CHE 572: ASSIGNMENT #1.

SOLUTIONS.

(1)

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = \begin{bmatrix} x_1^2 + 6x_1x_2 + x_2^2 + 4x_1 + 3x_2 + 12 \\ 2x_1^2 + 2x_2^2 - 2x_1x_2 \end{bmatrix} = 0$$

Jacobian of $f(x)$:

$$J[f(x)] = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}.$$

- $\frac{\partial f_1}{\partial X_1} = 2X_1 + 6X_2 + 4.$
- $\frac{\partial f_1}{\partial X_2} = 6X_1 + 2X_2 + 3.$
- $\frac{\partial f_2}{\partial X_1} = 4X_1 - 2X_2.$
- $\frac{\partial f_2}{\partial X_2} = 4X_2 - 2X_1.$

Substituting the differential terms into the expression $J[f(x)]$:

$$J[f(x)] = \begin{bmatrix} 2X_1 + 6X_2 + 4 & 6X_1 + 2X_2 + 3 \\ 4X_1 - 2X_2 & 4X_2 - 2X_1 \end{bmatrix}$$

(2)

$$r(x) = \frac{\mu_{max} \cdot x_1 x_2}{K_m + x_2}.$$

Gradient of $r(x)$ is given as:

$$\nabla r(x) = \frac{\partial r}{\partial x_1}\hat{i} + \frac{\partial r}{\partial x_2}\hat{j} \quad \text{—— (2a)}$$

Now, $\frac{\partial r}{\partial x_1} = \frac{\mu_{max} \cdot x_2}{K_m + X_2}$; $\frac{\partial r}{\partial X_2} = \frac{(K_m + x_2)\mu_{max} x_1 - \mu_{max} x_1 x_2}{[K_m + x_2]^2}$

$$= \frac{K_m \mu_{max} x_1}{[K_m + x_2]^2}$$

Substituting the differential terms into (2a):

$$\nabla r = \left[\frac{\mu_{max} X_2}{K_m + X_2} \hat{i} + \frac{K_m \mu_{max} X_1}{[K_m + X_2]^2} \hat{j} \right]$$

3) a)

Second-order Taylor series expansion of a single variable function $f(x)$ about $x = x_0$ is given as:

$$f(x) \approx f(x_0) + \left.\frac{df(x)}{dx}\right|_{x=x_0} (x - x_0) + \frac{1}{2!} \left.\frac{d^2f(x)}{dx^2}\right|_{x=x^0} (x - x_0)^2 \quad \text{—(3a)}$$

When $f(x) = xe^{-x}$, the differential terms in Eq.(3a) can be written as:

$$\frac{df(x)}{dx} = e^{-x} - xe^{-x} = (1-x)e^{-x};$$

$$\frac{d^2f(x)}{dx^2} = -e^{-x} - e^{-x} + xe^{-x} = (x-2)e^{-x}$$

Substituting the differential terms into (3a) yields:

$$xe^{-x} \approx x_0 e^{-x_0} + (1-x_0)e^{-x_0}(x - x_0) + \frac{1}{2!}(x_0 - 2)e^{-x_0}(x - x_0)^2$$

b) Second order Taylor series expansion of a multivariable function $f(\underline{x})$ about $\underline{x}_0$ is given as:

$$f(\underline{x}) \approx f(\underline{x}_0) + \left.\nabla f(\underline{x})\right|_{\underline{x}=x_0} (\underline{x} - \underline{x}_0) + \frac{1}{2!} (\underline{x} - \underline{x}_0)^T \left.\nabla^2 f(\underline{x})\right|_{\underline{x}=x_0} (\underline{x} - \underline{x}_0)$$

when $f(\underline{X}) = \dfrac{\mu_{max}\, X_1 X_2}{Km + X_2}$ and $\underline{X} = [X_1 \quad X_2]$

$\underline{X}_0 = [X_1^0 \quad X_2^0]$, the

differential terms in (3b) can be calculated as follows:

Jacobian matrix $\longrightarrow$ $$\nabla f(\underline{X}) = \begin{bmatrix} \dfrac{\partial f(\underline{X})}{\partial X_1} & \dfrac{\partial f(\underline{X})}{\partial X_2} \end{bmatrix}$$

