Browse Networks in the Matlab Command Window Using surfNet

Author(s): Siu Hung Joshua Chan, Department of Chemical Engineering, The Pennsylvania State University

Reviewer(s):

INTRODUCTION

In this tutorial, we will demonstrate how to browse a COBRA model in verbal format in the Matlab command window through an initial call and interactive mouse clicking.

MATERIALS

EQUIPMENT SETUP

Start CobraToolbox

```
initCobraToolbox(false) % false, as we don't want to update;
```

```
     _____   _____   _____   _____     _____     |
    /  ___| /  _  \ |  _  \ |  _  \   / ___ \    |   COnstraint-Based Reconstruction and Analysis
    | |     | | | | | |_| | | |_| |   | |___| |   |   The COBRA Toolbox - 2019
    | |     | | | | |  _  { |  _  /   |  ___  |   |
    | |___  | |_| | | |_| | | | \ \   | |   | |   |   Documentation:
    \_____| \_____/ |_____/ |_|  \_\ |_|   |_|   |   http://opencobra.github.io/cobratoolbox
                                                  |

> Checking if git is installed ...  Done (version: 2.17.1).
> Checking if the repository is tracked using git ...  Done.
> Checking if curl is installed ...  Done.
> Checking if remote can be reached ...  Done.
> Initializing and updating submodules (this may take a while)... Done.
> Adding all the files of The COBRA Toolbox ...  Done.
> Define CB map output... set to svg.
> TranslateSBML is installed and working properly.
> Configuring solver environment variables ...
  - [*---] ILOG_CPLEX_PATH: /opt/ibm/ILOG/CPLEX_Studio128/cplex/matlab/x86-64_linux
  - [*---] GUROBI_PATH: /opt/gurobi810/linux64/matlab
  - [----] TOMLAB_PATH: --> set this path manually after installing the solver ( see instructions )
  - [---*] MOSEK_PATH: /opt/mosek/8/
  Done.
> Checking available solvers and solver interfaces ... Done.
> Setting default solvers ... Done.
> Saving the MATLAB path ... Done.
  - The MATLAB path was saved as ~/pathdef.m.

> Summary of available solvers and solver interfaces

          Support        LP      MILP        QP      MIQP       NLP
   ----------------------------------------------------------------------
   gurobi          active              1         1         1         1         -
   ibm_cplex       active              1         1         1         1         -
   tomlab_cplex    active              0         0         0         0         -
   glpk            active              1         1         -         -         -
   mosek           active              1         -         1         -         -
   matlab          active              1         -         -         -         1
```

```
    cplex_direct     active               0        0        0        -        -
    dqqMinos         active               0        -        -        -        -
    pdco             active               1        -        1        -        -
    quadMinos        active               0        -        -        -        -
    qpng             passive              -        -        1        -        -
    tomlab_snopt     passive              -        -        -        -        0
    lp_solve         legacy               1        -        -        -        -
    ------------------------------------------------------------------------
    Total            -                    7        3        5        2        1

  + Legend: - = not applicable, 0 = solver not compatible or not installed, 1 = solver installed.


  > You can solve LP problems using: 'ibm_cplex' - 'glpk' - 'mosek' - 'matlab' - 'pdco'
  > You can solve MILP problems using: 'ibm_cplex' - 'glpk'
  > You can solve QP problems using: 'ibm_cplex' - 'mosek' - 'pdco' - 'qpng'
  > You can solve MIQP problems using: 'ibm_cplex'
  > You can solve NLP problems using: 'matlab'

> Checking for available updates ... skipped
```

PROCEDURE

Load the *E. coli* iJO1366 model as an example model.

```
modelFileName = 'iJO1366.mat';
modelDirectory = getDistributedModelFolder(modelFileName); %Look up the folder for the
modelFileName= [modelDirectory filesep modelFileName]; % Get the full path. Necessary t
iJO1366 = readCbModel(modelFileName);
```

```
Warning: Metabolite IDs will be adjusted to COBRA style metID[e] instead of metID_e
```

```
```

Browse a network

Browse the network by starting from an initial metabolite, e.g., D-glucose in the extracellular compartment.

```
surfNet(iJO1366, 'glc__D[e]')
```

```
Met #1195  glc__D[e], D-Glucose, C6H12O6

Consuming reactions:
  #164  EX_glc__D_e, Bd: -10 / 1000, D-Glucose exchange
glc__D[e] <=>
  #1355  GLCtex_copy1, Bd: -1000 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] <=> glc__D[p]
  #1356  GLCtex_copy2, Bd: 0 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] -> glc__D[p]
Producing reactions: none

Show previous steps...
```

All reactions producing or consuming '**glc__D_e**' will have their reaction indices (#xxx), ids (.rxns), bounds (.lb/.ub), names (.rxnNames) and formulae printed on the command window. All reactions and the participating metabolites are hyperlinked. For example, **click** on the reaction '**GLCtex_copy1**'. (This is equivalent to run the following command.)

```
% called by clicking 'GLCtex_copy1'
surfNet([], 'GLCtex_copy1', 0, 'none', 0, 1, [], 0)
```

```
Rxn #1355  GLCtex_copy1, Bd: -1000 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] <=> glc__D[p]
  id     Met        Stoich     metNames, metFormulas
Reactant:
 #1195   glc__D[e]  -1         D-Glucose, C6H12O6
Product:
 #1587   glc__D[p]  1          D-Glucose, C6H12O6

Show previous steps...
```

Details for the metabolites will appear, e.g., indeices, ids, stoichiometric coefficients, names and chemical formulae. By iteratively clicking on the reactions and metabolites that you are interested in, you can browse through the metabolic network.

Now, say you have gone through a series of metabolites and reactions (glc__D[e], GLCtex_copy1, glc__D[p], GLCptspp, g6p[c]):

Click glc__D_[p]:

```
% called by clicking 'glc__D_p'
surfNet([], 'glc__D[p]', 0, 'none', 0, 1, [], 0)
```

```
Met #1587  glc__D[p], D-Glucose, C6H12O6

Consuming reactions:
  #1336  GLCDpp, Bd: 0 / 1000, Glucose dehydrogenase (ubiquinone-8 as acceptor) (periplasm)
q8[c] + glc__D[p] + h2o[p] -> q8h2[c] + glcn[p] + h[p]
  #1352  GLCabcpp, Bd: 0 / 1000, D-glucose transport via ABC system (periplasm)
atp[c] + h2o[c] + glc__D[p] -> adp[c] + glc__D[c] + h[c] + pi[c]
  #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  #1354  GLCt2pp, Bd: 0 / 1000, D-glucose transport in via proton symport (periplasm)
glc__D[p] + h[p] -> glc__D[c] + h[c]
Producing reactions:
  #1252  G1PPpp, Bd: 0 / 1000, Glucose-1-phosphatase
g1p[p] + h2o[p] -> glc__D[p] + pi[p]
  #1355  GLCtex_copy1, Bd: -1000 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] <=> glc__D[p]
  #1356  GLCtex_copy2, Bd: 0 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] -> glc__D[p]
  #1607  LACZpp, Bd: 0 / 1000, B-galactosidase
h2o[p] + lcts[p] -> gal[p] + glc__D[p]
  #2463  TREHpp, Bd: 0 / 1000, Alpha,alpha-trehalase (periplasm)
h2o[p] + tre[p] -> 2 glc__D[p]

Show previous steps...
```

