Hesaraki et al. Model Overlay Fit on 1DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)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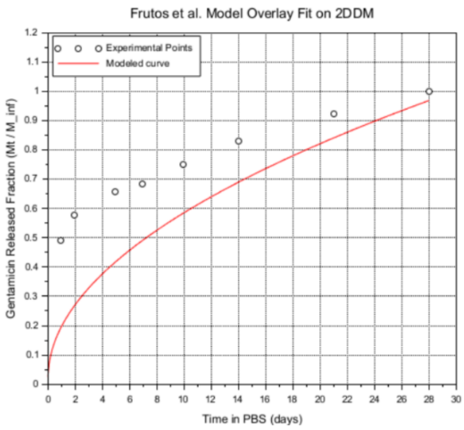
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)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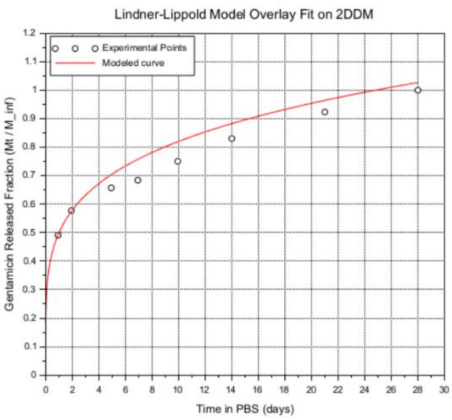
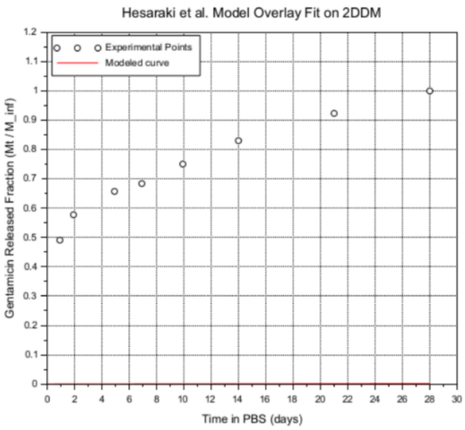
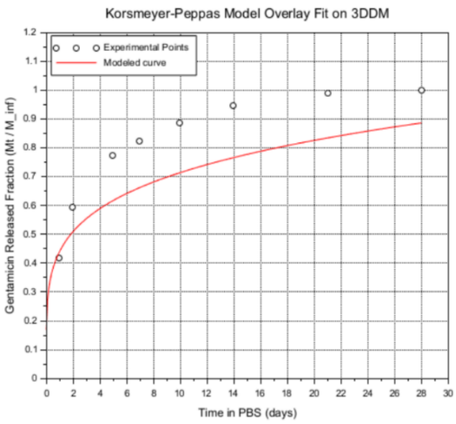
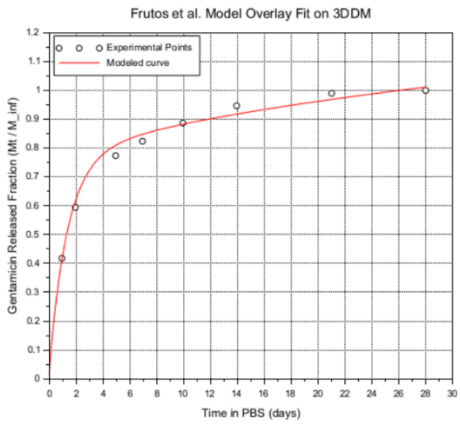
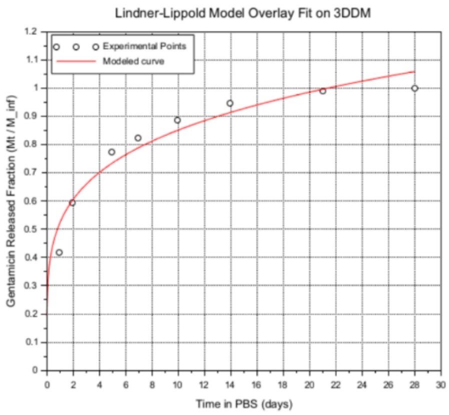
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

