% nlin_fit_kinetics.m

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%
% This MATLAB m-file predicts the concentrations
% of the species at several times for a reaction
% network of the two reactions :
%     A + B --> C
%     C + B --> D
%
% The two parameters to be fixed are the rate
% constants for each reaction.
%
% The data to be fit are the concentrations of
% species A, C, and D for various times for
% several experiments of initial concentrations
% of A and B.
%
% K. Beers
% MIT ChE
% 12/9/2001

function [yhat,iflag] = nlin_fit_kinetics(theta,Param_fix);

iflag = 0;

num_exp = 3;
num_species_data = 3;

% We now allocate memory for the vector of model predictions.
num_data = num_species_data*sum(Param_fix.num_time_data);
yhat = zeros(num_data,1);

% We now perform each dynamic simulation.
count = 0;
for iexp = 1:num_exp
   [t_traj,y_traj] = ode15s(@nlin_fit_kinetics_tdot, ...
      Param_fix.time_data(iexp,1:Param_fix.num_time_data(iexp)), ...
      Param_fix.conc_init(iexp,:)',[],theta);
   % We then extract the model predictions.
   % A
   yhat(count+1:count+Param_fix.num_time_data(iexp)) = ...
      y_traj(:,1);
   count = count + Param_fix.num_time_data(iexp);
   % C
   yhat(count+1:count+Param_fix.num_time_data(iexp)) = ...
      y_traj(:,3);
   count = count + Param_fix.num_time_data(iexp);
   % D
   yhat(count+1:count+Param_fix.num_time_data(iexp)) = ...
      y_traj(:,4);
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    count = count + Param_fix.num_time_data(iexp);
end

iflag = 1;

return;
```