Click GLCptspp:

```
% called by clicking 'GLCptspp'
surfNet([], 'GLCptspp', 0, 'none', 0, 1, [], 0)
```

```
Rxn #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  id     Met        Stoich     metNames, metFormulas
Reactant:
 #784       pep[c]  -1         Phosphoenolpyruvate, C3H2O6P
```

```
 #1587   glc__D[p]  -1         D-Glucose, C6H12O6
Product:
 #508       g6p[c]  1          D-Glucose 6-phosphate, C6H11O9P
 #853       pyr[c]  1          Pyruvate, C3H3O3

Show previous steps...
```

Click g6p_c:

```
% called by clicking 'g6p[c]'
surfNet([], 'g6p[c]', 0, 'none', 0, 1, [], 0)
```

```
Met #508  g6p[c], D-Glucose 6-phosphate, C6H11O9P

Consuming reactions:
  #1283  G6PDH2r, Bd: -1000 / 1000, Glucose 6-phosphate dehydrogenase
g6p[c] + nadp[c] <=> 6pgl[c] + h[c] + nadph[c]
  #1284  G6PP, Bd: 0 / 1000, Glucose-6-phosphate phosphatase
g6p[c] + h2o[c] -> glc__D[c] + pi[c]
  #2077  PGI, Bd: -1000 / 1000, Glucose-6-phosphate isomerase
g6p[c] <=> f6p[c]
  #2461  TRE6PS, Bd: 0 / 1000, Alpha,alpha-trehalose-phosphate synthase (UDP-forming)
g6p[c] + udpg[c] -> h[c] + tre6p[c] + udp[c]
Producing reactions:
  #477  AB6PGH, Bd: 0 / 1000, Arbutin 6-phosphate glucohydrolase
arbt6p[c] + h2o[c] -> g6p[c] + hqn[c]
  #1214  FFSD, Bd: 0 / 1000, Beta-fructofuranosidase
h2o[c] + suc6p[c] -> fru[c] + g6p[c]
  #1231  FRULYSDG, Bd: -1000 / 1000, Fructoselysine phosphate deglycase
frulysp[c] + h2o[c] <=> g6p[c] + lys__L[c]
  #1285  G6Pt6_2pp, Bd: 0 / 1000, Glucose-6-phosphate transport via phosphate antiport (periplasm)
2 pi[c] + g6p[p] -> g6p[c] + 2 pi[p]
  #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  #1500  HEX1, Bd: 0 / 1000, Hexokinase (D-glucose:ATP)
atp[c] + glc__D[c] -> adp[c] + g6p[c] + h[c]
  #2082  PGMT, Bd: -1000 / 1000, Phosphoglucomutase
g1p[c] <=> g6p[c]
  #2459  TRE6PH, Bd: 0 / 1000, Trehalose-6-phosphate hydrolase
h2o[c] + tre6p[c] -> g6p[c] + glc__D[c]

Show previous steps...
```

In each click, there is also a button '**Show previous steps...**' at the bottom. Clicking on it will show the metabolites and reactions that you have visited in order. This is equivalent to calling:

```
% called by clicking 'Show previous steps...'
surfNet([], [], 0, 'none', 0, 1, [], 0, struct('showPrev', true))
```

```
glc__D[e]>>GLCtex_copy1>>glc__D[p]>>GLCptspp>>g6p[c]>>
```

You can go back to any of the intermediate metabolites/reactions by clicking the hyperlinked `mets/rxns` shown.

Call options

Shown below are various call options for including flux vectors and customizing display. All call options are preserved during the interactive browsing by mouse clicking.

