A Programmed Solution to ARGESIM Comparison "C15 Clearance Identification" with MATLAB

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Simulator. MATLAB is a widely used software tool based on numerical vector and matrix manipulation. Additionally it provides several toolboxes for various tasks (Optimisation toolbox used here).

Model: The model ODEsare directly programmed in MATLAB code with a simple if-else-structure.

```
function xd = C15dgl(t,x)
C15data; k01 = 0.0041; k12 = 0.0585;
k21 = 0.0498; V1 = 7.3;
A = [-(k01+k21),      k12;...
          k21,     -k12];
b = [C15inf(t);0]; xd = A*x + b;
function inf = C15inf(t); C15data; n = length(t);
for j = 1:n
    if t < tau;inf(j) = D/tau;
    else ; inf(j) = 0; end; end;
```

Task a: Simulation of the System: The differential equations are numerically solved by MATLAB's ODE solver ODE23 (RKF-type solver), calling the above model description.

```
sol = ode23(@C15deq,tspan,x0);
```

Results for τ_1 = 0.5 min, τ_2 = 3 min und τ_3 = 240 are given in fig. 1. In fig. 2 one can already see the effect of the clearance: short injection time - very low concentration in the central compartment. Table 1 gives the numerical values.

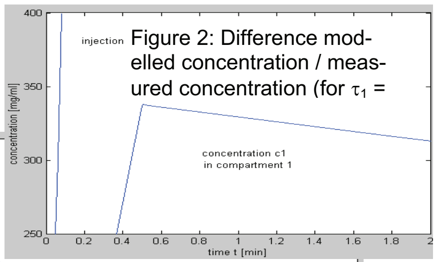

Figure 2: Difference modelled concentration / measured concentration (for τ_1 =

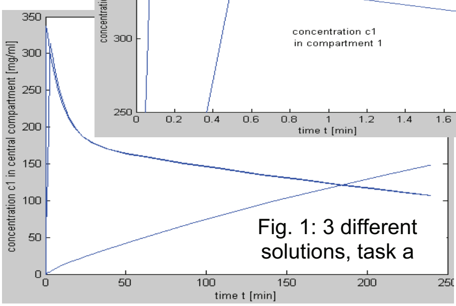

Fig. 1: 3 different solutions, task a

τ_1 = 0.5 min	τ_2 = 3 min	τ_3 = 240 min
$x_1(1.5)$= 2341.9	$x_1(4)$ = 2184.2	$x_1(240)$=1058.2
c_1 = 320.8	c_1 = 299.2	c_1 = 145.0

Table 1: Values of x_1 and c_1 1 min after injection ends (for τ_3=240 min at the end of the injection time)

Task b: Identification. The identification of the model was done with the Levenberg-Marquardt algorithm, using the known algebraic solutions of type $c_1(t) = b_1 \cdot e^{-\lambda_1 \cdot t} + b_2 \cdot e^{-\lambda_2 \cdot t}$

In order to improve efficiency of the identification, the parameters b_1, b_2 and λ_1, λ_2 were identified in two steps (b_i depend only linear). These "indirect" parameters then "recalculate" the "true" parameters:

```
% Caculate "linear" parameters
B = zeros(length(t),2); B(:,1) = exp(-lam(1)*t);…
%solve B*b = c1 for linear parameters b
z = B*b; f = z-c1;   %compute error (residual)
% Call Identification (Optimisation)
options = optimset
(…,'iter','LevenbergMarquardt','TolX',0.00,…)
[lam,resnorm,residual,exitflag,output]=
  lsqnonlin('C15conc',lam,[],[],options,Datas,h)
% Recalculation of true parameters
k01 = (lam(1)*lam(2)*(b(1)+b(2)))/   …
V1 = D/(b(1)+b(2))
```

The identified values are: k_{01} = 0.0042, k_{12} = 0.0581, k_{21} = 0.0501, V_1 = 7.2150; Clearance C = k_{01}*V_1*1000 = 30.303, residuum 260.8067. Fig. 3 shows result graphically

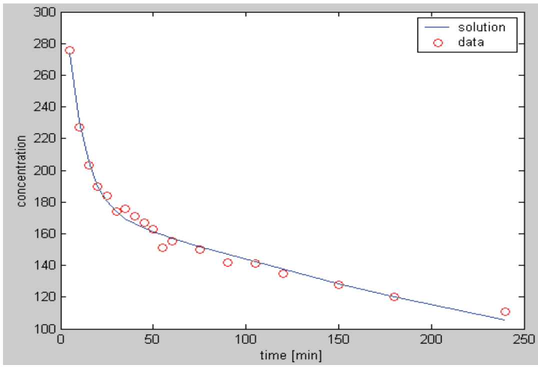

Figure 3: Identified model and measured data

Task c: Error Estimation. Data are disturbed at MATLAB level, for each set of the disturbed data the numerical identification is performed.

	k_{01}	k_{12}	k_{21}	V_1
mean	0.0042	0.0579	0.0512	7.2055
sd	0.0005	0.0085	0.0117	0.4411

Table 2: Mean and standard deviation (sd) of identified parameters, based of 1000 samples

C15 Classification: Programmed Fully Numerical Approach

Simulator: MATLAB Rel.12 with Optimisation Toolbox