
NOTE: The exam starts on Monday, April 23 at 9:30 AM and must be handed in at the Physics Main Office (MCD 124) on Wednesday, April 25 before 10:00 AM. **After that time no document will be accepted.** You can use your lecture notes and your subroutines library but you do not need anything else. In particular, you do not need the help of your classmates. For the first two questions, illustrate your solutions with appropriate graphs, briefly discuss your results and provide a copy of your code.

- If you are a student in **PHY 5340**, **do all questions** (no. 3 is analytical, but straightforward and quite short).
- If you are a student in **PHY 4140**, **do question 1** and **question 2.**

1. A CLASSICAL LENNARD-JONES MOLECULE

Consider the following classical diatomic molecule, made up of two atoms of mass m_1 and m_2 located at the vector-position $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. The interaction between the two atoms is of the Lennard-Jones type. The force $\mathbf{F}_{12}$ acting on m_1 due to m_2 is then:

$$\mathbf{F}_{12} = m_1\mathbf{a}_1 = -\nabla_1 V \; ; \quad V = 4V_o((a/r)^{12} - (a/r)^6) \tag{1}$$

where V_o is a positive energy scale (ionization energy), a is a length scale, $\mathbf{a}_1$ is the acceleration of the atom 1 and

$$r = |\mathbf{r}_1 - \mathbf{r}_2| \tag{2}$$

is the distance between the two atoms. Of course, from Newton's third law of motion, the force acting on m_2 due to m_1 is

$$\mathbf{F}_{21} = -\mathbf{F}_{12} = m_2\mathbf{a}_2 \,. \tag{3}$$

The force is central and, consequently, the orbits (trajectories) of the atoms will lie on a plane, the XY plane, say. The gradient term in Eq. (1) can then be written as derivative with respect to the Cartesian coordinates of atom 1:

$$\nabla_1 = \mathbf{i}\frac{\partial}{\partial x_1} + \mathbf{j}\frac{\partial}{\partial y_1} \tag{4}$$

where $\mathbf{i}$ and $\mathbf{j}$ are basis vectors in the X and Y direction, respectively.

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a) Choose your frame of reference so that the center of mass of the system is at rest and fixed at the origin:

$$m_1\mathbf{r}_1 + m_2\mathbf{r}_2 = 0; \quad m_1\mathbf{v}_1 + m_2\mathbf{v}_2 = 0\,. \tag{5}$$

Show that the equation of motion of the first atom can be written in terms of its coordinates $\mathbf{r}_1$=$\mathbf{i}x_1$+$\mathbf{j}y_1$ as:

$$m_1\mathbf{a}_1 = 24\frac{V_0}{r_1^2}\alpha^7\left[2\alpha^6\left(\frac{a}{r_1}\right)^{12} - \left(\frac{a}{r_1}\right)^6\right]\mathbf{r}_1\,. \tag{6}$$

where $\alpha = \dfrac{m_2}{m_1 + m_2}$ (with $0<\alpha<1$).

b) Choose a as length scale and $a\sqrt{m_1/V_0}$ as time scale. Simplify the equation of motion (6) in terms of scaled variables.

c) Using appropriate initial conditions for the two atoms, find their orbit (numerically) by using the Størmer-Verlet algorithm. Use the predictor-corrector approach suggested at the end of chapter 3 in order to estimate the position vector of the first atom $\mathbf{r}_1(h)$ at the first time step $t = h$:

$$\mathbf{r}_1(h) \approx \mathbf{r}_1(0) + h\mathbf{v}_1(0) + \frac{h^2}{2}(\mathbf{a}_1(0) + \mathbf{a}_1(h))/2\,.$$

Here, h is the time step. The acceleration of the first atom at time h, $\mathbf{a}_1(h)$, is estimated using the approximate position $\mathbf{r}_1$* defined as:

$$\mathbf{r}_1^* \approx \mathbf{r}_1(0) + h\mathbf{v}_1(0) + \frac{h^2}{2}\mathbf{a}_1(0)\,.$$

In particular, obtain orbits for the following three cases:

- The two atoms are just vibrating about their equilibrium position.
- The two atoms are just rotating about their center of mass.
- A more general case where you have both vibration and rotation.