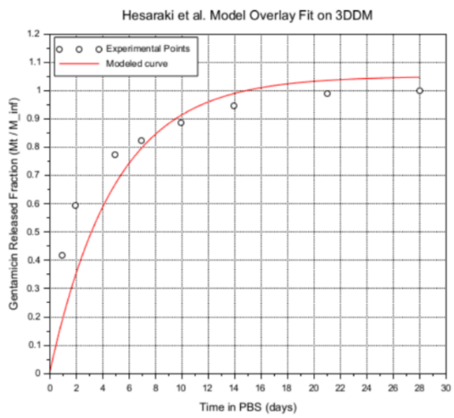

Lindner-Lippold Model Overlay Fit on 2DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Hesaraki et al. Model Overlay Fit on 2DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Korsmeyer-Peppas Model Overlay Fit on 3DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Frutos et al. Model Overlay Fit on 3DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Lindner-Lippold Model Overlay Fit on 3DDM
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)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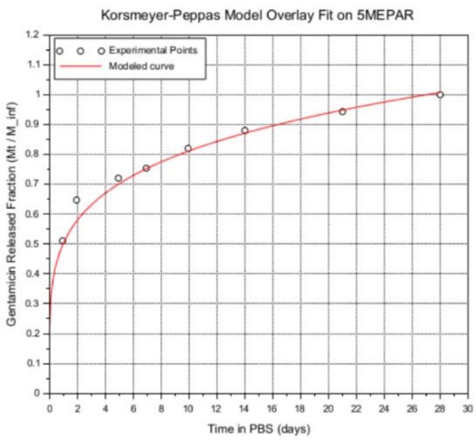
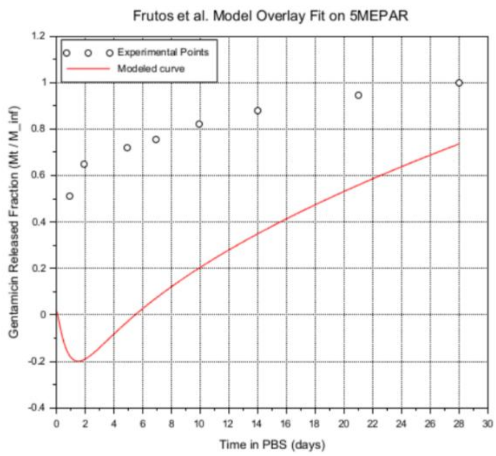
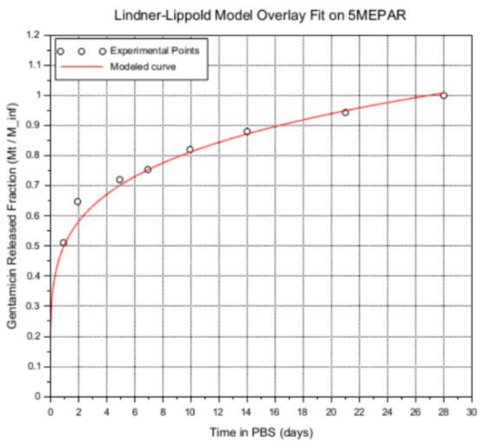
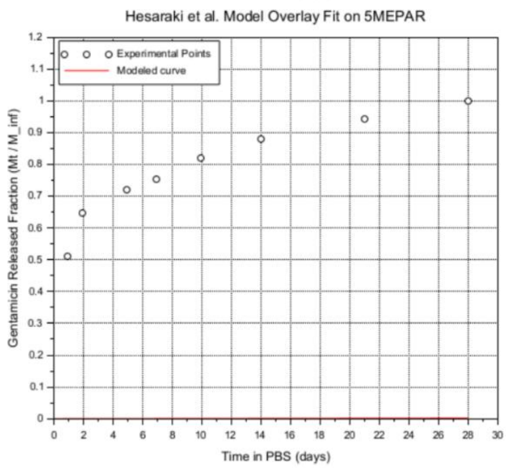
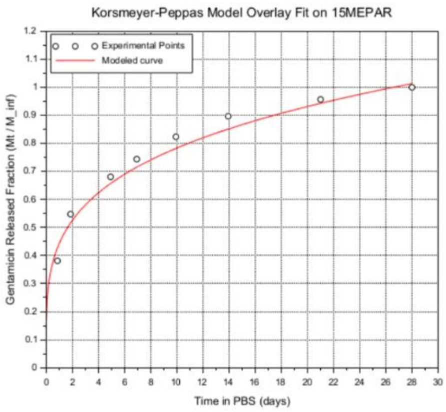
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

