Solution of a Partial Differential Equations using the Method of Lines

Partial differential equations where there are several independent variables have a typical general form

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

A problem involving PDE's requires specification of initial values and boundary conditions.

Solved Examples are available in the Cutlip and Shacham (2007) book (Probs. 6.8 and 9.14) and in the publication:

Cutlip, M. B. and M. Shacham, "The Numerical Method of Lines for Partial Differential Equations", CACHE News, No. 47, 18-21(1998) (http://www.polymath-software.com/papers/cachen2.pdf)

Unsteady-state Diffusion and Reaction in a Semi-Infinite Slab
Solution by the Method of Lines

Differential Equations: 20 | Auxiliary Equations: 5 | Ready for solution

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d(CA2)/d(t) = DAB * (CA3 - 2 * CA2 + CA1) / deltax ^ 2 - kprime * CA2 # Concentration of A at distance of deltax from the top
d(CA3)/d(t) = DAB * (CA4 - 2 * CA3 + CA2) / deltax ^ 2 - kprime * CA3 # Concentration of A at distance of 2*deltax from the top
d(CA4)/d(t) = DAB * (CA5 - 2 * CA4 + CA3) / deltax ^ 2 - kprime * CA4 # Concentration of A at distance of 3*deltax from the top
d(CA5)/d(t) = DAB * (CA6 - 2 * CA5 + CA4) / deltax ^ 2 - kprime * CA5 # Concentration of A at distance of 4*deltax from the top
d(CA6)/d(t) = DAB * (CA7 - 2 * CA6 + CA5) / deltax ^ 2 - kprime * CA6 # Concentration of A at distance of 5*deltax from the top
d(CA7)/d(t) = DAB * (CA8 - 2 * CA7 + CA6) / deltax ^ 2 - kprime * CA7 # Concentration of A at distance of 6*deltax from the top
d(CA8)/d(t) = DAB * (CA9 - 2 * CA8 + CA7) / deltax ^ 2 - kprime * CA8 # Concentration of A at distance of 7*deltax from the top
d(CA9)/d(t) = DAB * (CA10 - 2 * CA9 + CA8) / deltax ^ 2 - kprime * CA9 # Concentration of A at distance of 8*deltax from the top
d(CA10)/d(t) = DAB * (CA11 - 2 * CA10 + CA9) / deltax ^ 2 - kprime * CA10 # Concentration of A at distance of 9*deltax from the top
d(CA11)/d(t) = DAB * (CA12 - 2 * CA11 + CA10) / deltax ^ 2 - kprime * CA11 # Concentration of A at distance of 10*deltax from the top
d(CA12)/d(t) = DAB * (CA13 - 2 * CA12 + CA11) / deltax ^ 2 - kprime * CA12 # Concentration of A at distance of 11*deltax from the top
d(CA13)/d(t) = DAB * (CA14 - 2 * CA13 + CA12) / deltax ^ 2 - kprime * CA13 # Concentration of A at distance of 12*deltax from the top
d(CA14)/d(t) = DAB * (CA15 - 2 * CA14 + CA13) / deltax ^ 2 - kprime * CA14 # Concentration of A at distance of 13*deltax from the top
d(CA15)/d(t) = DAB * (CA16 - 2 * CA15 + CA14) / deltax ^ 2 - kprime * CA15 # Concentration of A at distance of 14*deltax from the top
d(CA16)/d(t) = DAB * (CA17 - 2 * CA16 + CA15) / deltax ^ 2 - kprime * CA16 # Concentration of A at distance of 15*deltax from the top
d(CA17)/d(t) = DAB * (CA18 - 2 * CA17 + CA16) / deltax ^ 2 - kprime * CA17 # Concentration of A at distance of 16*deltax from the top
d(CA18)/d(t) = DAB * (CA19 - 2 * CA18 + CA17) / deltax ^ 2 - kprime * CA18 # Concentration of A at distance of 17*deltax from the top
d(CA19)/d(t) = DAB * (CA20 - 2 * CA19 + CA18) / deltax ^ 2 - kprime * CA19 # Concentration of A at distance of 18*deltax from the top
d(CA20)/d(t) = DAB * (CA21 - 2 * CA20 + CA19) / deltax ^ 2 - kprime * CA20 # Concentration of A at distance of 19*deltax from the top
d(Q)/d(t) =  - DAB * ( - 3 * CA1 + 4 * CA2 - CA3) / (2 * deltax) # Total amount of A transferred to the solution (kg-mol/m^2)

