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% Kathryn Atherton
% ABE 202 Homework
% Alcohol Metabolism

function ABE202homework20417
    % dose
    D = 8 * 46.2 * 0.5 * 0.78924;

    [t,y] = ode45(@metmodel, [0 24], [0;0;0], [], D);
    figure(1)
    plot(t,y(:,2))
    hold on
    plot (t,y(:,3))
    title('Alcohol and Acetaldehyde Concentrations')
    xlabel('Time, hours')
    ylabel('Concentrations, g/ml')
    legend('Alcohol', 'Acetaldehyde')

    peakethanol = max(y(:,2));
    peakacetaldehyde = max(y(:,3));
    maxtimeethanol = find(y(:,2) == peakethanol);
    maxtimeacetaldehyde = find(y(:,3) == peakacetaldehyde);
    timeethanol = t(maxtimeethanol);
    timeacetaldehyde = t(maxtimeacetaldehyde);

    D = 0;
    peakethanoldrive = 0;

    while peakethanoldrive < 0.08
        D = D + 1;
        [t,y] = ode45(@metmodel, [0 24], [0;0;0], [], D);
        peakethanoldrive = max(y(:,2));
    end

    drinks = D / (46.2 * 0.5 * 0.78924);

    D = 0;
    peakethanoldrivehet = 0;

    while peakethanoldrivehet < 0.08
        D = D + 1;
        [t,y] = ode45(@metmodelhet, [0 24], [0;0;0], [], D);
        peakethanoldrivehet = max(y(:,2));
    end

    drinkshet = D / (46.2 * 0.5 * 0.78924);

    D = 0;
    peakethanoldrivehom = 0;

    while peakethanoldrivehom < 0.08
        D = D + 1;
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        [t,y] = ode45(@metmodelhom, [0 24], [0;0;0], [], D);
        peakethanoldrivehom = max(y(:,2));
    end

    drinkshom = D / (46.2 * 0.5 * 0.78924);

    % Number One %
    fprintf('1): \n');
    fprintf('    Full equation for dB/dt: \n');
    fprintf('        dB/dt = Ka * I - (Vadhmax * B - A * Vadhrev) / \n'
        (Kmadh + B + A * Kadhrev)\n');
    fprintf('    Full equation for dA/dt: \n');
    fprintf('        dA/dt = dAdt = ((Vadhmax * B - A * Vadhrev) / \n'
        (Kmadh + B + A * Kadhrev)) - ((Valdhmax * A) / (Kmal dh + A))\n');
    fprintf('\n');

    % Number Two %
    fprintf('2): \n');
    fprintf('    Plot alcohol and acetaldehyde concentration for \n'
        situation:\n');
    fprintf('        see plot.\n');
    fprintf('    Peak blood alcohol content:\n');
    fprintf('        %f M\n', peakethanol);
    fprintf('    Peak blood acetaldehyde content:\n');
    fprintf('        %f M\n', peakacetaldehyde);
    fprintf('    Time after consumption peak blood alcohol level \n'
        occurs:\n');
    fprintf('        %f hrs\n', timeethanol);
    fprintf('    Time after consumption peak blood acetaldehyde level \n'
        occurs:\n');
    fprintf('        %f hrs\n', timeacetaldehyde);
    fprintf('\n');

    % Number Three %
    fprintf('3): \n');
    fprintf('    Drinks to reach Indiana legal limit for driving:\n');
    fprintf('        %f drinks\n', drinks);
    fprintf('\n');

    % Number Four %
    fprintf('4): \n');
    fprintf('    Does slower ALDH rate affect blood alcohol content in \n'
        mutants? \n');
    fprintf('        Yes, as the amount of acetaldehyde affects the dB/\n'
        dt equation (A). The mutation makes the dB/dt process slower, which \n'
        keeps the blood-alcohol content higher, longer. \n');
    fprintf('    Number of drinks to reach legal limit for mutant \n'
        genotypes: \n');
    fprintf('        Heterozygous: %f drinks\n', drinkshet);
    fprintf('        Homozygous: %f drinks\n', drinkshom);
    fprintf('\n');

