Calculation of conversion factors for model parameters

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```
library(biogas)
```

Last run:

```
Sys.time()
```

```
## [1] "2021-05-19 12:11:12 EDT"
```

Note on inputs

Chemical formulas from biogas package. Document values of macromolecular composition. These match the SoftwareX paper.

```
biogas:::std.forms
```

```
##           vfa       protein  carbohydrate         lipid       lignin   tripalmitin       biomass        acetic
##      "C2H4O2" "C4H6.1O1.2N"     "C6H10O5"   "C57H104O6"    "C10H13O3"    "C51H98O6"     "C5H7O2N"     "CH3COOH"
##       lactic       ethanol     cellulose       glucose      fructose       sucrose       lactose           ash
##      "C3H6O3"    "CH3CH2OH"     "C6H10O5"     "C6H12O6"     "C6H12O6"   "C12H22O11"   "C12H22O11"        "NaCl"
```

Composition of manure based on macromolecular groups from Appendix S3 in the paper, as g/g VS.

1. COD:VS ratios

A. Pig, degradable, no VFA

```
pred <- predBg(mcomp = c(protein = 0.18, lipid = 0.12, carbohydrate = 0.39),
               mass = 1, value = 'all')
```

```
## Warning in predBg(mcomp = c(protein = 0.18, lipid = 0.12, carbohydrate = 0.39), : Sum of mcomp != 1.0 so dividing all
## elements by the sum for calculation of formula.
```

```
pred
```

```
##                         form mass mol.mass       moles      COD     hydro      fCH4     vCH4      mCH4      mCO2
## 1 C14.7566H24.619707.43355N    1 334.9872 0.002985188 1.570902 0.3568326 0.5571998 548.8482 0.3937563 0.8584544
```

```
1/pred$COD
```

```
## [1] 0.6365771
```

C. Cattle, degradable, no VFA

```
pred <- predBg(mcomp = c(protein = 0.15, lipid = 0.07, carbohydrate = 0.43),
               mass = 1, value = 'all')
```

```
## Warning in predBg(mcomp = c(protein = 0.15, lipid = 0.07, carbohydrate = 0.43), : Sum of mcomp != 1.0 so dividing all
## elements by the sum for calculation of formula.
```

```
pred
```

```
##                         form mass mol.mass       moles     COD     hydro      fCH4     vCH4     mCH4      mCO2
## 1 C15.895H26.339509.20092N    1 378.6709 0.002640816 1.44754 0.3073311 0.5388303 505.7476 0.362835 0.8519434
```

```
1/pred$COD
```

```
## [1] 0.6908272
```

2. Chemical formulas and CO2:COD ratios

These all use degradable VS plus VFA to give CO2 mass produced per g COD converted. We need to reduce CO2 (and any other "energy reaction" products) by the fraction of substrate used for microbial biomass synthesis. This is a bit sketchy because this biomass contributes to slurry OM (VS and COD). But we only explicitly include it in the model for methanogens. So for the others (fermentation, aerobic, sulfate reduction?) we should include an effective fraction that represents slowly degradable or nondegradable biomass.

Yields in g COD/g COD. Below I took about 20% off the yields from Table 3.1 in Rittmann and McCarty.

```
yaer <- 0.1
yanaer <- 0.03
ysr <- 0.01
```

A. Pig, degradable, with VFA

```
pred <- predBg(mcomp = c(acetic = 0.08, protein = 0.18, lipid = 0.12, carbohydrate = 0.39),
               mass = 1, value = 'all')
```

```
## Warning in predBg(mcomp = c(acetic = 0.08, protein = 0.18, lipid = 0.12, : Sum of mcomp != 1.0 so dividing all
## elements by the sum for calculation of formula.
```

```
pred
```

```
##                         form mass mol.mass       moles      COD    hydro      fCH4     vCH4      mCH4      mCO2
## 1 C16.0499H27.20630.72684N    1 373.8197 0.002675086 1.518427 0.319765 0.5525908 530.5142 0.3806031 0.8454081
```

```
1/pred$COD
```

```
## [1] 0.6585765
```

Round for the following formula for degradable pig slurry organic matter (OM).