Show objective reactions

Omit the '`metrxn`' (2nd) argument to print objective reactions:

```
surfNet(iJO1366)
```

```
Rxn #8  BIOMASS_Ec_iJO1366_core_53p95M, Bd: 0 / 1000, E. coli biomass objective function (iJO1366) - core
0.000223 10fthf[c] + 2.6e-05 2fe2s[c] + 0.000223 2ohph[c] + 0.00026 4fe4s[c] + 0.513689 ala__L[c] + 0.0002
  0.295792 arg__L[c] + 0.241055 asn__L[c] + 0.241055 asp__L[c] + 54.1248 atp[c] + 0.000122 bmocogdp[c] + 2
  0.005205 ca2[c] + 0.005205 cl[c] + 0.000576 coa[c] + 2.5e-05 cobalt2[c] + 0.133508 ctp[c] + 0.000709 cu2
  0.09158 cys__L[c] + 0.026166 datp[c] + 0.027017 dctp[c] + 0.027017 dgtp[c] + 0.026166 dttp[c] + 0.000223
  0.006715 fe2[c] + 0.007808 fe3[c] + 0.26316 gln__L[c] + 0.26316 glu__L[c] + 0.612638 gly[c] + 0.215096 g
  + 0.094738 his__L[c] + 0.290529 ile__L[c] + 0.195193 k[c] + 0.450531 leu__L[c] + 0.343161 lys__L[c] + 0.
  0.008675 mg2[c] + 0.000223 mlthf[c] + 0.000691 mn2[c] + 7e-06 mobd[c] + 0.001831 nad[c] + 0.000447 nadp[
  0.000323 ni2[c] + 0.017868 pe160[c] + 0.054154 pe161[c] + 0.185265 phe__L[c] + 0.000223 pheme[c] + 0.221
  0.000223 pydx5p[c] + 0.000223 ribflv[c] + 0.215792 ser__L[c] + 0.000223 sheme[c] + 0.004338 so4[c] + 0.0
  0.000223 thmpp[c] + 0.253687 thr__L[c] + 0.056843 trp__L[c] + 0.137896 tyr__L[c] + 5.5e-05 udcpdp[c] + 0
  0.423162 val__L[c] + 0.000341 zn2[c] + 0.019456 kdo2lipid4[e] + 0.013894 murein5px4p[p] + 0.045946 pe160
  -> 53.95 adp[c] + 53.95 h[c] + 53.9457 pi[c] + 0.773903 ppi[c]
  id     Met             Stoich     metNames, metFormulas
Reactant:
 #1           10fthf[c]  -0.000223  10-Formyltetrahydrofolate, C20H21N7O7
 #69           2fe2s[c]  -0.000026  [2Fe-2S] iron-sulfur cluster, S2Fe2
 #82           2ohph[c]  -0.000223  2-Octaprenyl-6-hydroxyphenol, C46H70O2
 #167          4fe4s[c]  -0.00026   [4Fe-4S] iron-sulfur cluster, S4Fe4
 #255         ala__L[c]  -0.513689  L-Alanine, C3H7NO2
 #265           amet[c]  -0.000223  S-Adenosyl-L-methionine, C15H23N6O5S
 #294         arg__L[c]  -0.295792  L-Arginine, C6H15N4O2
 #298         asn__L[c]  -0.241055  L-Asparagine, C4H8N2O3
 #302         asp__L[c]  -0.241055  L-Aspartate, C4H6NO4
 #307            atp[c]  -54.124831  ATP C10H12N5O13P3, C10H12N5O13P3
 #314       bmocogdp[c]  -0.000122  Bis-molybdopterin guanine dinucleotide, C40H44N20O27P4S4Mo
 #317            btn[c]  -0.000002  Biotin, C10H15N2O3S
 #326            ca2[c]  -0.005205  Calcium, Ca
 #355             cl[c]  -0.005205  Chloride, Cl
 #358            coa[c]  -0.000576  Coenzyme A, C21H32N7O16P3S
 #359        cobalt2[c]  -0.000025  Co2+, Co
 #377            ctp[c]  -0.133508  CTP C9H12N3O14P3, C9H12N3O14P3
 #379            cu2[c]  -0.000709  Copper, Cu
 #383         cys__L[c]  -0.09158   L-Cysteine, C3H7NO2S
 #392           datp[c]  -0.026166  DATP C10H12N5O12P3, C10H12N5O12P3
 #401           dctp[c]  -0.027017  DCTP C9H12N3O13P3, C9H12N3O13P3
 #412           dgtp[c]  -0.027017  DGTP C10H12N5O13P3, C10H12N5O13P3
 #451           dttp[c]  -0.026166  DTTP C10H13N2O14P3, C10H13N2O14P3
 #468            fad[c]  -0.000223  Flavin adenine dinucleotide oxidized, C27H31N9O15P2
 #474            fe2[c]  -0.006715  Fe2+ mitochondria, Fe
 #475            fe3[c]  -0.007808  Iron (Fe3+), Fe
 #541         gln__L[c]  -0.26316   L-Glutamine, C5H10N2O3
 #544         glu__L[c]  -0.26316   L-Glutamate, C5H8NO4
 #551            gly[c]  -0.612638  Glycine, C2H5NO2
 #574            gtp[c]  -0.215096  GTP C10H12N5O14P3, C10H12N5O14P3
 #580            h2o[c]  -48.601527  H2O H2O, H2O
 #597         his__L[c]  -0.094738  L-Histidine, C6H9N3O2
 #621         ile__L[c]  -0.290529  L-Isoleucine, C6H13NO2
 #637              k[c]  -0.195193  Potassium, K
 #650         leu__L[c]  -0.450531  L-Leucine, C6H13NO2
 #661         lys__L[c]  -0.343161  L-Lysine, C6H15N2O2
 #686         met__L[c]  -0.153686  L-Methionine, C5H11NO2S
 #691            mg2[c]  -0.008675  Magnesium, Mg
 #694          mlthf[c]  -0.000223  5,10-Methylenetetrahydrofolate, C20H21N7O6
 #697            mn2[c]  -0.000691  Manganese, Mn
 #702           mobd[c]  -0.000007  Molybdate, MoO4
 #720            nad[c]  -0.001831  Nicotinamide adenine dinucleotide, C21H26N7O14P2
```

```
 #722           nadp[c]  -0.000447  Nicotinamide adenine dinucleotide phosphate, C21H25N7O17P3
 #725            nh4[c]  -0.013013  Ammonium, H4N
 #726            ni2[c]  -0.000323  Nickel, Ni
 #780          pe160[c]  -0.017868  Phosphatidylethanolamine (dihexadecanoyl, n-C16:0), C37H74N1O8P1
 #781          pe161[c]  -0.054154  Phosphatidylethanolamine (dihexadec-9enoyl, n-C16:1), C37H70N1O8P1
 #800         phe__L[c]  -0.185265  L-Phenylalanine, C9H11NO2