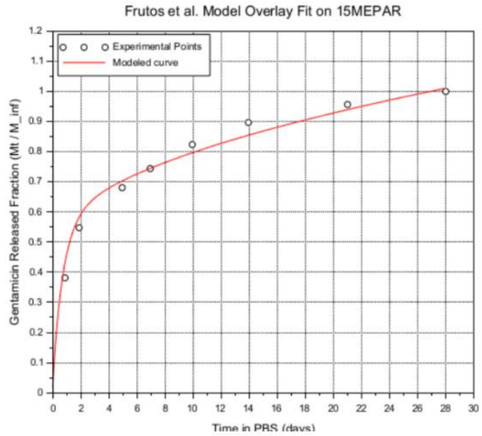

Korsmeyer-Peppas Model Overlay Fit on 5MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

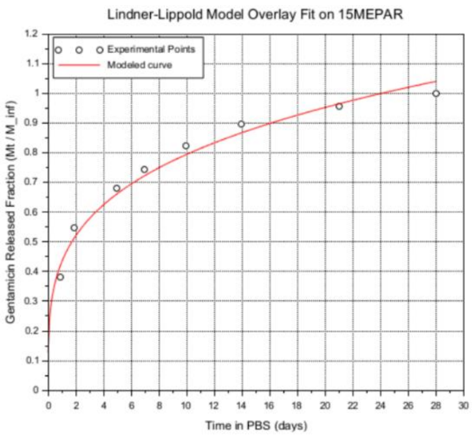

Frutos et al. Model Overlay Fit on 5MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

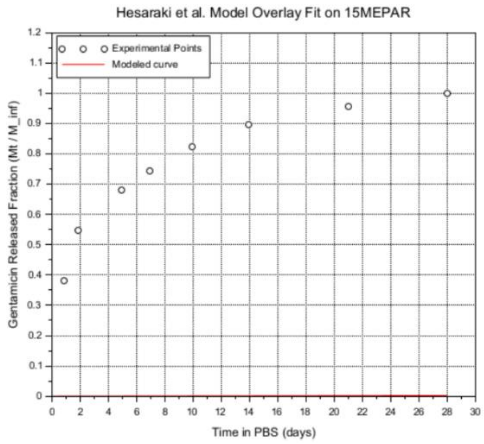

Lindner-Lippold Model Overlay Fit on 5MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

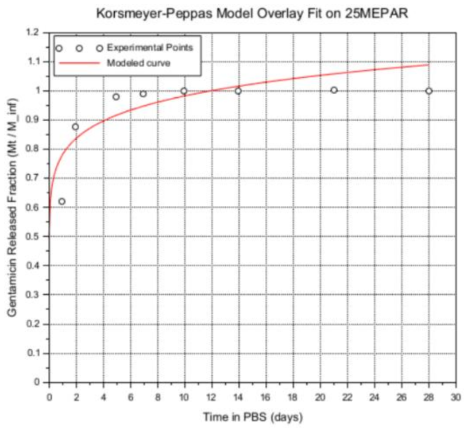

Hesaraki et al. Model Overlay Fit on 5MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

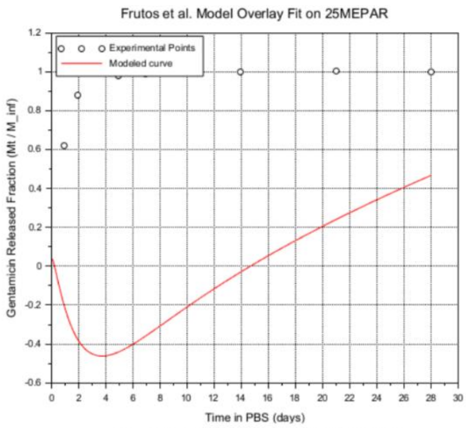

Korsmeyer-Peppas Model Overlay Fit on 15MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

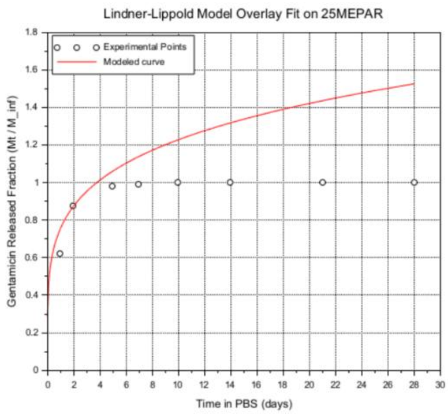

Frutos et al. Model Overlay Fit on 15MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