2. MAKING CHATEAU FORTRAN

In this problem, you are going to code a simple but realistic problem in population biology. You will explore numerically the dynamics of grape juice fermentation in a tank of length *L*, whereby micro-organisms (yeasts) transform glucose ($C_6H_{12}O_6$) into alcohol (ethanol, C_2H_5OH) while releasing CO_2. We put the fermentation tank in the horizontal position, so that the effect of yeast settling by gravity is neglected. The chemical reaction of interest is:

$$C_6H_{12}O_6 \xrightarrow{k} 2CO_2 + 2C_2H_5OH + \text{heat}.$$

k(*T*) is the reaction rate coefficient and it depends on temperature *T*. There are a few interesting feedbacks. First, the action of the yeasts is inhibited by a high concentration of ethanol (negative feedback) as is the case for humans. Also, fermentation releases heat, which then accelerates the action of the yeast (positive feedback). This is true up to a point, since the yeasts cease to work when the temperature is too high.

Let's write a simple kinetic model for the time evolution of the yeast population. We set

S = sugar concentration in grams/litre (g/L)
Y = yeast concentration in g/L
A = alcohol concentration in g/L.

The kinetics of *S* is given by:

$$\boxed{\frac{dS}{dt} = -k(T)\frac{YS}{S+K}} \qquad (1)$$

where a so-called Monod kinetic law has been used to describe the activity of the micro-organisms on sugar substrate. *K* is the so-called saturation constant in g/L. The kinetics of *A* is given by:

$$\boxed{\frac{dA}{dt} = 2k(T)\frac{YS}{S+K}\frac{M_A}{M_S}} \qquad (2)$$

where the factor 2 comes from the stoichiometry of the chemical reaction and M_A/M_S is the ratio of the molar mass of ethanol and glucose (necessary to go to concentration units in grams/litre). The kinetics of the yeast population is described by:

$$\boxed{\frac{dY}{dt} = \alpha k(T)\frac{YS}{S+K} - bAY - cY} \qquad (3)$$

where the dimensionless factor α (the yield) describes the efficiency with which the yeasts feed on glucose and reproduce, *b* is the inhibition (death) rate due to alcohol and c is an intrinsic death rate. These parameters depend on temperature in principle, but we will take them as constants. The temperature (in degrees K) is defined by the conduction problem:

$$\boxed{\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} + hk(T)\frac{YS}{S+K};} \qquad (4)$$

where D is the thermal diffusivity of the grape juice (considered constant) and the second term describes the temperature raise due to the heat of reaction. h is a constant expressed in degrees per sugar concentration unit. The boundary conditions and initial condition are:

$$\boxed{T(x,0) = T_0; \quad T(0,t) = T_0; \quad \frac{\partial T}{\partial x}(L,t) = 0}. \qquad (5)$$

They correspond to a fixed temperature at the origin (x=0) of the fermentation tank and a thermally insulated condition at the other end of the tank (x=L).
Finally, we model the rate coefficient $k(T)$ as:

$$\boxed{k(T) = k_0 \exp(-E/T)\Theta(T)} \qquad (6)$$

where k_0 is a constant, E is an activation energy describing the fact that the rate is faster at higher temperatures and Θ is a piecewise decaying function:

$$\boxed{\Theta(T) = \begin{cases} \exp(-d(T-T_s)) \text{ for } T > T_s, \\ = 1 \text{ for } T \le T_s. \end{cases}}. \qquad (7)$$

This function represents the fact that the action of the yeasts slows down substantially when the temperature is higher than some threshold T_s. d is the efficiency factor for this slowing down.

So far, so good. First, we can easily eliminate the alcohol concentration A by adding 2 times M_A/M_S times Eq. (1) to Eq. (2). The result is:

$$2\frac{M_A}{M_S}S + A = \text{constant} = 2\frac{M_A}{M_S}S_0 \Rightarrow$$

$$\boxed{A = 2\frac{M_A}{M_S}(S_0 - S)} \qquad (8)$$

where S_0 is the initial sugar concentration and we have taken into account that there is no alcohol in the initial grape juice. Thus, Eq. (3) becomes:

$$\boxed{\frac{dY}{dt} = \alpha k(T)\frac{YS}{S+K} - 2\frac{M_A}{M_S}b(S_0 - S)Y - cY}. \qquad (9)$$

In summary, the problem is defined by the two ODE (1) and (9), the PDE (4) with its boundary and initial conditions (5) and the rate expression (6, 7). Eq. (8) solves for A.

a) Now, get to work! First, you should scale the problem. Use

- $\bar{t} = [\alpha k_0 \exp(-E/T_0)]^{-1}$ as the time scale, where T_0 is the initial temperature.
- $\bar{x} = \sqrt{D\bar{t}}$ as the space scale,
- the initial (constant in space) yeast concentration Y_0 as the Y scale,
- the initial (constant in space) glucose concentration S_0 as the S scale,
- $\theta = (T - T_0)/T_0$ as the scaled temperature.

