

Background

- Compartment models of nuclides in body are used in bioassay analysis, and many analyses are done with an approach using a restricted number of terms.
- An example: Integrated Modules for Bioassay (IMBA) models internal radiation doses and uses only 10 terms.
- The eigensolution of a 22-compartment plutonium biokinetic model (Figure 1) must be fit with models with 10 or fewer terms.
- The required input form for the IMBA model is

$$R(t) = \sum_{i=1}^N A_i e^{-B_i t} \text{ where } N \leq 10.$$

$$\frac{d\bar{R}}{dt} = T\bar{R}$$

Equation representing the plutonium biokinetic model in Figure 1. The matrix T represents transfer of material as a function of time between different compartments in the model.

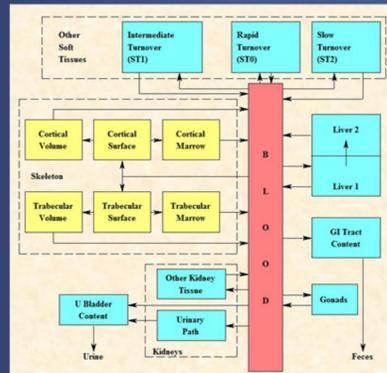


Figure 1. Plutonium biokinetic model

Purpose

- Confirm the results of the updated differential equation solver DIFSOL using *Mathematica*
- Develop an automated method to fit DIFSOL's eigensolution for the plutonium biokinetic model to the functional form required by IMBA

Methodology

- Using *Mathematica's* command "DSolve," the system of first order linear differential equations are solved and compared to the equations outputted by the program DIFSOL.
- The previously used fitting method involved trial and error by deleting terms with small coefficients and renormalizing the coefficients to a given sum. The process fit successfully, but was not automated. The new procedure developed is automated.

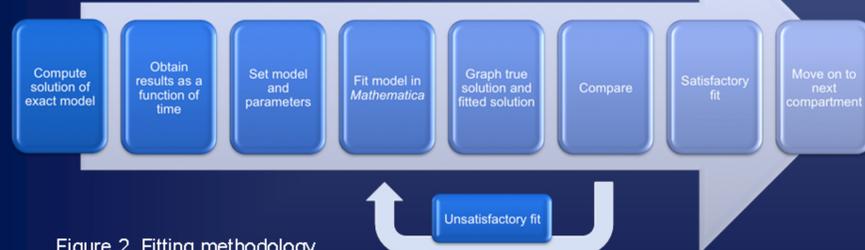


Figure 2. Fitting methodology.

Fitting the Eigensolution of Compartment Models

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Results

- The results obtained using *Mathematica's* "DSolve" correspond to the results obtained by DIFSOL, so Killough and Eckerman's differential equation solver is confirmed to function correctly.
- Automated fitting approach using *Mathematica* worked very well in some cases (e.g., blood) but poorly in others (e.g., liver).

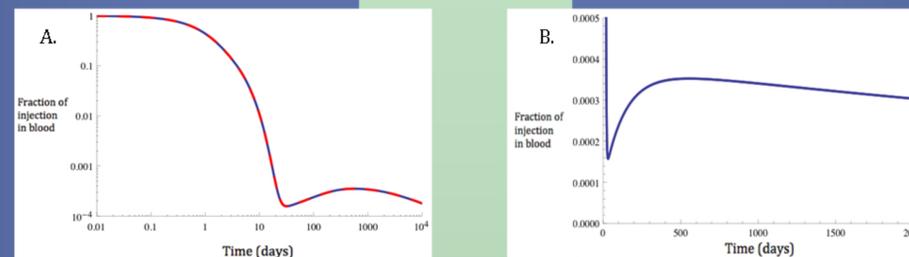


Figure 3. (A.) Log-log plot and (B.) Linear-linear plot of **blood** fitted curve (red) and exact solution (blue). Original 15-term equation fits using 10 terms with multiple terms of the same exponent. Fitted data begins at time = 1 day. The results are for a unit bolus injection into blood. Fit quality diminishes with increased time domain.