# The explicit equations
CA1 = .03 # Concentration of A at top
CA21 = 0 # Concentration of A at bottom
DAB = 1.5e-9 # Diffusivity coefficient (m^2/s)
deltax = 5.0e-7 # Length of finite difference section
kprime = 35 # First order reaction rate constant (1/s)

# Initial values of the differential variables
CA2(0) = 0
CA3(0) = 0
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Solving Differential-Algebraic System of Equations (DAE's) using the Controlled Integration Method

The system defined by the equations:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(\mathbf{y}, \mathbf{z}, x)$$

$$\mathbf{g}(\mathbf{y}, \mathbf{z}) = 0$$

with the initial conditions $\mathbf{y}(\mathbf{x}_0) = \mathbf{y}_0$ is called a system of differential-algebraic equations. Solved examples are available in the Cutlip and Shacham (2007) book (Prob 6.7) and in the reference:

Shacham, M., N. Brauner and M. B. Cutlip, "Prediction and Prevention of Chemical Reaction Hazards – Learning by Simulation", *Chem. Eng. Educ.*, 35(4), 268-273(2001) (http://www.polymath-software.com/papers/CEE_35_268_01.pdf)

Batch distillation of an ideal binary mixture

Line	Equation
1	d(L)/d(x2)=L/(k2*x2-x2)
2	d(T)/d(x2)=Kc*err
3	Kc=0.5e6
4	k2=10^(6.95464-1344.8/(T+219.482))/(760*1.2)
5	x1=1-x2
6	k1=10^(6.90565-1211.033/(T+220.79))/(760*1.2)
7	err=(1-k1*x1-k2*x2)
8	x2(0)=0.4
9	L(0)=100
10	T(0)=95.5851
11	x2(f)=0.8

Variable	Initial value	Minimal value	Maximal value	Final value
err	-3.646E-07	-3.646E-07	7.747E-05	7.747E-05
k1	1.311644	1.311644	1.856602	1.856602
k2	0.5325348	0.5325348	0.7857526	0.7857526
Kc	5.0E+05	5.0E+05	5.0E+05	5.0E+05
L	100.	14.04555	100.	14.04555
T	95.5851	95.5851	108.5693	108.5693
x1	0.6	0.2	0.6	0.2
x2	0.4	0.4	0.8	0.8

Stiff Systems of First-Order ODE's

Systems of ODE's where the dependent variables change on various time (independent variable) scales which differ by many orders of magnitude are called "Stiff" systems.

The characterization of stiff systems and the special techniques that are used for solving such systems are described in detail in problem 6.2 in the Cutlip and Shacham (2007) book. Detailed analysis of a problem for stiffness is demonstrated in the publication:

Shacham, M., N. Brauner, W. R. Ashurst and M. B. Cutlip, "Can I Trust this Software Package? – An Exercise in Validation of Computational Results ", *Chem. Eng. Educ.*, (in press, 2008) (ftp://ftp.bgu.ac.il/shacham/publ_papers/CEE_08.pdf)

Using MATLAB Symbolic Manipulation Capabilities for Investigation Stiffness of an ODE system