Hessian matrix $\longrightarrow$ $$\nabla^2 f(X) = \begin{bmatrix} \dfrac{\partial^2 f(\underline{X})}{\partial X_1^2} & \dfrac{\partial^2 f(\underline{X})}{\partial X_1 \partial X_2} \\ \dfrac{\partial^2 f(\underline{X})}{\partial X_2 \partial X_1} & \dfrac{\partial f^2(\underline{X})}{\partial X_2^2} \end{bmatrix}$$

where:

$$\frac{\partial f(\underline{X})}{\partial X_1} = \frac{\mu_{max}\, X_2}{Km + X_2};$$

$$\frac{\partial f(X)}{\partial X_2} = \frac{Km\, \mu_{max}\, X_1}{[Km + X_2]^2};$$

$$\frac{\partial^2 f(\underline{X})}{\partial X_1^2} = 0 \; ; \; \frac{\partial^2 f(\underline{X})}{\partial X_1 \partial X_2} = \frac{\partial^2 f(X_1)}{\partial X_2 \partial X_1} = \frac{Km\, \mu_{max}}{[Km + X_2]^2};$$

$$\frac{d^2 f(\underline{X})}{\partial X_2^2} = -\frac{2 Km\, \mu_{max}\, X_1}{[Km + X_2]^3}$$

Substituting the differential terms into (3b) yields:

$$f(\underline{X}) \approx \frac{\mu_{max}\, X_1^0 X_2^0}{Km + X_2^0} + \begin{bmatrix} \dfrac{\mu_{max}\, X_2^0}{Km + X_2^0} & \dfrac{Km\, \mu_{max}\, X_1^0}{[Km + X_2^0]^2} \end{bmatrix} [\underline{X} - \underline{X}_0]$$

$$+ \frac{1}{2!} [\underline{X} - \underline{X}_0]^T \begin{bmatrix} 0 & \dfrac{Km\, \mu_{max}}{[Km + X_2^0]^2} \\ \dfrac{Km\, \mu_{max}}{[Km + X_2^0]^2} & \dfrac{-2 Km\, \mu_{max}\, X_1^0}{[Km + X_2^0]^3} \end{bmatrix} [\underline{X} - \underline{X}_0].$$

4) a)

Solver	Method
ode45	Runge-kutta
ode23	Runge-kutta
ode113	Adams-Bashforth-Moolton
ode15s	Numerical differentiation formulas
ode23s	Rosenbrock formula
ode23t	Trapizoidal rule
ode23tb	Trapizoidal + backward differentiation formula

b) $$\begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix} \frac{dx}{dt} = \begin{bmatrix} 10^6 & 0 \\ 0 & 1 \end{bmatrix} \underline{x} + \begin{bmatrix} 473 \\ 5 \end{bmatrix} \underline{u}$$

inverting the matrix premultiplying $\frac{dx}{dt}$ term, we obtain the state-space model in the standard form

$$\frac{dx}{dt} = \begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 10^6 & 0 \\ 0 & 1 \end{bmatrix} \underline{x} + \begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 473 \\ 5 \end{bmatrix} \underline{u}$$

$$\frac{dx}{dt} = \underbrace{\begin{bmatrix} 0 & 0.5 \\ 10^6 & 0 \end{bmatrix}}_{\to \underline{\underline{A}}} \underline{x} + \begin{bmatrix} 2.5 \\ 473 \end{bmatrix} \underline{u}$$

The eigenvalues of $\underline{\underline{A}}$ are: 707.1068 ; -707.1068 .

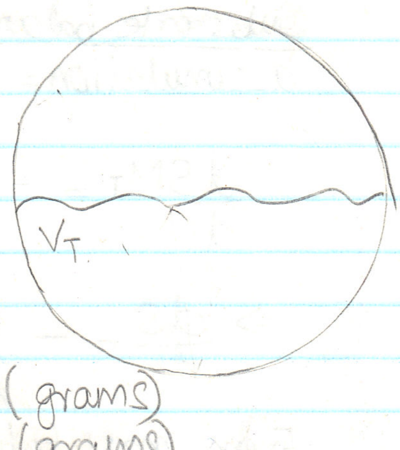
from the eigenvalues of $\underline{\underline{A}}$, it is evident that the dynamics of both x_1 and x_2 change equally fast. The opposite signs just indicate the direction of that change.

Therefore, the given set of ODEs constitute a non-stiff problem for which, use of any Runge-kutta based solver would suffice.

c) ode45 : (i) Non-stiff problem solver (ii) medium order of accuracy. (iii) Computationally fast.

Notations.

M_T : Total mass of the liquid inside the kettle (grams)



V_T : Total volume of the liquid inside the kettle (litres).

S : Mass fraction of substrate

E : Mass fraction of ethanol.