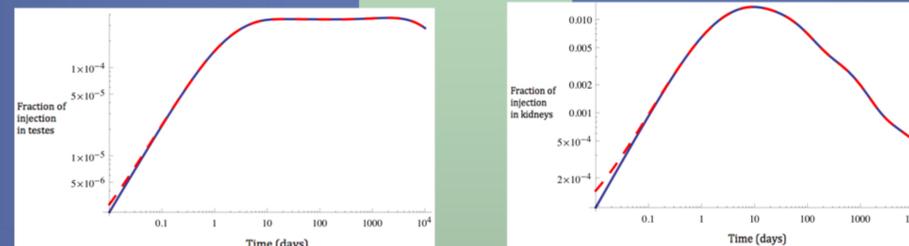


Figure 4. Log-log plot of **testes** fitted curve and true solutions. Original 15-term equation fits using 10 terms with multiple terms of the same exponent. Fitted data begins at time = 1 day.

Figure 5. Log-log plot of **kidneys** fit and true solutions. Original 16-term equation fits using 9 terms with multiple terms of the same exponent. Fitted data begins at time = 1 day. Results for the fit improved when the fit model had fewer than 10 terms.

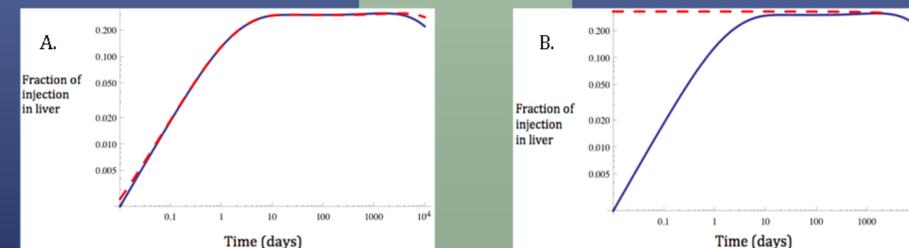


Figure 6. Log-log plot of (A.) adjusted and (B.) unadjusted **liver** fit and true solutions. The adjusted solution fits original 15-term solution using 8 terms, 5 of which are part of the true solution. The unadjusted solution fits original solution using a single term. Fitted data begins at time = 1 day.

Worse

True solution
Fitted solution

Table of Results

	Good fit (w/ 10 terms)	Bad fit (w/ 10 terms)	Multiple terms with same exponent	Needs more iterations (time)	Better fit when adjusted	Better fit with different model
blood	X		X			
liver		X			X	
cBoneS		X			X	
tBoneS		X	X		X	
kidneys			X			X
testes	X		X			
other	X			X		
cBoneV		X		X		
rMarrow		X				
tBoneV	X					
ubCont		X	X		X	
uliCont		X				
lllCont	X		X			
siCont	X		X			
ovaries	X		X			

Figure 7. Different situations encountered when fitting in *Mathematica*.

Conclusions

- Mathematica* provides a simpler data fitting method than previously used trial-and-error fitting method.
- Problems encountered using *Mathematica*:
 - More difficult to control numerical fitting method used
 - A few bad fits which could not be resolved
 - Excessive time to obtain fits on PC, (e.g. 24 hours to run enough iterations for blood compartment)
 - Multiple terms occurred with same exponent

Future Work

- Increase accuracy of fits
 - Using more precise data
 - Finding most appropriate numerical fitting method
- Find best fit model for each compartment
 - Number of terms
 - Automated adjustment of model
- Run additional iterations on compartments using workstation on high performance computers

References

- Wolfram Research, Inc., *Mathematica*, Version 7.0, Champaign, IL (2008).
- Killough, G. G. and Eckerman, K. F. "A conversational eigenanalysis program for solving differential equations," in *Computer Applications in Health Physics*, Eds R.L. Kathern, D.F. Higby, and M.A. McKinney, Columbia Chapter of Health Physics Society, Richland WA, 1984.
- Leggett, R. W. "A model of the retention, translocation, and excretion of systemic plutonium." *Health Phys.* 49,1115-1137, 1985.
- ICRP. Age-dependent Doses to Members of the Public from Intake of Radionuclides, Part 2: Ingestion Dose Coefficients, ICRP Publication 67. *Annals of the ICRP* 23(3/4) 1993.