```
fpd <- 'C16 H27 O8.7 N'
```

Anaerobic CO2.

```
predBg(fpd, fs = yanaer, value = 'reactionc')
```

```
## [1] "C16 H27 O8.7 N + 6.226H2O --> 8.56CH4 + 6.016CO2 + 0.1059C5H7O2N + 0.8941NH4+ + 0.8941HCO3-"
```

```
pred <- predBg(fpd, fs = 0.10, value = 'all')
pred
```

```
##             form mass mol.mass       moles      COD  fs  fe fd   hydro      fCH4     vCH4      mCH4      mCO2
## 1 C16 H27 O8.7 N    1  372.583 0.002683966 1.515904 0.1 0.9  1 0.25328 0.5579557 476.6695 0.3419737 0.7432785
##       m.bio       N.req
## 1 0.1071678 -0.02432352
```

```
pred$mCO2 / pred$COD
```

```
## [1] 0.4903203
```

So we have 0.49 CO2 per g COD.

Aerobic CO2. Here we need the mass of CO2 assuming all C goes to CO2, per g COD.

```
(1 - yaer) * molMass('CO2') * 16 / (calcCOD(fpd) * molMass(fpd))
```

```
## [1] 1.122068
```

Sulfate reduction:

```
(1 - ysr) * molMass('CO2') * 16 / (calcCOD(fpd) * molMass(fpd))
```

```
## [1] 1.234275
```

B. Cattle, degradable, with VFA

```
pred <- predBg(mcomp = c(acetic = 0.04, protein = 0.15, lipid = 0.07, carbohydrate = 0.43),
               mass = 1, value = 'all')
```

```
## Warning in predBg(mcomp = c(acetic = 0.04, protein = 0.15, lipid = 0.07, : Sum of mcomp != 1.0 so dividing all
## elements by the sum for calculation of formula.
```

```
pred
```

```
##                         form mass mol.mass       moles      COD    hydro      fCH4     vCH4      mCH4      mCO2
## 1 C16.6711H27.891809.97706N    1 401.9748 0.002487718 1.425404 0.289512 0.5370228 498.0137 0.3572865 0.8450384
```

```
1/pred$COD
```

```
## [1] 0.7015553
```

Round for the following formula for degradable pig slurry organic matter (OM).

```
fcd <- 'C16.6 H27.9 O10 N'
```

Anaerobic CO2.

```
predBg(fcd, fs = yanaer, value = 'reactionc')
```

```
## [1] "C16.6 H27.9 O10 N + 5.947H2O --> 8.645CH4 + 6.527CO2 + 0.107C5H7O2N + 0.893NH4+ + 0.893HCO3-"
```

```
pred <- predBg(fcd, fs = yanaer, value = 'all')
pred
```

```
##                form mass mol.mass       moles      COD   fs   fe fd     hydro      fCH4     vCH4      mCH4      mCO2
## 1 C16.6 H27.9 O10 N    1 401.4962 0.002490684 1.420686 0.03 0.97  1 0.2668637 0.5381258 481.4742 0.3454207 0.8133569
##        m.bio       N.req
## 1 0.03013088 -0.03115584
```

```
pred$mCO2 / pred$COD
```

```
## [1] 0.57251
```

0.57 g CO2 per g COD.

Aerobic CO2:

```
(1 - yaer) * molMass('CO2') * 16.6 / (calcCOD(fcd) * molMass(fcd))
```

```
## [1] 1.152716
```

```
(1 - ysr) * molMass('CO2') * 16.6 / (calcCOD(fcd) * molMass(fcd))
```

```
## [1] 1.267988
```