No.	Commands
1	syms q1 q2 q3 g h1 h2 h3 H1 Ao D1 D2 g
2	f(1)= (q1 - (Ao * sqrt(2 * g * (h1 - h2)))) / ((pi / 4) * ((D2 + ((D1 - D2) / H1) * h1) ^ 2));
3	f(2)= (q2 + (Ao * sqrt(2 * g * (h1 - h2))- (Ao * sqrt(2 * g * (h2 - h3)))) / (pi * exp(2 * h2));
4	f(3)= ((Ao * sqrt(2 * g * (h2 - h3))) + q3 - ((Ao * sqrt((2 * g * h3))))) / (h3 ^ 2);
5	for i=1:3
6	df(i,1)=diff(f(i),h1);
7	df(i,2)=diff(f(i),h2);
8	df(i,3)=diff(f(i),h3);
9	end
10	Ao = pi / 100; g = 9.81; q1 = 0.05; q2 = 0.05; q3=0.05 + 0.05 * 0.1;
11	H1 = 4; H2 = 2.5; H3 = 2.5; D1 = 4; D2 = 1;
12	h1=1.8656; h2= 1.7367; h3=1.2282;
13	df_numeric=subs(df);
14	format long g
15	Lambda=eig(df_numeric)

Derive the elements of the Jacobian matrix

Introduce numerical values into the Jacobian

The ratio between the max. and min. eigenvalues of the Jacobian matrix serves as an indicator for the stiffness of the problem

Parameter Estimation in Dynamic Systems

The (system) of ordinary differential equations

$$\frac{d\hat{y}}{dt} = f(a_0, a_1 \ldots a_n, x_1, x_2, \ldots x_n, t)$$

is used to model the data by finding the values of the parameters a_0, a_1 … a_n that minimize the squares of the errors

$$S = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Solution of such problems requires the integration of the differential equations in an inner loop in order to obtain the $\hat{y}_i$ values and minimizing S as function of a_0, a_1 … a_n in an outer loop.

A solved example is available in the Cutlip and Shacham (2007) book (Prob. 6.9)

ESTIMATING MODEL PARAMETERS INVOLVING ODE'S USING FERMENTATION DATA

When the microorganism *Penicillium Chrysogenum* is grown in a batch fermenter under carefully controlled conditions, the cells reproduce at a rate which can be modeled by the logistic law

$$\frac{dy_1}{dt} = b_1 y_1\left(1 - \frac{y_1}{b_2}\right) \qquad \textbf{(6-49)}$$

where y_1 is the concentration of the cells expressed as percent dry weight. In addition, the rate of production of penicillin has been mathematically quantified by the equation where y_2 is the units of penicillin per mL.

$$\frac{dy_2}{dt} = b_3 y_1 - b_4 y_2 \qquad \textbf{(6-50)}$$

(a) Use the experimental data in Table 6–22 to find the values of the parameters b_1, b_2, b_3 and b_4 which minimize the sum of squares of the differences between the calculated and experimental concentrations (y_1 and y_2) for all the data points. The following initial estimates can be used: $b_1 = 0.1$; $b_2 = 4.0$; $b_3 = 0.02$ and $b_4 = 0.02$.

(b) Plot the calculated and experimental values of y_1 and y_2 using the optimal parameter values.