Y : Mass fraction of yeast

M_E : Mass of ethanol inside the kettle (grams)

M_S : Mass of substrate " " " (grams)

M_Y : Mass of yeast " " " (grams)

M_W : Mass of water " " " (grams)

ρ : density of liquid at any given time 't' (grams/litre).

S_0 : initial mass fraction of substrate

E_0 : initial mass fraction of ethanol.

a)

Variables	INPUTS		OUTPUTS			States
	manip.	dist.	meas.	unmeas.	control	
M_T						✓
M_E						✓
M_Y						✓
M_W						✓
S				✓		
E				✓		
Y				✓		

6) **Assumptions:**

1.) ideal mixing conditions.

2.) Net change in the density & volume of the solution is negligible.

3) No initial mass of ethanol or yeast i.e., $E_0 = 0$ & $Y_0 = 0$

Substrate balance

$$\text{accumulation} = \cancelto{0}{\text{flow in}} - \cancelto{0}{\text{flow out}} + \cancelto{0}{\text{generation}} - \text{consumption}$$

$$\frac{dSM_T}{dt} = -\mu SM_T \qquad \text{where } SM_T \doteq M_S$$

$$\Rightarrow \frac{dS}{dt} = -\frac{\mu_{max} S}{K_m + S} \quad \text{— (1)}$$

From mass balance, we also know that mass of substrate consumed = mass of yeast and ethanol produced:

$$\text{i.e., } \underbrace{S_0M_T - SM_T}_{\text{mass of substrate consumed}} = \underbrace{EM_T}_{\text{mass of ethanol produced}} + \underbrace{YM_T}_{\text{mass of yeast produced}} \quad \text{— (2)}$$

Also: $EM_T = YM_T$ (given) — (3)

∴ Substituting (3) into (2) yields:

$$S_0M_T - SM_T = 2EM_T$$

$$\Rightarrow \frac{S_0 - S}{2} = E = Y \quad \text{— (4)}$$

differentiating (4) w.r.t. 't':

$$\frac{dE}{dt} = \frac{-1}{2}\frac{dS}{dt} = \frac{1}{2}\frac{\mu_{max} \cdot S}{K_m + S} \quad \text{— (5)}$$

Similarly, $$\frac{dY}{dt} = \frac{1}{2}\frac{\mu_{max} S}{K_m + S} \quad \text{— (6)}$$

Finally, the dynamic model of the system is given as

$$\frac{dS}{dt} = -\frac{\mu_{max} S}{k_m + S}$$

$$\frac{dE}{dt} = \frac{1}{2}\frac{\mu_{max} S}{k_m + S}$$

$$\frac{dY}{dt} = \frac{1}{2}\frac{\mu_{max} S}{k_m + S}.$$

d) The above model is non-linear w.r.t the variable 'S'.

e.) Refer to Fig. 1.

f) Refer to Fig 2.

g) liquid level 'h' in the kettle doesn't depend on the length of time. See Assumption (2)

Appendix

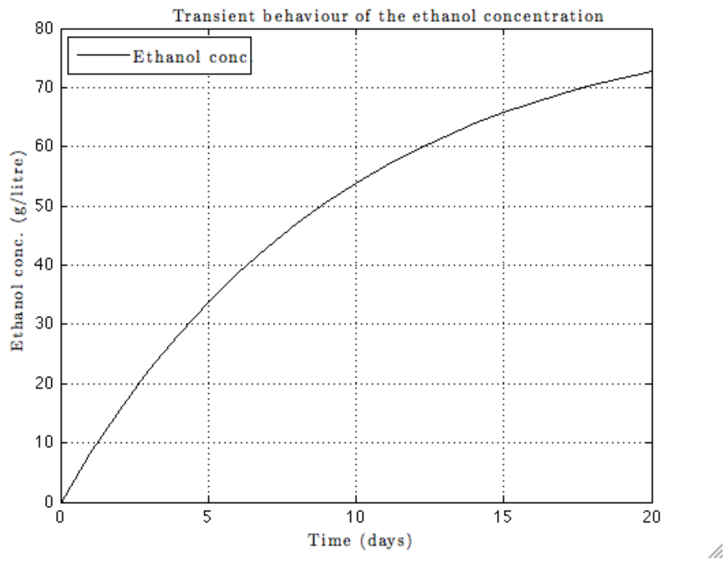
- $V_T = 20$ litres (See Assumption (2))
- $M_T = \underbrace{17 \times 1000}_{\text{mass of water}} + \underbrace{3200}_{\text{mass of malt}} + \underbrace{100}_{\text{mass of hops}} = 20300$ grams