 #801          pheme[c]  -0.000223  Protoheme C34H30FeN4O4, C34H30FeN4O4
 #834         pro__L[c]  -0.221055  L-Proline, C5H9NO2
 #851         pydx5p[c]  -0.000223  Pyridoxal 5'-phosphate, C8H8NO6P
 #868         ribflv[c]  -0.000223  Riboflavin C17H20N4O6, C17H20N4O6
 #885         ser__L[c]  -0.215792  L-Serine, C3H7NO3
 #889          sheme[c]  -0.000223  Siroheme C42H36FeN4O16, C42H36FeN4O16
 #897            so4[c]  -0.004338  Sulfate, O4S
 #936            thf[c]  -0.000223  5,6,7,8-Tetrahydrofolate, C19H21N7O6
 #940          thmpp[c]  -0.000223  Thiamine diphosphate, C12H16N4O7P2S
 #942         thr__L[c]  -0.253687  L-Threonine, C4H9NO3
 #977         trp__L[c]  -0.056843  L-Tryptophan, C11H12N2O2
 #985         tyr__L[c]  -0.137896  L-Tyrosine, C9H11NO3
 #1001        udcpdp[c]  -0.000055  Undecaprenyl diphosphate, C55H89O7P2
 #1025           utp[c]  -0.144104  UTP C9H11N2O15P3, C9H11N2O15P3
 #1026        val__L[c]  -0.423162  L-Valine, C5H11NO2
 #1039           zn2[c]  -0.000341  Zinc, Zn
 #1238    kdo2lipid4[e]  -0.019456  KDO(2)-lipid IV(A), C84H148N2O37P2
 #1676   murein5px4p[p]  -0.013894  Two disacharide linked murein units, pentapeptide crosslinked tetrapep
 #1711         pe160[p]  -0.045946  Phosphatidylethanolamine (dihexadecanoyl, n-C16:0), C37H74N1O8P1
 #1712         pe161[p]  -0.02106   Phosphatidylethanolamine (dihexadec-9enoyl, n-C16:1), C37H70N1O8P1
Product:
 #240            adp[c]  53.95      ADP C10H12N5O10P2, C10H12N5O10P2
 #577              h[c]  53.95      H+, H
 #808             pi[c]  53.945662  Phosphate, HO4P
 #821            ppi[c]  0.773903   Diphosphate, HO7P2

Show previous steps...
```

Call with a list of mets/rxns

The 'metrxn' arguement can be a string of id for a metabolite or reaction. It can also be a cell array of ids, e.g.,

```
surfNet(iJO1366, {'glc__D[p]'; 'GLCptspp'; 'g6p[c]'})
```

```
Met #1587  glc__D[p], D-Glucose, C6H12O6

Consuming reactions:
  #1336  GLCDpp, Bd: 0 / 1000, Glucose dehydrogenase (ubiquinone-8 as acceptor) (periplasm)
q8[c] + glc__D[p] + h2o[p] -> q8h2[c] + glcn[p] + h[p]
  #1352  GLCabcpp, Bd: 0 / 1000, D-glucose transport via ABC system (periplasm)
atp[c] + h2o[c] + glc__D[p] -> adp[c] + glc__D[c] + h[c] + pi[c]
  #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  #1354  GLCt2pp, Bd: 0 / 1000, D-glucose transport in via proton symport (periplasm)
glc__D[p] + h[p] -> glc__D[c] + h[c]
Producing reactions:
  #1252  G1PPpp, Bd: 0 / 1000, Glucose-1-phosphatase
g1p[p] + h2o[p] -> glc__D[p] + pi[p]
  #1355  GLCtex_copy1, Bd: -1000 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] <=> glc__D[p]
  #1356  GLCtex_copy2, Bd: 0 / 1000, Glucose transport via diffusion (extracellular to periplasm)
glc__D[e] -> glc__D[p]
  #1607  LACZpp, Bd: 0 / 1000, B-galactosidase
h2o[p] + lcts[p] -> gal[p] + glc__D[p]
  #2463  TREHpp, Bd: 0 / 1000, Alpha,alpha-trehalase (periplasm)
h2o[p] + tre[p] -> 2 glc__D[p]
```

```
Rxn #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  id     Met        Stoich     metNames, metFormulas
Reactant:
 #784       pep[c]  -1         Phosphoenolpyruvate, C3H2O6P
 #1587   glc__D[p]  -1         D-Glucose, C6H12O6
Product:
 #508       g6p[c]  1          D-Glucose 6-phosphate, C6H11O9P
 #853       pyr[c]  1          Pyruvate, C3H3O3

Met #508  g6p[c], D-Glucose 6-phosphate, C6H11O9P

Consuming reactions:
  #1283  G6PDH2r, Bd: -1000 / 1000, Glucose 6-phosphate dehydrogenase
g6p[c] + nadp[c] <=> 6pgl[c] + h[c] + nadph[c]
  #1284  G6PP, Bd: 0 / 1000, Glucose-6-phosphate phosphatase
g6p[c] + h2o[c] -> glc__D[c] + pi[c]
  #2077  PGI, Bd: -1000 / 1000, Glucose-6-phosphate isomerase
g6p[c] <=> f6p[c]
  #2461  TRE6PS, Bd: 0 / 1000, Alpha,alpha-trehalose-phosphate synthase (UDP-forming)
g6p[c] + udpg[c] -> h[c] + tre6p[c] + udp[c]
Producing reactions:
  #477  AB6PGH, Bd: 0 / 1000, Arbutin 6-phosphate glucohydrolase
arbt6p[c] + h2o[c] -> g6p[c] + hqn[c]
  #1214  FFSD, Bd: 0 / 1000, Beta-fructofuranosidase
h2o[c] + suc6p[c] -> fru[c] + g6p[c]
  #1231  FRULYSDG, Bd: -1000 / 1000, Fructoselysine phosphate deglycase
frulysp[c] + h2o[c] <=> g6p[c] + lys__L[c]
  #1285  G6Pt6_2pp, Bd: 0 / 1000, Glucose-6-phosphate transport via phosphate antiport (periplasm)
2 pi[c] + g6p[p] -> g6p[c] + 2 pi[p]
  #1353  GLCptspp, Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  #1500  HEX1, Bd: 0 / 1000, Hexokinase (D-glucose:ATP)
atp[c] + glc__D[c] -> adp[c] + g6p[c] + h[c]
  #2082  PGMT, Bd: -1000 / 1000, Phosphoglucomutase
g1p[c] <=> g6p[c]
  #2459  TRE6PH, Bd: 0 / 1000, Trehalose-6-phosphate hydrolase
h2o[c] + tre6p[c] -> g6p[c] + glc__D[c]

Show previous steps...
```