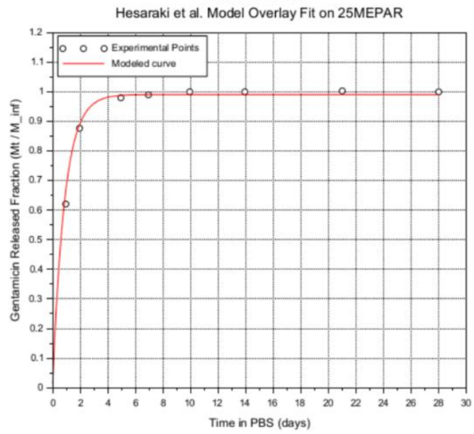

Lindner-Lippold Model Overlay Fit on 15MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Hesaraki et al. Model Overlay Fit on 15MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Korsmeyer-Peppas Model Overlay Fit on 25MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

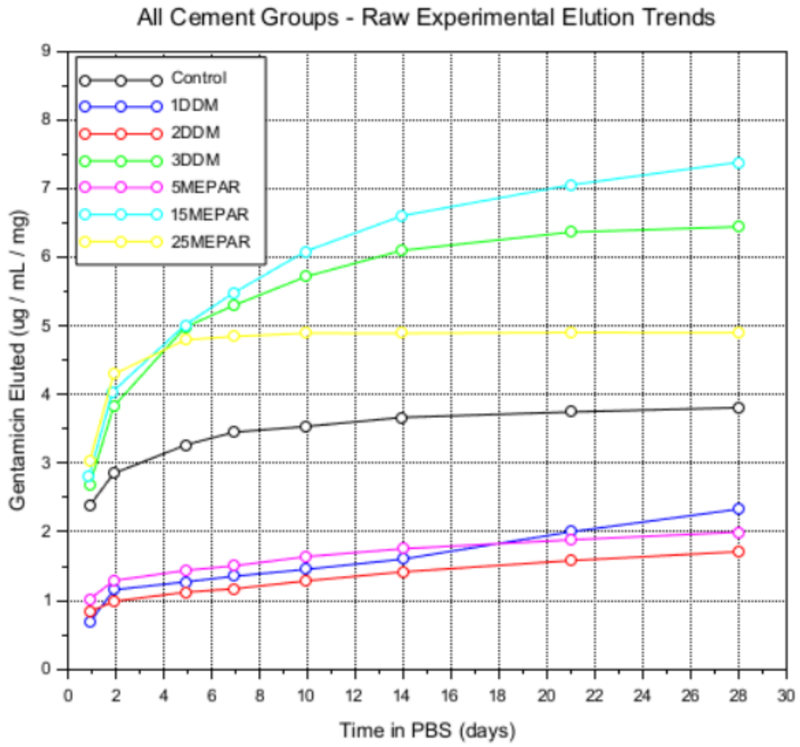

Frutos et al. Model Overlay Fit on 25MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Lindner-Lippold Model Overlay Fit on 25MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)


Hesaraki et al. Model Overlay Fit on 25MEPAR
Experimental Points
Modeled curve
Gentamicin Released Fraction (Mt / M_inf)
Time in PBS (days)