    % Bonus %
    fprintf('Bonus): \n');

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fprintf('    Component used in hangover "cures": \n');
fprintf('        ALDH\n');
fprintf('    Why?\n');
fprintf('        ALDH is the enzyme which breaks down the toxic
byproduct of the breakdown of ethanol, acetaldehyde.\n');
fprintf('        If ALDH malfunctions or is inhibited, acetaldehyde
cannot be properly broken down, leading to adverse \n');
fprintf('        side effects that are seen in hangovers.\n');
fprintf('\n');

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end

function dydt = metmodel(t,y,D)

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% Constants %
Kemax = 10.2; % per hour
a = 0.00167; % g^-2
Ka = 25.1; % per hour
V = 44.100; % ml
Vm = 0.202; % mg/ml * hr
Km = 0.0818; % %mg/ml
Vadhmax = 0.184;
Valdhmax = 0.246;
Kadhrev = 1;
Vadhrev = 3.26;
Kmadh = 0.014; % %mg/ml
Kmal dh = 0.0000528; % %mg/ml

Ke = Kemax / (1 + a * D^2);

% Amount of Alcohol in Places Tracked %

I = y(1); % amount of alcohol in intestine
B = y(2); % amount of alcohol in body/blood
A = y(3); % amount of acetaldehyde in body/blood

% determining F
if D <= 11.2
    F = 0.785;
elseif D <= 22.4
    F = 0.96;
else
    F = 1;
end

% Differential Equations %

dIdt = Ke * (F * D / V) * exp(-(Ke * t)) - Ka * I; % need to find
I
dBdt = Ka * I - (Vadhmax * B - A * Vadhrev) / (Kmadh + B + A *
Kadhrev); % need to find B
dAdt = ((Vadhmax * B) - (A * Vadhrev)) / (Kmadh + B + (A *
Kadhrev)) - (Valdhmax * A) / (Kmal dh + A); % ???, need to find A

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    dydt = [dIdt; dBdt; dAdt];
end

function dydt = metmodelhet(t,y,D)

    % Constants %
    Kemax = 10.2; % per hour
    a = 0.00167; % g-2
    Ka = 25.1; % per hour
    V = 44.100; % ml
    Vm = 0.202; % mg/ml * hr
    Km = 0.0818; % %mg/ml
    Vadhmax = 0.184;
    Valdhmax = 0.246;
    Kadhrev = 1;
    Vadhrev = 3.26;
    Kmadh = 0.014; % %mg/ml
    Kmaldh = 0.0000528 * 0.7; % %mg/ml

    Ke = Kemax / (1 + a * D^2);

    % Amount of Alcohol in Places Tracked %

    I = y(1); % amount of alcohol in intestine
    B = y(2); % amount of alcohol in body/blood
    A = y(3); % amount of acetaldehyde in body/blood

    % determining F
    if D <= 11.2
        F = 0.785;
    elseif D <= 22.4
        F = 0.96;
    else
        F = 1;
    end

    % Differential Equations %

    dIdt = Ke * (F * D / V) * exp(-(Ke * t)) - Ka * I; % need to find
I
    dBdt = Ka * I - (Vadhmax * B - A * Vadhrev) / (Kmadh + B + A *
Kadhrev); % need to find B
    dAdt = ((Vadhmax * B) - (A * Vadhrev)) / (Kmadh + B + (A *
Kadhrev)) - (Valdhmax * A) / (Kmaldh + A); % ???, need to find A

    dydt = [dIdt; dBdt; dAdt];
end

function dydt = metmodelhom(t,y,D)

    % Constants %
    Kemax = 10.2; % per hour
    a = 0.00167; % g-2
    Ka = 25.1; % per hour