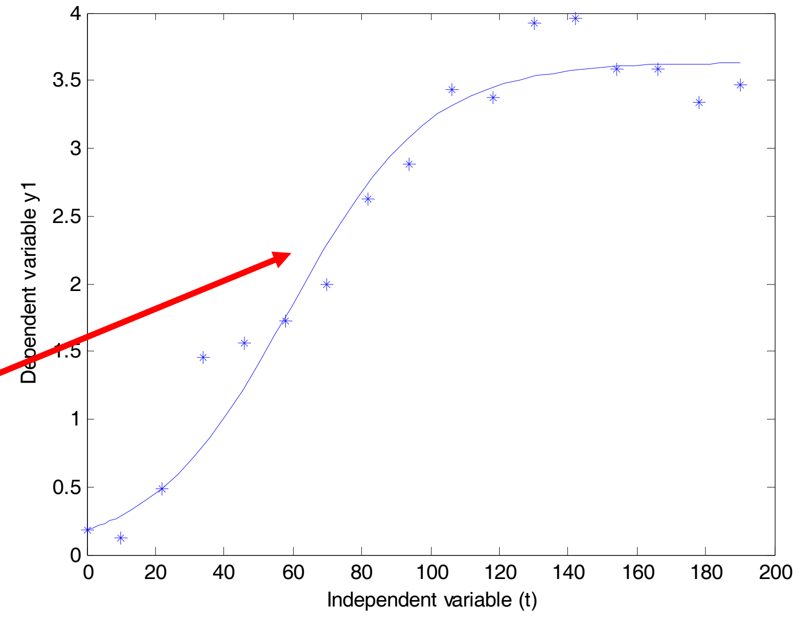
ESTIMATING MODEL PARAMETERS INVOLVING ODE'S USING FERMENTATION DATA

Data

Time h	Cell Concentration Percent Dry Weight y_1	Penicillin Concentration Units/mL y_2
0	0.18	0
10	0.12	0
22	0.48	0.0089
34	1.46	0.0642
46	1.56	0.2266
58	1.73	0.4373
70	1.99	0.6943
82	2.62	1.2459
94	2.88	1.4315
106	3.43	2.0402
118	3.37	1.9278
130	3.92	2.1848
142	3.96	2.4204
154	3.58	2.4615
166	3.58	2.283
178	3.34	2.7078
190	3.47	2.6542

Function evaluation No. 1 Sum of Squares 36.1271	
Function evaluation No. 63 Sum of Squares 1.5582	
Optimal Results	
Parameter Number	Value
1	0.049875
2	3.634
3	0.020459
4	0.02652
Final Sum of Squares 1.4358 Function evaluations 268	

Parameter values



Plot of experimental vs. calculated

Nonlinear Programming (Optimization) with Equity Constraints

The nonlinear programming problem with equity constrains is defined by:

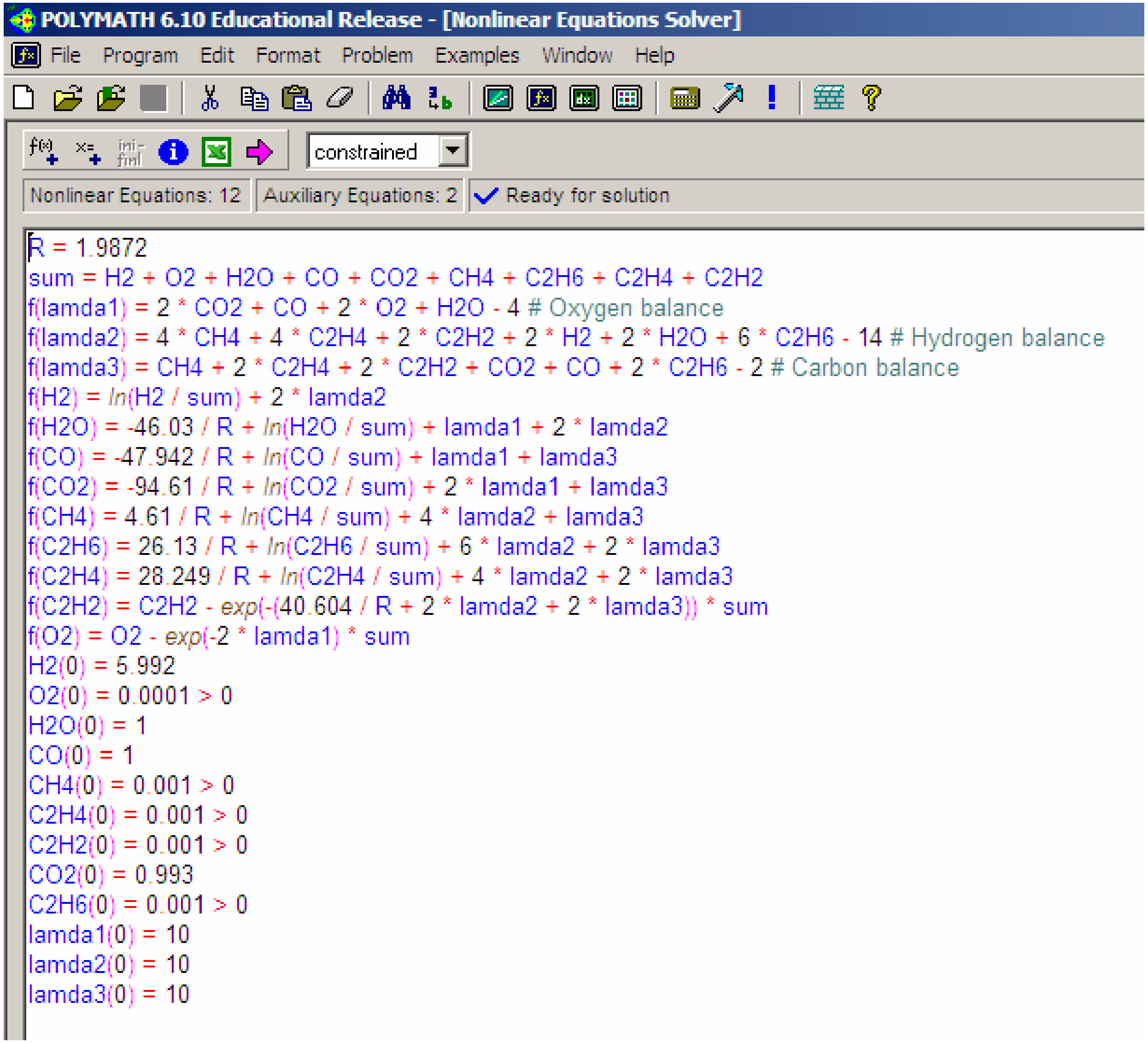
$$\begin{aligned} &\textit{Minimize} \quad f(\mathbf{x}) \\ &\textit{Subject to} \quad \mathbf{h}(\mathbf{x}) = \mathbf{0} \end{aligned}$$