Show metabolite names in reaction formulae

Some models may use generic ids for `mets/rxns`. In this case, call `surfNet()` with the '`metNameFlag`' (3rd) arguement turned on to show the names for metabolites (`.metNames`) in the reaction formulae, e.g.,

```
surfNet(iJO1366, 'fgam[c]', 1)
```

```
Met #484  fgam[c], N2-Formyl-N1-(5-phospho-D-ribosyl)glycinamide, C8H13N2O9P

Consuming reactions:
  #2207  PRFGS, Bd: 0 / 1000, Phosphoribosylformylglycinamidine synthase
ATP C10H12N5O13P3 + N2-Formyl-N1-(5-phospho-D-ribosyl)glycinamide + L-Glutamine + H2O H2O -> ADP C10H12N5O
  + L-Glutamate + H+ + Phosphate
Producing reactions:
  #1316  GARFT, Bd: -1000 / 1000, Phosphoribosylglycinamide formyltransferase
10-Formyltetrahydrofolate + N1-(5-Phospho-D-ribosyl)glycinamide <=> N2-Formyl-N1-(5-phospho-D-ribosyl)glyc

  #1317  GART, Bd: 0 / 1000, GAR transformylase-T
ATP C10H12N5O13P3 + Formate + N1-(5-Phospho-D-ribosyl)glycinamide -> ADP C10H12N5O10P2 + N2-Formyl-N1-(5-p
  + H+ + Phosphate
```

```
Show previous steps...
```

Hide reaction detials

Turn off the '`showMets`' (6th) arguement to suppress details for reactions, e.g.,

```
surfNet(iJO1366, iJO1366.rxns(1001:1010), [], [], [], 0)
```

```
Rxn #1001  DHPPDA2, Bd: 0 / 1000, Diaminohydroxyphosphoribosylaminopryrimidine deaminase (25drapp)
25drapp[c] + h[c] + h2o[c] -> 5apru[c] + nh4[c]

Rxn #1002  DHPS2, Bd: 0 / 1000, Dihydropteroate synthase
4abz[c] + 6hmhptpp[c] -> dhpt[c] + ppi[c]

Rxn #1003  DHPTDCs2, Bd: 0 / 1000, 4,5-dihydroxy-2,3-pentanedione cyclization (spontaneous)
dhptd[c] -> mdhdhf[c]

Rxn #1004  DHPTDNR, Bd: 0 / 0, Dihydropteridine reductase
dhptdn[c] + 3 h[c] + nadph[c] -> nadp[c] + thptdn[c]

Rxn #1005  DHPTDNRN, Bd: 0 / 0, Dihydropteridine reductase (NADH)
dhptdn[c] + 3 h[c] + nadh[c] -> nad[c] + thptdn[c]

Rxn #1006  DHPTPE, Bd: -1000 / 1000, Dihydroneopterin triphosphate 2'-epimerase
ahdt[c] <=> dhmptp[c]

Rxn #1007  DHQS, Bd: 0 / 1000, 3-dehydroquinate synthase
2dda7p[c] -> 3dhq[c] + pi[c]

Rxn #1008  DHQTi, Bd: 0 / 1000, 3-dehydroquinate dehydratase, irreversible
3dhq[c] -> 3dhsk[c] + h2o[c]

Rxn #1009  DIMPtex, Bd: -1000 / 1000, DIMP transport via diffusion (extracellular to periplasm)
dimp[e] <=> dimp[p]

Rxn #1010  DINSt2pp, Bd: 0 / 1000, Deoxyinosine transport in via proton symport (periplasm)
din[p] + h[p] -> din[c] + h[c]

Show previous steps...
```

Look at one or more flux distributions

First, get a flux distribution by optimizing the biomass production of the model (the standard flux balance analysis[1]). Then call surfNet with the flux distribution (4th argument) to look at how the flux through pyruvate is distributed:

```
s = optimizeCbModel(iJO1366, 'max', 'one');
surfNet(iJO1366, 'pyr[c]', [], s.x)
```

```
Met #853  pyr[c], Pyruvate, C3H3O3

Consuming reactions with non-zero fluxes :
  #511  ACHBS (0.28541), Bd: 0 / 1000, 2-aceto-2-hydroxybutanoate synthase
2obut[c] + h[c] + pyr[c] -> 2ahbut[c] + co2[c]
  #513  ACLS (0.85886), Bd: 0 / 1000, Acetolactate synthase
h[c] + 2 pyr[c] -> alac__S[c] + co2[c]
  #618  ALATA_L (-0.57111), Bd: -1000 / 1000, L-alanine transaminase
akg[c] + ala__L[c] <=> glu__L[c] + pyr[c]
  #987  DHDPS (0.36441), Bd: 0 / 1000, Dihydrodipicolinate synthase
aspsa[c] + pyr[c] -> 23dhdp[c] + h[c] + 2 h2o[c]
```

```
  #1053  DXPS (0.00279), Bd: 0 / 1000, 1-deoxy-D-xylulose 5-phosphate synthase
g3p[c] + h[c] + pyr[c] -> co2[c] + dxyl5p[c]
  #2047  PDH (7.96919), Bd: 0 / 1000, Pyruvate dehydrogenase
coa[c] + nad[c] + pyr[c] -> accoa[c] + co2[c] + nadh[c]
  #2171  POR5 (0.10684), Bd: -1000 / 1000, Pyruvate synthase
coa[c] + 2 flxso[c] + pyr[c] <=> accoa[c] + co2[c] + 2 flxr[c] + h[c]
  #2466  TRPAS2 (-0.05584), Bd: -1000 / 1000, Tryptophanase (L-tryptophan)
h2o[c] + trp__L[c] <=> indole[c] + nh4[c] + pyr[c]
Producing reactions with non-zero fluxes :
  #554  ADCL (0.00066), Bd: 0 / 1000, 4-aminobenzoate synthase
4adcho[c] -> 4abz[c] + h[c] + pyr[c]
  #666  ANS (0.05584), Bd: 0 / 1000, Anthranilate synthase
chor[c] + gln__L[c] -> anth[c] + glu__L[c] + h[c] + pyr[c]
  #813  CHRPL (0.00022), Bd: 0 / 1000, Chorismate pyruvate lyase
chor[c] -> 4hbz[c] + pyr[c]
  #908  CYSTL (0.1512), Bd: 0 / 1000, Cystathionine b-lyase
cyst__L[c] + h2o[c] -> hcys__L[c] + nh4[c] + pyr[c]
  #978  DHAPT (0.86538), Bd: 0 / 1000, Dihydroxyacetone phosphotransferase
dha[c] + pep[c] -> dhap[c] + pyr[c]
  #1353  GLCptspp (10), Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]

Show previous steps...
```