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V = 44.100; % ml
Vm = 0.202; % mg/ml * hr
Km = 0.0818; % %mg/ml
Vadhmax = 0.184;
Valdhmax = 0.246;
Kadhrev = 1;
Vadhrev = 3.26;
Kmadh = 0.014; % %mg/ml
Kmal dh = 0.0000528 * 0.55; % %mg/ml

Ke = Kemax / (1 + a * D^2);

% Amount of Alcohol in Places Tracked %

I = y(1); % amount of alcohol in intestine
B = y(2); % amount of alcohol in body/blood
A = y(3); % amount of acetaldehyde in body/blood

% determining F
if D <= 11.2
    F = 0.785;
elseif D <= 22.4
    F = 0.96;
else
    F = 1;
end

% Differential Equations %

dIdt = Ke * (F * D / V) * exp(-(Ke * t)) - Ka * I; % need to find
I
dBdt = Ka * I - (Vadhmax * B - A * Vadhrev) / (Kmadh + B + A *
Kadhrev); % need to find B
dAdt = ((Vadhmax * B) - (A * Vadhrev)) / (Kmadh + B + (A *
Kadhrev)) - (Valdhmax * A) / (Kmal dh + A); % ???, need to find A

dydt = [dIdt; dBdt; dAdt];
end

1):
    Full equation for dB/dt:
        dB/dt = Ka * I - (Vadhmax * B - A * Vadhrev) / (Kmadh + B + A *
Kadhrev)
    Full equation for dA/dt:
        dA/dt = dAdt = ((Vadhmax * B - A * Vadhrev) / (Kmadh + B + A *
Kadhrev)) - ((Valdhmax * A) / (Kmal dh + A))

2):
    Plot alcohol and acetaldehyde concentration for situation:
        see plot.
    Peak blood alcohol content:
        1.610078 M
    Peak blood acetaldehyde content:
        0.000151 M

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Time after consumption peak blood alcohol level occurs:  
5.854020 hrs  
Time after consumption peak blood acetaldehyde level occurs:  
5.861963 hrs

3):

Drinks to reach Indiana legal limit for driving:  
0.438802 drinks

4):

Does slower ALDH rate affect blood alcohol content in mutants?  
Yes, as the amount of acetaldehyde affects the  $dB/dt$  equation  
(A). The mutation makes the  $dB/dt$  process slower, which keeps the  
blood-alcohol content higher, longer.

Number of drinks to reach legal limit for mutant genotypes:  
Heterozygous: 0.438802 drinks  
Homozygous: 0.438802 drinks

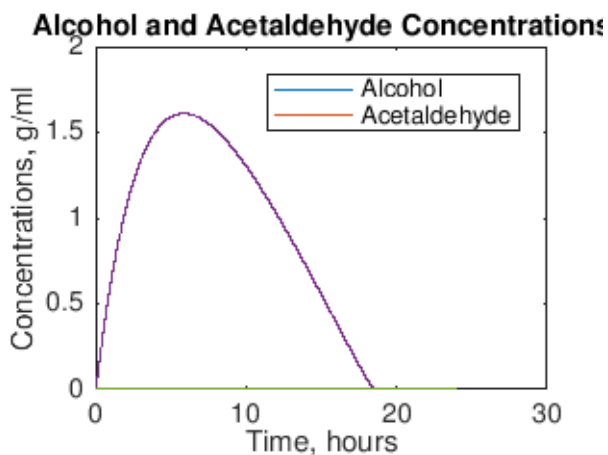
Bonus):

Component used in hangover "cures":  
ALDH

Why?

ALDH is the enzyme which breaks down the toxic byproduct of the  
breakdown of ethanol, acetaldehyde.

If ALDH malfunctions or is inhibited, acetaldehyde cannot be  
properly broken down, leading to adverse  
side effects that are seen in hangovers.



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