where f is a function, **x** is an *n* - vector of variables and **h** is an *m*-vector (*m*<*n*) of

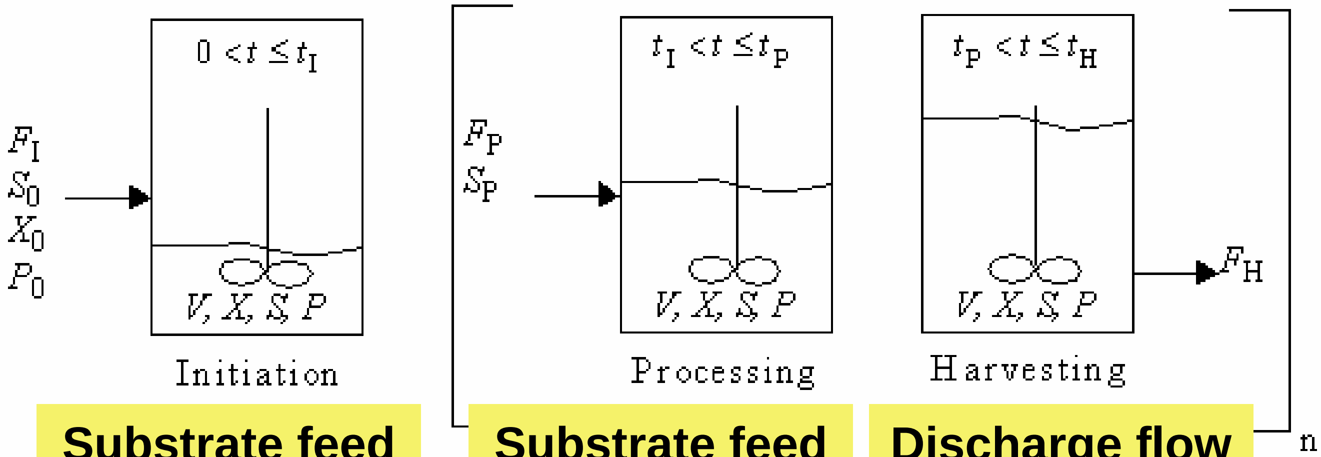
Solution of such problems requires the inclusion of the constraints in the objective function using Lagrange multipliers, differentiating the objective function and solving the resultant system of NLEs.