- $S_0 = \dfrac{3200 + 100}{M_T} = \dfrac{3300}{20300} = 0.1626$

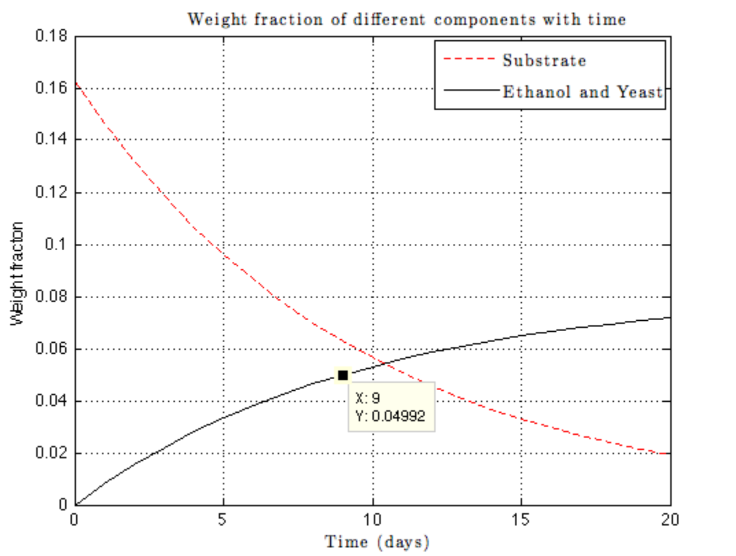
- $E_0 = 0$
- $Y_0 = 0$ } (See Assumption 3)

- $k_M = 5$
- $\mu_{max} = 0.54 \text{ days}^{-1}$

e)



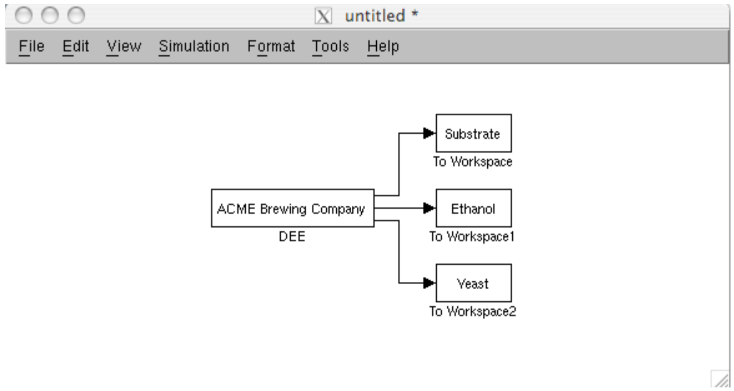
f)



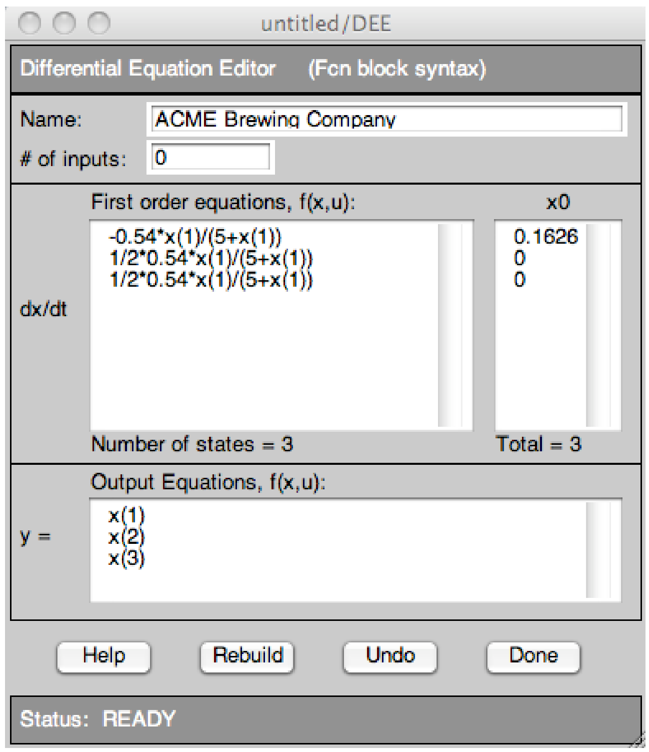
A batch of beer with 5wt% ethanol content takes approximately 9 days of brewing time.

Mixture composition at the end of a batch:

Ethanol=	5%	(see the DataTip on the graph)
Yeast=	5%	(since Ethanol production=Yeast production)
Substrate=	6.27%	(Also from the graph)
Water=	83.33%	



SIMULINK sheet



System model with initial conditions