```
% This file calculates maintenance energy for the A. acidocaldarius model
% and can be used for EFMA or FBA applications. To run, the file requires the
% model output from efmtool (run with no GAM or NGAM in the biomass reaction)
% be loaded into the MATLAB workspace.
% See the EFM Calculation page on the Biochemical Engineering Laboratory
% website for details on running efmtool
(http://www.chbe.montana.edu/biochemenglab/efm.html).
% CO2            C44 out 44
% oxygen         C45 in  45
% ammonium       C50 in  50
% glucose        C51 in  51
% H2O            C56 out 56
% H+             C57 out 57
% phosphate      C61 in  61
% sulfate        C62 in  62
% biomass        B0  out 207
% energy         C60 out 213

% Widely used relationship between the observed specific substrate uptake
rate, q,
% and the specific growth rate, mu, in terms of the biomass yield, Y, and a
% nongrowing cellular maintenance term, m:
% qobs = mu / Y + m  (Equation 1).

% Equation 1 can be rearranged to solve for the observed biomass yield,
% Yobs, by dividing each term by the specific growth rate, mu:
% 1 / Yobs = 1 / Y + m / mu  (Equation 2).

% The theoretical yield, Y, can be deconstructed into a biomass yield for
theoretical
% stoichiometric chemical transformations, Yc, which is the stoichiometric
conversion
% and polymerization cost in a model, and an energy/error biomass yield, Ym,
which
% accounts for everything else that varies with growth:
% 1 / Yobs = 1 / Yc + 1 / Ym + m / mu  (Equation 3).

% Treating the energy/error term as a energy based cost, Ym can be
% decomposed into the energy yield, Ye, and a growth associated cost, GAM:
% 1 / Yobs = 1 / Yc + GAM / Ye + m / mu  (Equation 4).

% Nongrowth cellular maintenance, m, can be similarly decomposed to Ye and
% NGAM:
% 1 / Yobs = 1 / Yc + GAM / Ye + NGAM / Ye / mu  (Equation 5).

% Equation 5 can be rearranged to extract the GAM and NGAM for a given model
% from the observed growth associated yield and nongrowth associated
% specific uptake rate, as done in lines 66 and 69, respectively.

% Yobs = observed biomass yield on a given substrate          [g bio / mol
sub]
% mu   = specific growth rate                                 [g bio / g bio
/ h]
% Y    = observed growth associated biomass yield             [g bio / mol
sub]
```

```
% Yc   = theoretical biomass yield from the model without GAM [g bio / mol
sub]
% Ym   = theoretical growth associated biomass yield          [g bio / mol
sub]
% Ye   = theoretical energy yield determined from the model   [g bio / mol
sub]
% m    = observed nongrowth associated maintenance energy     [mol sub / g
bio / h]
% GAM  = Growth Associated Maintenance energy                 [mol energy / g
bio]
% NGAM = NonGrowth Associated Maintenance energy              [mol energy / g
bio / h]

% Determine the highest biomass and energy yields on carbon
Ybc = mnet.efms(207,:) * 1000 ./ mnet.efms(51,:);
Yec = mnet.efms(213,:) ./ mnet.efms(51,:);
[Ymbc,ibc] = max(Ybc) % g per mol
[Ymec,iec] = max(Yec)  % mol per mol

% Calculate biomass and energy yields on oxygen
Ybo = mnet.efms(207,:) * 1000 ./ mnet.efms(45,:);
Yeo = mnet.efms(213,:) ./ mnet.efms(45,:);

% From Table 1 in  Farrand et al 1983; DOI:10.1007/BF00413481
Ymaxbioglucose= 83.5; % g biomass per mol glucose
Ymaxbiooxygen = 28.1; % g biomass per mol oxygen
Mglucose = 0.00053; % mol glucose per h per g biomass
Moxygen  = 0.00232; % mol oxgyen per h per g biomass

% Calculate the Growth Associated Maintenance (GAM) for carbon limitation
GAMc = ((1 / Ymaxbioglucose) - (1 / Ybc(ibc))) / (1 / Yec(iec)) % mol energy
per g biomass
GAMo = ((1 / Ymaxbiooxygen) - (1 / Ybo(ibc))) / (1 / Yeo(iec))  % mol energy
per g biomass

% Calculate the NonGrowth Associated Maintenance (NGAM)
NGAMc = Mglucose / (1 / Yec(iec)) % mol energy per g biomass per hour
NGAMo = Moxygen / (1 / Yeo(iec))  % mol energy per g biomass per hour

% Calculate the Combined Maintenance for EFMA at a growth rate of 0.1 1/h
Maintc = (GAMc + (NGAMc / 0.1)) * 1000 % mmol energy per g biomass
Mainto = (GAMo + (NGAMo / 0.1)) * 1000 % mmol energy per g biomass

% EFMA model: include an energy_maintenance term in the biomass reaction and
set
% its coefficient to Maintc. After rerunning the model, the maximum biomass
% yield per substrate used to calibrate, in this case, glucose should be
% ~57.9 g biomass per mol of glucose. (Rounding propagates so it may not be
% identical.)
% FBA model: include an energy_maintenance term in the biomass reaction and
export
% from CellNetAnalyzer, then set the energy specific production rate lower
% bound (lb) and upper bound (ub) to NGAM and the energy_maintenance
% coefficient in the biomass reaction to GAM. The resulting model should
% match your calibrated data.
```

```
% Example code to set parameters in exported FBA model:
%     CobraModel.S(51,207) = -13.4;
%     CobraModel.lb(213) = 4.2;
%     CobraModel.ub(213) = 4.2;
%
% The following code was used to recreate Figure 1 in Farrand et al 1983;
% DOI:10.1007/BF00413481:
% for i = 1:20
%     cobramodel.ub(207) = i * 0.01;
%     cobramodel.lb(207) = i * 0.01;
%     t = optimizeCbModel(cobramodel,'Min','one',1);
%     q(i) = t.f;
% end

% If used correctly, running this file on a model with the correct settings
% should indicate no need for additional Maintc.
```