All reactions involving pyruvate with non-zero fluxes are printed. The flux values are in the parentheses following the reaction ids. Note that reactions stated as consuming or producing the metabolite have taken the directions of the fluxes into account. Therefore, supplying a different flux distribution or not supplying may give different display. By default, only reactions with non-zero fluxes are printed if a flux distribution is supplied. Turn the '`nonzeroFluxFlag`' (5th) argument off to show all reactions:

```
surfNet(iJO1366, 'pyr[c]', [], s.x, 0)
```

```
Met #853  pyr[c], Pyruvate, C3H3O3

Consuming reactions:
  #511  ACHBS (0.28541), Bd: 0 / 1000, 2-aceto-2-hydroxybutanoate synthase
2obut[c] + h[c] + pyr[c] -> 2ahbut[c] + co2[c]
  #513  ACLS (0.85886), Bd: 0 / 1000, Acetolactate synthase
h[c] + 2 pyr[c] -> alac__S[c] + co2[c]
  #618  ALATA_L (-0.57111), Bd: -1000 / 1000, L-alanine transaminase
akg[c] + ala__L[c] <=> glu__L[c] + pyr[c]
  #987  DHDPS (0.36441), Bd: 0 / 1000, Dihydrodipicolinate synthase
aspsa[c] + pyr[c] -> 23dhdp[c] + h[c] + 2 h2o[c]
  #1053  DXPS (0.00279), Bd: 0 / 1000, 1-deoxy-D-xylulose 5-phosphate synthase
g3p[c] + h[c] + pyr[c] -> co2[c] + dxyl5p[c]
  #2047  PDH (7.96919), Bd: 0 / 1000, Pyruvate dehydrogenase
coa[c] + nad[c] + pyr[c] -> accoa[c] + co2[c] + nadh[c]
  #2067  PFL (0), Bd: 0 / 1000, Pyruvate formate lyase
coa[c] + pyr[c] -> accoa[c] + for[c]
  #2171  POR5 (0.10684), Bd: -1000 / 1000, Pyruvate synthase
coa[c] + 2 flxso[c] + pyr[c] <=> accoa[c] + co2[c] + 2 flxr[c] + h[c]
  #2172  POX (0), Bd: 0 / 1000, Pyruvate oxidase
h2o[c] + pyr[c] + q8[c] -> ac[c] + co2[c] + q8h2[c]
  #2198  PPS (0), Bd: 0 / 1000, Phosphoenolpyruvate synthase
atp[c] + h2o[c] + pyr[c] -> amp[c] + 2 h[c] + pep[c] + pi[c]
  #2466  TRPAS2 (-0.05584), Bd: -1000 / 1000, Tryptophanase (L-tryptophan)
h2o[c] + trp__L[c] <=> indole[c] + nh4[c] + pyr[c]
Producing reactions:
  #507  ACGAptspp (0), Bd: 0 / 1000, N-Acetyl-D-glucosamine transport via PEP:Pyr PTS  (periplasm)
pep[c] + acgam[p] -> acgam6p[c] + pyr[c]
  #516  ACMANAptspp (0), Bd: 0 / 1000, N-acetyl-D-mannosamine transport via PTS  (periplasm)
```

```
pep[c] + acmana[p] -> acmanap[c] + pyr[c]
  #518  ACMUMptspp (0), Bd: 0 / 1000, N-acetylmuramate transport via PEP:Pyr PTS (periplasm)
pep[c] + acmum[p] -> acmum6p[c] + pyr[c]
  #522  ACNML (0), Bd: 0 / 1000, N-Acetylneuraminate lyase
acnam[c] -> acmana[c] + pyr[c]
  #554  ADCL (0.00066), Bd: 0 / 1000, 4-aminobenzoate synthase
4adcho[c] -> 4abz[c] + h[c] + pyr[c]
  #617  ALATA_D2 (0), Bd: 0 / 1000, D-alanine transaminase
ala__D[c] + pydx5p[c] -> pyam5p[c] + pyr[c]
  #619  ALATA_L2 (0), Bd: 0 / 1000, Alanine transaminase
ala__L[c] + pydx5p[c] -> pyam5p[c] + pyr[c]
  #666  ANS (0.05584), Bd: 0 / 1000, Anthranilate synthase
chor[c] + gln__L[c] -> anth[c] + glu__L[c] + h[c] + pyr[c]
  #698  ARBTptspp (0), Bd: 0 / 1000, Arbutin transport via PEP:Pyr PTS (periplasm)
pep[c] + arbt[p] -> arbt6p[c] + pyr[c]
  #716  ASCBptspp (0), Bd: 0 / 1000, L-ascorbate transport via PEP:Pyr PTS (periplasm)
pep[c] + ascb__L[p] -> ascb6p[c] + pyr[c]
  #813  CHRPL (0.00022), Bd: 0 / 1000, Chorismate pyruvate lyase
chor[c] -> 4hbz[c] + pyr[c]
  #814  CHTBSptspp (0), Bd: 0 / 1000, Chitobiose transport via PEP:Pyr PTS (periplasm)
pep[c] + chtbs[p] -> chtbs6p[c] + pyr[c]
  #902  CYSDDS (0), Bd: 0 / 1000, D-cysteine desulfhydrase
cys__D[c] + h2o[c] -> h2s[c] + nh4[c] + pyr[c]
  #903  CYSDS (0), Bd: 0 / 1000, Cysteine Desulfhydrase
cys__L[c] + h2o[c] -> h2s[c] + nh4[c] + pyr[c]
  #908  CYSTL (0.1512), Bd: 0 / 1000, Cystathionine b-lyase
cyst__L[c] + h2o[c] -> hcys__L[c] + nh4[c] + pyr[c]
  #927  DAAD (0), Bd: 0 / 1000, D-Amino acid dehydrogenase
ala__D[c] + fad[c] + h2o[c] -> fadh2[c] + nh4[c] + pyr[c]
  #942  DAPAL (0), Bd: 0 / 1000, 2,3-diaminopropionate amonnia lyase
23dappa[c] + h2o[c] -> 2 nh4[c] + pyr[c]
  #970  DDPGALA (-0), Bd: -1000 / 1000, 2-dehydro-3-deoxy-6-phosphogalactonate aldolase
2dh3dgal6p[c] <=> g3p[c] + pyr[c]
  #978  DHAPT (0.86538), Bd: 0 / 1000, Dihydroxyacetone phosphotransferase
dha[c] + pep[c] -> dhap[c] + pyr[c]
  #1094  EDA (0), Bd: 0 / 1000, 2-dehydro-3-deoxy-phosphogluconate aldolase
2ddg6p[c] -> g3p[c] + pyr[c]
  #1238  FRUpts2pp (0), Bd: 0 / 1000, Fructose transport via PEP:Pyr PTS (f6p generating) (periplasm)
pep[c] + fru[p] -> f6p[c] + pyr[c]
  #1239  FRUptspp (0), Bd: 0 / 1000, D-fructose transport via PEP:Pyr PTS (periplasm)
pep[c] + fru[p] -> f1p[c] + pyr[c]
  #1303  GALTptspp (0), Bd: 0 / 1000, Galactitol transport via PEP:Pyr PTS (periplasm)
pep[c] + galt[p] -> galt1p[c] + pyr[c]
  #1313  GAMptspp (0), Bd: 0 / 1000, D-glucosamine transport via PEP:Pyr PTS (periplasm)
pep[c] + gam[p] -> gam6p[c] + pyr[c]
  #1341  GLCRAL (0), Bd: 0 / 1000, 5-dehydro-4-deoxyglucarate aldolase
5dh4dglc[c] -> 2h3oppan[c] + pyr[c]
  #1353  GLCptspp (10), Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]
  #1519  HOPNTAL (0), Bd: 0 / 1000, 4-hydroxy-2-oxopentanoate aldolase
4h2opntn[c] -> acald[c] + pyr[c]
  #1551  ICHORT (0), Bd: 0 / 1000, Isochorismatase
h2o[c] + ichor[c] -> 23ddhb[c] + pyr[c]
  #1601  L_LACD2 (0), Bd: 0 / 1000, L-Lactate dehydrogenase (ubiquinone)
lac__L[c] + q8[c] -> pyr[c] + q8h2[c]
  #1602  L_LACD3 (0), Bd: 0 / 1000, L-Lactate dehydrogenase (menaquinone)
lac__L[c] + mqn8[c] -> mql8[c] + pyr[c]
  #1622  LDH_D (0), Bd: -1000 / 1000, D-lactate dehydrogenase
lac__D[c] + nad[c] <=> h[c] + nadh[c] + pyr[c]
  #1623  LDH_D2 (0), Bd: 0 / 1000, D-lactate dehydrogenase
lac__D[c] + q8[c] -> pyr[c] + q8h2[c]
  #1711  MALDDH (0), Bd: 0 / 1000, Malate decarboxylating oxidoreductase (decarboxylating)
mal__D[c] + nad[c] -> co2[c] + nadh[c] + pyr[c]
  #1725  MALTptspp (0), Bd: 0 / 1000, Maltose transport via PEP:Pyr PTS (periplasm)
```

```
pep[c] + malt[p] -> malt6p[c] + pyr[c]
  #1736  MANGLYCptspp (0), Bd: 0 / 1000, 2-O-alpha-mannosyl-D-glycerate transport via PEP:Pyr PTS (peripla
pep[c] + manglyc[p] -> man6pglyc[c] + pyr[c]
  #1739  MANptspp (0), Bd: 0 / 1000, D-mannose transport via PEP:Pyr PTS (periplasm)
pep[c] + man[p] -> man6p[c] + pyr[c]
  #1742  MCITL2 (0), Bd: -1000 / 1000, Methylisocitrate lyase
micit[c] <=> pyr[c] + succ[c]
  #1745  MCPST (0), Bd: 0 / 1000, 3-mercaptopyruvate sulfurtransferase
cyan[c] + mercppyr[c] -> h[c] + pyr[c] + tcynt[c]
  #1761  ME1 (0), Bd: 0 / 1000, Malic enzyme (NAD)
mal__L[c] + nad[c] -> co2[c] + nadh[c] + pyr[c]
  #1762  ME2 (0), Bd: 0 / 1000, Malic enzyme (NADP)
mal__L[c] + nadp[c] -> co2[c] + nadph[c] + pyr[c]
  #1822  MNLptspp (0), Bd: 0 / 1000, Mannitol transport via PEP:Pyr PTS (periplasm)
pep[c] + mnl[p] -> mnl1p[c] + pyr[c]
  #1977  OAADC (0), Bd: 0 / 1000, Oxaloacetate decarboxylase
h[c] + oaa[c] -> co2[c] + pyr[c]
  #2266  PYK (0), Bd: 0 / 1000, Pyruvate kinase
adp[c] + h[c] + pep[c] -> atp[c] + pyr[c]
  #2269  PYRt2rpp (0), Bd: -1000 / 1000, Pyruvate reversible transport via proton symport (periplasm)
h[p] + pyr[p] <=> h[c] + pyr[c]
  #2326  SBTptspp (0), Bd: 0 / 1000, D-sorbitol transport via PEP:Pyr PTS (periplasm)
pep[c] + sbt__D[p] -> pyr[c] + sbt6p[c]
  #2342  SERD_D (0), Bd: 0 / 1000, D-serine deaminase
ser__D[c] -> nh4[c] + pyr[c]
  #2343  SERD_L (0), Bd: 0 / 1000, L-serine deaminase
ser__L[c] -> nh4[c] + pyr[c]
  #2352  SHCHCS3 (0), Bd: 0 / 1000, 2-succinyl-6-hydroxy-2,4-cyclohexadiene 1-carboxylate synthase
2sephchc[c] -> 2shchc[c] + pyr[c]
  #2391  SUCptspp (0), Bd: 0 / 1000, Sucrose transport via PEP:Pyr  (periplasm)
pep[c] + sucr[p] -> pyr[c] + suc6p[c]
  #2464  TREptspp (0), Bd: 0 / 1000, Trehalose transport via PEP:Pyr PTS (periplasm)
pep[c] + tre[p] -> pyr[c] + tre6p[c]
  #2558  VPAMTr (0), Bd: -1000 / 1000, Valine-pyruvate aminotransferase
3mob[c] + ala__L[c] <=> pyr[c] + val__L[c]

Show previous steps...
```