Introduce the dimensionless parameters:

- $\varepsilon = E/T_0$, a scaled activation energy,
- $\mu = hY_0/\alpha T_0$, a scaled heat production term,
- $\upsilon = Y_0/\alpha S_0$, a ratio of initial concentrations,
- $\kappa = K/S_0$, a scaled saturation constant,
- $\beta = 2b\bar{t}S_0(M_A/M_S)$, a scaled alcoholic inhibition rate,
- $\gamma = c\bar{t}$, a scaled death rate,
- $\lambda = L/\bar{x}$, a scaled tank length,
- $\Delta = d\,T_0$, a scaled slowing down factor.

Obtain the scaled version of the model, Eq. (1, 9, 4, 5, 6, 7, 8) in terms of these parameters and scaled variables.

b) Adopt the following realistic parameter values to do the next question:

$K = 112$ g/L; $D = 1.39 \times 10^{-3}$ cm^2/s; $L = 1$ m; $T_0 = 18^\circ$C $= 291$ K;
$T_s = 30^\circ$C $= 303$ K; $d = 0.1$ K^{-1}; $S_0 = 200$ g/L; $Y_0 = 5$ g/L; $\alpha = 0.05$; $c = 3 \times 10^{-5}$ h^{-1};
$k_0 = 1.76 \times 10^6$ h^{-1}; $h = 0.113$ KL/g; $b = 8.5 \times 10^{-5}$ Lg^{-1}h^{-1}; $E = 4594$ K;
$M_A = 46.07$ g/mole; $M_S = 180.16$ g/mole.
(Here, h is the symbol for hour.)

Use a Crank-Nicholson algorithm to obtain the temperature and concentrations profiles. In particular:

- After 400 hours (of fermentation time!), obtain the spatial temperature, yeast population and sugar concentration profiles. Do the yeasts prefer to live where it is warm of cool?

- Obtain and interpret the time evolution of the spatially-averaged temperature, spatially-averaged yeast population, spatially-averaged glucose concentration and (using the scaled version of Eq. 8) the spatially-averaged ethanol concentration. Here, the spatial average of a quantity *f* is defined as:

  $$\bar{f}(t) = \frac{1}{L}\int_0^L dx f(x,t)$$

  and should be evaluated numerically.

- After 800 hours, the fermentation should be very slow, if present. How warm is the resulting wine?

- After 800 hours, determine whether the final wine is dry (S < 4 g/L), semi-sweet (4 g/L < S <45 g/L) or sweet (S>45 g/L).

- Using Eq. (8), find the spatially-averaged ethanol concentration after 800 hours. To convert from g/L to % per volume, divide the alcohol concentration by its density 0.789 g/cm^3 and multiply by 0.1 (to convert litre to cm^3 and to %). What is the alcoholic strength (in %vol) of the final wine?

Hints:

i) The dynamics of the glucose consumption and the yeast population are described by ordinary differential equations that can still be solved using a Crank-Nicholson-like algorithm, whereby these equations are evaluated at the half-time step. The only difference is that no spatial derivative occurs for these ODE, so that no inversion of tridiagonal matrices is necessary.

ii) The terms coupling each variable to the others and the non-linear terms can be evaluated using the advanced projection method (section H of chap. 6.2).

iii) The yeast population and the glucose concentration are obviously positive (or zero) quantities. As is often the case in computational problems of that kind, you may need to artificially set these variables to zero if the algorithm would blindly make them negative.

3. HARMONIC OSCILLATOR (AGAIN)

In this problem, consider the (dimensionless) classical harmonic oscillator:

$$\frac{dx}{dt} = v; \quad \frac{dv}{dt} = -x.$$

a) Establish the second order Runge-Kutta (RK2) scheme for this system.

b) Establish the numerical stability criteria for this scheme.