Solved examples are available in the Cutlip and Shacham (2007) book (Probs. 4.5 and 5.5)

Complex Chemical Equilibrium by Gibbs Energy Minimization



Three Modes in the Operation of the Semi-batch Bioreactor



Substrate feed rate F_I **Final volume V_I**	**Substrate feed rate F_P** **Final Volume V_H**	**Discharge flow rate F_H** **Final Volume V_I**

***n* – cycle number**

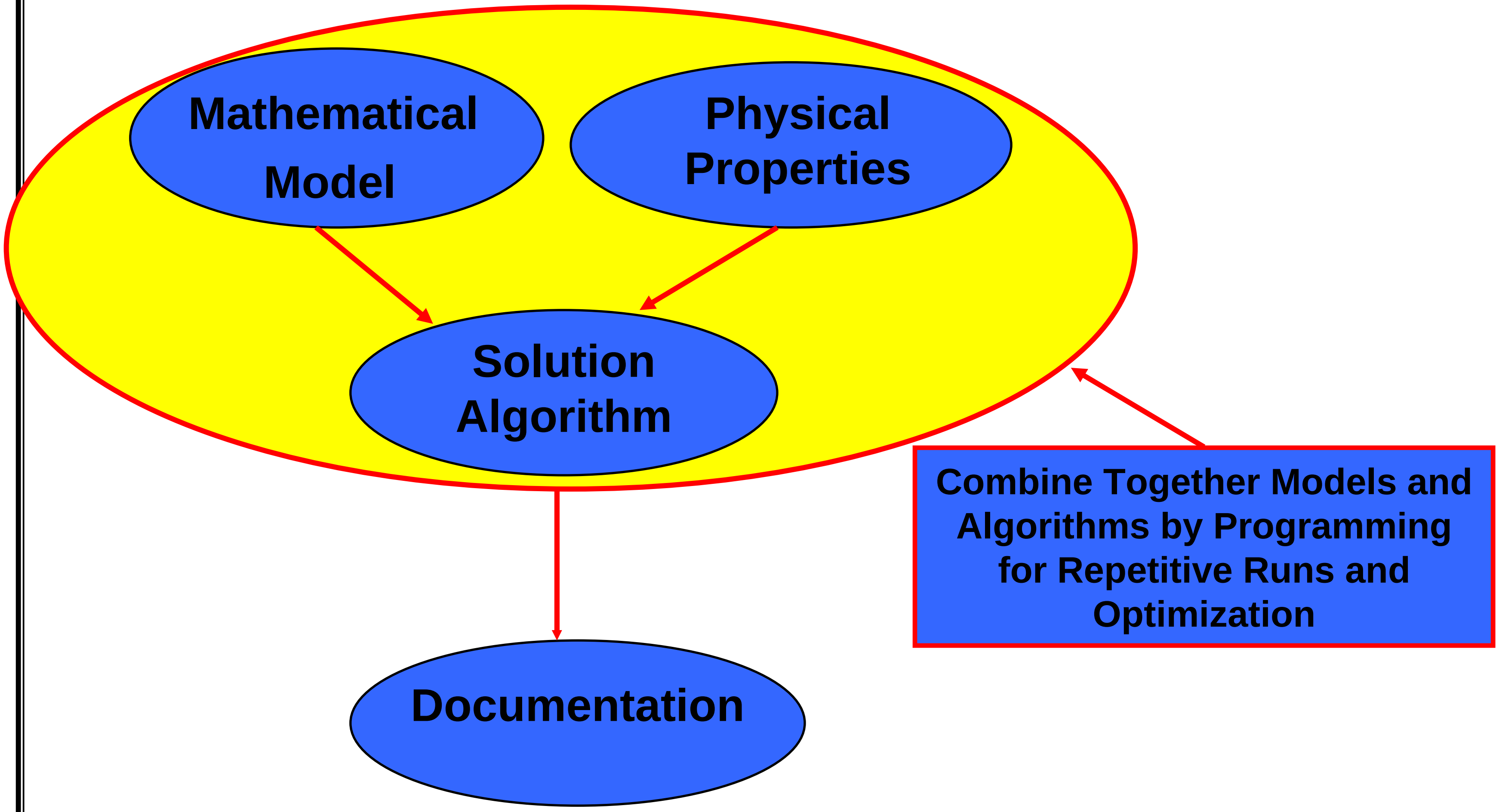
***n* = 1 fed-batch operation**

S (substrate reactant) + X (cell) = P (product) + nX

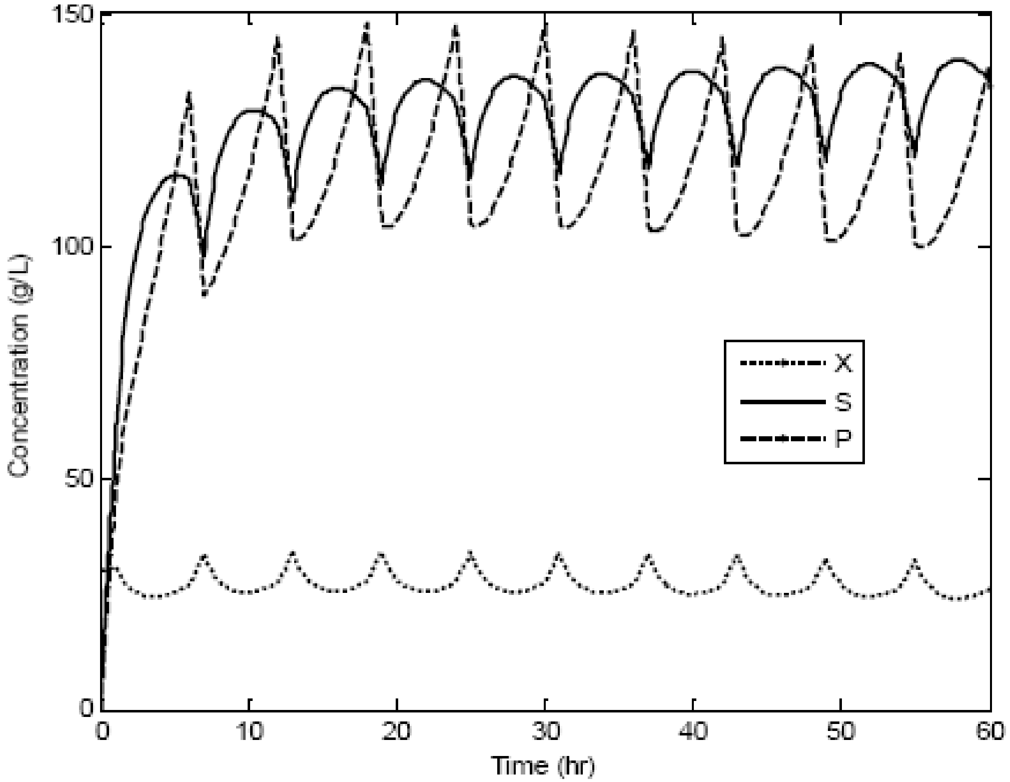
The biochemical reaction is inhibited by the substrate

Optimal substrate feed concentration is required with fixed set of operating conditions

Solution of Multiple Model – Multiple Algorithm Problems



Three Modes in the Operation of the Semi-batch Bioreactor Results of Ten Cycles of Processing and Harvesting



Complete details of the solution can be found in the Cutlip and Shacham (2007) book (Prob.14.13) and the site: http://www.engr.uconn.edu/~cutlipm/escape17

Skills Needed for Solving Various Types of Problems

Introductory Level – Linear Eqs., NLEs, ODE – IVP, Regression

1. Categorize the problem according to the numerical solution technique to be used for its solution.

2. Use one software package (say, POLYMATH) to solve single model – single algorithm problems for one or a few sets of parameter values

3. Use 95% confidence intervals and residual plots to analyze regression results

4. Use a spreadsheet or programming for parametric runs and for preparing graphical and tabular summaries of the results

Skills Needed for Solving Various Types of Problems

Advanced Level – NLEs, ODE – BVP, DAE, PDE and Multiple Model – Multiple Algorithm Problems

1. Acquire familiarity with the basic numerical methods for solving NLEs, ODEs, DAEs and PDEs

2. Use programming to combine several algorithms to solve single model multiple algorithm problems (i.e. ODE BVP)

3. Use programming to combine several models to solve multiple model single algorithm problems (i.e. various stages of operation of a reactor)

4. Use programming to combine several models and algorithms to solve multiple model- multiple algorithm problems