You can also compare multiple flux distributions by supplying them in a matrix format, each column being a flux distribution. For example, get another flux distribution maximizing the biomass production using D-fructose instead of glucose as substrate. Then call surfNet to look at reactions with different fluxes.

Original uptake rates:

```
printUptakeBound(iJO1366);
```

```
EX_ca2_e                    -1000
EX_cbl1_e                   -0.01
EX_cl_e                     -1000
EX_co2_e                    -1000
EX_cobalt2_e                -1000
EX_cu2_e                    -1000
EX_fe2_e                    -1000
EX_fe3_e                    -1000
EX_glc__D_e                   -10
EX_h_e                      -1000
EX_h2o_e                    -1000
EX_k_e                      -1000
EX_mg2_e                    -1000
EX_mn2_e                    -1000
EX_mobd_e                   -1000
EX_na1_e                    -1000
```

```
EX_nh4_e                    -1000
EX_ni2_e                    -1000
EX_o2_e                     -1000
EX_pi_e                     -1000
EX_sel_e                    -1000
EX_slnt_e                   -1000
EX_so4_e                    -1000
EX_tungs_e                  -1000
EX_zn2_e                    -1000
```

Use fructose instead of glucose as substrate:

```
iJO1366 = changeRxnBounds(iJO1366, {'EX_glc__D_e'; 'EX_fru_e'},...
    [0; -10], {'L'; 'L'});
printUptakeBound(iJO1366);
```

```
EX_ca2_e                    -1000
EX_cbl1_e                   -0.01
EX_cl_e                     -1000
EX_co2_e                    -1000
EX_cobalt2_e                -1000
EX_cu2_e                    -1000
EX_fe2_e                    -1000
EX_fe3_e                    -1000
EX_fru_e                      -10
EX_h_e                      -1000
EX_h2o_e                    -1000
EX_k_e                      -1000
EX_mg2_e                    -1000
EX_mn2_e                    -1000
EX_mobd_e                   -1000
EX_na1_e                    -1000
EX_nh4_e                    -1000
EX_ni2_e                    -1000
EX_o2_e                     -1000
EX_pi_e                     -1000
EX_sel_e                    -1000
EX_slnt_e                   -1000
EX_so4_e                    -1000
EX_tungs_e                  -1000
EX_zn2_e                    -1000
```

Run FBA again to get a flux distribution using fructose as substrate. Then look at reactions with different fluxes in the glucose and fructose cases using `surfNet`.

```
sFru = optimizeCbModel(iJO1366, 'max', 'one');  % FBA
fluxMatrix = [s.x, sFru.x];  % put two flux vectors in a matrix
% reactions with different fluxes
rxnDiff = abs(fluxMatrix(:, 1) - fluxMatrix(:, 2)) > 1e-6;
surfNet(iJO1366, iJO1366.rxns(rxnDiff), [], fluxMatrix, [], 0)
```

```
Rxn #139  EX_fru_e (0, -10), Bd: -10 / 1000, D-Fructose exchange
fru[e] <=>

Rxn #164  EX_glc__D_e (-10, 0), Bd: 0 / 1000, D-Glucose exchange
glc__D[e] ->

Rxn #623  ALAt2pp_copy2 (-0.00511, 0), Bd: -1000 / 1000, L-alanine transport in via proton symport (peripl
ala__L[p] + h[p] <=> ala__L[c] + h[c]

Rxn #624  ALAt4pp (0.00511, 0), Bd: 0 / 1000, L-alanine transport in via sodium symport (periplasm)
```

```
ala__L[p] + na1[p] -> ala__L[c] + na1[c]

Rxn #1230  FRUK (0, 5.75203), Bd: 0 / 1000, Fructose-1-phosphate kinase
atp[c] + f1p[c] -> adp[c] + fdp[c] + h[c]

Rxn #1238  FRUpts2pp (0, 4.24797), Bd: 0 / 1000, Fructose transport via PEP:Pyr PTS (f6p generating) (peri
pep[c] + fru[p] -> f6p[c] + pyr[c]

Rxn #1239  FRUptspp (0, 5.75203), Bd: 0 / 1000, D-fructose transport via PEP:Pyr PTS (periplasm)
pep[c] + fru[p] -> f1p[c] + pyr[c]

Rxn #1240  FRUtex (-0, 10), Bd: -1000 / 1000, D-fructose transport via diffusion (extracellular to peripla
fru[e] <=> fru[p]

Rxn #1353  GLCptspp (10, 0), Bd: 0 / 1000, D-glucose transport via PEP:Pyr PTS (periplasm)
pep[c] + glc__D[p] -> g6p[c] + pyr[c]

Rxn #1356  GLCtex_copy2 (10, 0), Bd: 0 / 1000, Glucose transport via diffusion (extracellular to periplasm
glc__D[e] -> glc__D[p]

Rxn #1377  GLUt2rpp (0, -0.00511), Bd: -1000 / 1000, L-glutamate transport via proton symport, reversible
glu__L[p] + h[p] <=> glu__L[c] + h[c]

Rxn #1378  GLUt4pp (0, 0.00511), Bd: 0 / 1000, Na+/glutamate symport (periplasm)
glu__L[p] + na1[p] -> glu__L[c] + na1[c]

Rxn #1758  MDH (4.82506, 4.82528), Bd: -1000 / 1000, Malate dehydrogenase
mal__L[c] + nad[c] <=> h[c] + nadh[c] + oaa[c]

Rxn #1837  MOX (0.0016, 0.00138), Bd: -1000 / 1000, Malate oxidase
mal__L[c] + o2[c] <=> h2o2[c] + oaa[c]

Rxn #2048  PDX5PO2 (0.00022, 0), Bd: 0 / 1000, Pyridoxine 5'-phosphate oxidase (anaerboic
nad[c] + pdx5p[c] -> h[c] + nadh[c] + pydx5p[c]

Rxn #2049  PDX5POi (0, 0.00022), Bd: 0 / 1000, Pyridoxine 5'-phosphate oxidase
o2[c] + pdx5p[c] -> h2o2[c] + pydx5p[c]

Rxn #2064  PFK (5.75203, 0), Bd: 0 / 1000, Phosphofructokinase
atp[c] + f6p[c] -> adp[c] + fdp[c] + h[c]

Rxn #2077  PGI (5.91807, -4.08193), Bd: -1000 / 1000, Glucose-6-phosphate isomerase
g6p[c] <=> f6p[c]

Show previous steps...
```

Customize model data to be displayed

Customize the fields for metabolites and reactions to be printed by supplying the '`field2print`' (7th) argument. It is defaulted to be:

`{{'metNames','metFormulas'}, {'rxnNames','lb','ub'}}`

The first cell contains the metabolite-related fields to be printed and the second cell contains the reaction-related fields to be printed. It can also be inputted as a single cell array of strings, as long as from the size (equal to `#mets` or `#rxns`) or from the name of the field (starting with '`met`' or '`rxn`'), the fields are recognizable to be met- or rxn-related. For example, show the `grRules` for rxns but omit the bounds and show the constraint sense (`csense`) associated with each metabolite. Note the difference from the original call:

```
surfNet(iJO1366, 'fdp[c]', [], [], [], [],...
```

```
    {'metNames', 'metFormulas', 'rxnNames', 'grRules', 'csense'})
```

```
Met #473  fdp[c], D-Fructose 1,6-bisphosphate, C6H10O12P2, csense: E

Consuming reactions:
  #1151  FBA, Fructose-bisphosphate aldolase, grRules: b2097 or b1773 or b2925
fdp[c] <=> dhap[c] + g3p[c]
  #1153  FBP, Fructose-bisphosphatase, grRules: b3925 or b4232 or b2930
fdp[c] + h2o[c] -> f6p[c] + pi[c]
Producing reactions:
  #1230  FRUK, Fructose-1-phosphate kinase, grRules: b2168
atp[c] + f1p[c] -> adp[c] + fdp[c] + h[c]
  #2064  PFK, Phosphofructokinase, grRules: b3916 or b1723
atp[c] + f6p[c] -> adp[c] + fdp[c] + h[c]

Show previous steps...
```

```
surfNet(iJO1366, 'fdp[c]')
```

```
Warning: The 2nd input is neither a metabolite nor reaction of the model.
```

The last argument (8th) 'nCharBreak' sets the number of characters printed per line. By default, it is equal to the width of the Matlab command window. Note the difference:

Characters per line = width of the command window (default):

```
surfNet(iJO1366, [], [], [], [], 0)
```

```
Rxn #8  BIOMASS_Ec_iJO1366_core_53p95M, Bd: 0 / 1000, E. coli biomass objective function (iJO1366) - core
0.000223 10fthf[c] + 2.6e-05 2fe2s[c] + 0.000223 2ohph[c] + 0.00026 4fe4s[c] + 0.513689 ala__L[c] + 0.0002
  0.295792 arg__L[c] + 0.241055 asn__L[c] + 0.241055 asp__L[c] + 54.1248 atp[c] + 0.000122 bmocogdp[c] + 2
  0.005205 ca2[c] + 0.005205 cl[c] + 0.000576 coa[c] + 2.5e-05 cobalt2[c] + 0.133508 ctp[c] + 0.000709 cu2
  0.09158 cys__L[c] + 0.026166 datp[c] + 0.027017 dctp[c] + 0.027017 dgtp[c] + 0.026166 dttp[c] + 0.000223
  0.006715 fe2[c] + 0.007808 fe3[c] + 0.26316 gln__L[c] + 0.26316 glu__L[c] + 0.612638 gly[c] + 0.215096 g
  + 0.094738 his__L[c] + 0.290529 ile__L[c] + 0.195193 k[c] + 0.450531 leu__L[c] + 0.343161 lys__L[c] + 0.
  0.008675 mg2[c] + 0.000223 mlthf[c] + 0.000691 mn2[c] + 7e-06 mobd[c] + 0.001831 nad[c] + 0.000447 nadp[
  0.000323 ni2[c] + 0.017868 pe160[c] + 0.054154 pe161[c] + 0.185265 phe__L[c] + 0.000223 pheme[c] + 0.221
  0.000223 pydx5p[c] + 0.000223 ribflv[c] + 0.215792 ser__L[c] + 0.000223 sheme[c] + 0.004338 so4[c] + 0.0
  0.000223 thmpp[c] + 0.253687 thr__L[c] + 0.056843 trp__L[c] + 0.137896 tyr__L[c] + 5.5e-05 udcpdp[c] + 0
  0.423162 val__L[c] + 0.000341 zn2[c] + 0.019456 kdo2lipid4[e] + 0.013894 murein5px4p[p] + 0.045946 pe160
  -> 53.95 adp[c] + 53.95 h[c] + 53.9457 pi[c] + 0.773903 ppi[c]

Show previous steps...
```

40 characters per line:

```
surfNet(iJO1366, [], [], [], [], 0, [], 40)
```

```
Rxn #8  BIOMASS_Ec_iJO1366_core_53p95M, Bd: 0 / 1000, E. coli biomass objective function (iJO1366) - core
0.000223 10fthf[c] + 2.6e-05 2fe2s[c] +
  0.000223 2ohph[c] + 0.00026 4fe4s[c] +
  0.513689 ala__L[c] + 0.000223 amet[c]
  + 0.295792 arg__L[c] +
  0.241055 asn__L[c] +
  0.241055 asp__L[c] + 54.1248 atp[c] +
  0.000122 bmocogdp[c] + 2e-06 btn[c] +
  0.005205 ca2[c] + 0.005205 cl[c] +
  0.000576 coa[c] + 2.5e-05 cobalt2[c] +
  0.133508 ctp[c] + 0.000709 cu2[c] +
  0.09158 cys__L[c] + 0.026166 datp[c] +
  0.027017 dctp[c] + 0.027017 dgtp[c] +
  0.026166 dttp[c] + 0.000223 fad[c] +
```

```
  0.006715 fe2[c] + 0.007808 fe3[c] +
  0.26316 gln__L[c] + 0.26316 glu__L[c]
  + 0.612638 gly[c] + 0.215096 gtp[c] +
  48.6015 h2o[c] + 0.094738 his__L[c] +
  0.290529 ile__L[c] + 0.195193 k[c] +
  0.450531 leu__L[c] +
  0.343161 lys__L[c] +
  0.153686 met__L[c] + 0.008675 mg2[c] +
  0.000223 mlthf[c] + 0.000691 mn2[c] +
  7e-06 mobd[c] + 0.001831 nad[c] +
  0.000447 nadp[c] + 0.013013 nh4[c] +
  0.000323 ni2[c] + 0.017868 pe160[c] +
  0.054154 pe161[c] + 0.185265 phe__L[c]
  + 0.000223 pheme[c] +
  0.221055 pro__L[c] +
  0.000223 pydx5p[c] +
  0.000223 ribflv[c] +
  0.215792 ser__L[c] + 0.000223 sheme[c]
  + 0.004338 so4[c] + 0.000223 thf[c] +
  0.000223 thmpp[c] + 0.253687 thr__L[c]
  + 0.056843 trp__L[c] +
  0.137896 tyr__L[c] + 5.5e-05 udcpdp[c]
  + 0.144104 utp[c] + 0.423162 val__L[c]
  + 0.000341 zn2[c] +
  0.019456 kdo2lipid4[e] +
  0.013894 murein5px4p[p] +
  0.045946 pe160[p] + 0.02106 pe161[p]
  -> 53.95 adp[c] + 53.95 h[c] +
  53.9457 pi[c] + 0.773903 ppi[c]

Show previous steps...
```

80 characters per line:

```
surfNet(iJO1366, [], [], [], [], 0, [], 80)
```

```
Rxn #8  BIOMASS_Ec_iJO1366_core_53p95M, Bd: 0 / 1000, E. coli biomass objective function (iJO1366) - core
0.000223 10fthf[c] + 2.6e-05 2fe2s[c] + 0.000223 2ohph[c] + 0.00026 4fe4s[c] +
  0.513689 ala__L[c] + 0.000223 amet[c] + 0.295792 arg__L[c] +
  0.241055 asn__L[c] + 0.241055 asp__L[c] + 54.1248 atp[c] +
  0.000122 bmocogdp[c] + 2e-06 btn[c] + 0.005205 ca2[c] + 0.005205 cl[c] +
  0.000576 coa[c] + 2.5e-05 cobalt2[c] + 0.133508 ctp[c] + 0.000709 cu2[c] +
  0.09158 cys__L[c] + 0.026166 datp[c] + 0.027017 dctp[c] + 0.027017 dgtp[c] +
  0.026166 dttp[c] + 0.000223 fad[c] + 0.006715 fe2[c] + 0.007808 fe3[c] +
  0.26316 gln__L[c] + 0.26316 glu__L[c] + 0.612638 gly[c] + 0.215096 gtp[c] +
  48.6015 h2o[c] + 0.094738 his__L[c] + 0.290529 ile__L[c] + 0.195193 k[c] +
  0.450531 leu__L[c] + 0.343161 lys__L[c] + 0.153686 met__L[c] + 0.008675 mg2[c]
  + 0.000223 mlthf[c] + 0.000691 mn2[c] + 7e-06 mobd[c] + 0.001831 nad[c] +
  0.000447 nadp[c] + 0.013013 nh4[c] + 0.000323 ni2[c] + 0.017868 pe160[c] +
  0.054154 pe161[c] + 0.185265 phe__L[c] + 0.000223 pheme[c] +
  0.221055 pro__L[c] + 0.000223 pydx5p[c] + 0.000223 ribflv[c] +
  0.215792 ser__L[c] + 0.000223 sheme[c] + 0.004338 so4[c] + 0.000223 thf[c] +
  0.000223 thmpp[c] + 0.253687 thr__L[c] + 0.056843 trp__L[c] +
  0.137896 tyr__L[c] + 5.5e-05 udcpdp[c] + 0.144104 utp[c] + 0.423162 val__L[c]
  + 0.000341 zn2[c] + 0.019456 kdo2lipid4[e] + 0.013894 murein5px4p[p] +
  0.045946 pe160[p] + 0.02106 pe161[p] -> 53.95 adp[c] + 53.95 h[c] +
  53.9457 pi[c] + 0.773903 ppi[c]

Show previous steps...
```

REFERENCES

[1] Orth, J. D., Thiele I., and Palsson, B. Ø. What is flux balance analysis? *Nat. Biotechnol., 28*(3), 245–248 (2010).