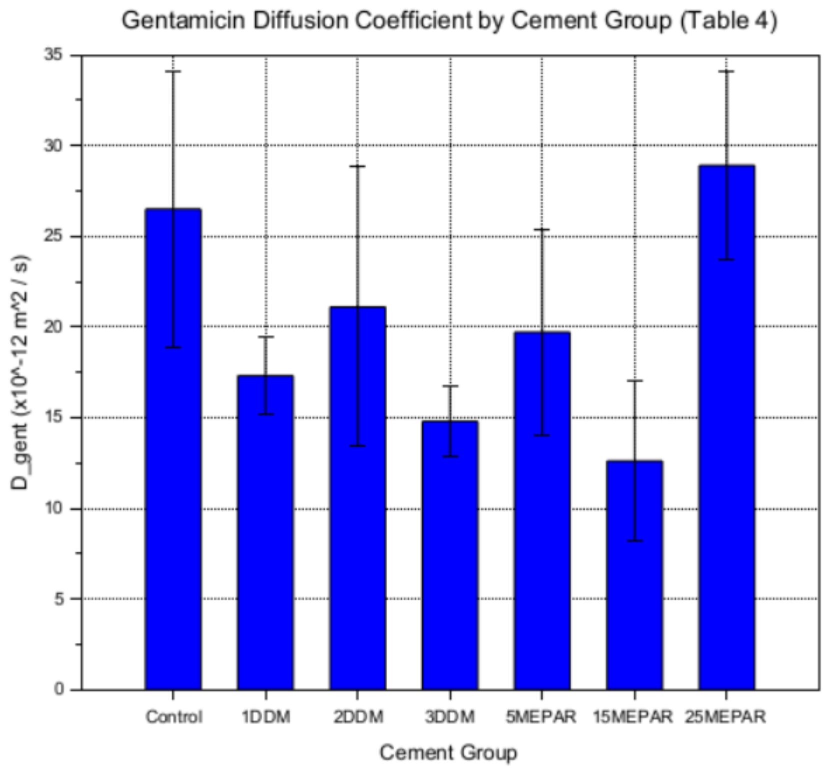
7.3 Cross-Group Overlay Plot

The overlay of all seven groups replicates figure 1 of the paper:



7.4 Dgent Bar Chart

Dgent values range from 12.6×10^{-12} m²/s (15MEPAR) to 28.9×10^{-12} m²/s (25MEPAR) as can be seen below:



7.5 Adjusted R^2 Values

The table below summarizes computed $adjR^2$ across all groups and equations.

Group	Eq2 AdjR²	Eq3 AdjR²	Eq4 AdjR²	Eq5 AdjR²
Control	0.9389	0.4945	-38.187	-38.58
1DDM	0.9177	-100.34	-77.74	-38560
2DDM	0.5061	0.9171	-0.6	-20.8
3DDM	0.4613	0.9370	0.9877	0.5388
5MEPAR	0.9677	0.9677	-16.12	-27.27
15MEPAR	0.9716	0.9768	0.9750	-14.38
25MEPAR	0.6488	-4.31	-75.14	0.9833

7.6 Conclusions and Project Scope

This case study implemented a Scilab GUI to replicate and visualize the gentamicin elution kinetics results from the reference paper. All four kinetic release models from the paper: Korsmeyer-Peppas (Eq. 2), Lindner-Lippold (Eq. 3), Frutos et al. (Eq. 4), and Hesaraki et al. (Eq. 5) were implemented using the best-fit coefficients from table 5, across all seven cement formulations. The GUI allows direct visual comparison of how well each model describes the elution behaviour of a given formulation, which is the core purpose of the tool.

As concluded in the paper, Dgent values across all seven groups show not significant difference between the experimental formulations and the control and $n2 < 0.5$ for Equation 3 which implies that neither MEPAR nor DDM addition meaningfully alters how gentamicin diffuses out of the cement matrix.

Fully implemented from the paper

All four kinetic model equations (Eq. 2–5) with coefficients exactly as reported in Table 5, Dgent mean and population SD values from Table 4 for all seven groups were coded. Experimental elution data from Figure 1 was digitized via WebPlotDigitizer for all seven groups at all eight time points (1, 2, 5, 7, 10, 14, 21, 28 days). Model curve plots (M_t/M_∞ vs time) and Cross-group overlay of raw elution data replicating Figure 1 and Dgent bar chart with error bars replicating Table 4 was plotted.

Modifications Made

The paper used actual M∞ values computed from Equation 1 (cylindrical diffusion governing equation, solved in Wolfram Mathematica) to normalize the experimental data before fitting. Those M∞ values are not tabulated in the paper. In this implementation, M∞ is approximated as the day-28 raw eluted value for each group. This introduces a small normalization error for groups still rising at day 28 (Control, 1DDM, 2DDM, 5MEPAR).

The paper's figure 2 uses per specimen Mt/M∞ experimental data whereas this GUI uses digitized data from figure 1 since it has not been tabulated in the paper. Since this involves manual identification of data points from a printed graph, the digitized values carry some uncertainity typically within ±0.1 to 0.2 units on both axes. As a result, the experimental plot shown in the model fits plots is an approximation of the original data.

Not implemented

Equation 1 (cylindrical diffusion governing equation) and the associated Dgent computation were not implemented. The paper solved this numerically in Mathematica using nonlinear fitting; replicating this would require the raw perspecimen elution data in absolute µg, which is not available. The nonlinear leastsquares fitting routine used to obtain the Table 5 coefficients (OriginPro 8.6) was not reimplemented and coefficients are hardcoded directly from the paper. Statistical analysis (Kruskal-Wallis test with Bonferroni correction, SAS Version 11.5) comparing Dgent and n2 across groups was not reimplemented.

8. References

Lewis, G. and Li, L. (2019) Kinetics of Elution of Gentamicin from a GentamicinLoaded PMMA Bone Cement. World Journal of Engineering and Technology, 7, 418428. https://doi.org/10.4236/wjet.2019.73031