Analyse combinedModel, input to component contribution

Author: Ronan Fleming, NUI Galway, Leiden University

Reviewers:

INTRODUCTION

PROCEDURE

Configure the environment

All the installation instructions are in a separate .md file named vonBertalanffy.md in docs/source/installation

With all dependencies installed correctly, we configure our environment, verfy all dependencies, and add required fields and directories to the matlab path.

```
aPath = which('initVonBertalanffy');
basePath = strrep(aPath,'vonBertalanffy/initVonBertalanffy.m','');
addpath(genpath(basePath))
folderPattern=[filesep 'old'];
method = 'remove';
editCobraToolboxPath(basePath,folderPattern,method)
```

```
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/componentContribution/ol
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/directionalityReport/old
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/groupContribution/old
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/inchi/old
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/molFiles/old
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/protons/old
removing: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/trainingModel/old
```

```
aPath = which('initVonBertalanffy');
basePath = strrep(aPath,'vonBertalanffy/initVonBertalanffy.m','');
addpath(genpath(basePath))
folderPattern=[filesep 'new'];
method = 'add';
editCobraToolboxPath(basePath,folderPattern,method)
```

```
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/componentContribution/new
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/groupContribution/new
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/inchi/new
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/molFiles/new
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/protons/new
adding: /home/rfleming/work/sbgCloud/code/fork-cobratoolbox/src/analysis/thermo/trainingModel/new
```

```
initVonBertalanffy
```

```
ChemAxon Marvin Beans is installed and working.
    linux-vdso.so.1 (0x00007fff445d9000)
    libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00007f91d2049000)
    libopenbabel.so.5 => /usr/lib/libopenbabel.so.5 (0x00007f91d1df9000)
    libstdc++.so.6 => /usr/lib/x86_64-linux-gnu/libstdc++.so.6 (0x00007f91d1bdf000)
```

```
	libgcc_s.so.1 => /usr/local/bin/MATLAB/R2021a/sys/os/glnxa64/libgcc_s.so.1 (0x00007f91d19c7000)
	/lib64/ld-linux-x86-64.so.2 (0x00007f91d2269000)
	libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00007f91d19bf000)
	libz.so.1 => /lib/x86_64-linux-gnu/libz.so.1 (0x00007f91d19a3000)
	libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6 (0x00007f91d1854000)
	libgomp.so.1 => /usr/lib/x86_64-linux-gnu/libgomp.so.1 (0x00007f91d180f000)
	libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x00007f91d17ec000)

babel must depend on the system libstdc++.so.6 not the one from MATLAB
Trying to edit the 'LD_LIBRARY_PATH' to make sure that it has the correct system path before the Matlab pa
The solution will be arch dependent
```

Load combined model

```
load('data_prior_to_componentContribution')
```

Statistics on the combined model

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool),' training metabolites')
```

```
672 training metabolites
```

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool &
combinedModel.groupDecomposableBool),' of which are Moiety decomposable.')
```

```
627 of which are Moiety decomposable.
```

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool &
~combinedModel.inchiBool),' of which have no inchi.')
```

```
45 of which have no inchi.
```

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool & combinedModel.inchiBool
& ~combinedModel.groupDecomposableBool),' of which are not Moiety
decomposable.')
```

```
0 of which are not Moiety decomposable.
```

```
fprintf('%u%s\n',nnz(combinedModel.testMetBool),' test metabolites')
```

```
2994 test metabolites
```

```
fprintf('%u%s\n',nnz(combinedModel.testMetBool &
combinedModel.groupDecomposableBool),' of which are Moiety decomposable.')
```

```
1997 of which are Moiety decomposable.
```

```
fprintf('%u%s\n',nnz(combinedModel.testMetBool & ~combinedModel.inchiBool),'
of which have no inchi.')
```

```
994 of which have no inchi.
```

```
fprintf('%u%s\n',nnz(combinedModel.testMetBool & combinedModel.inchiBool
& ~combinedModel.groupDecomposableBool),' ... of which are not Moiety
decomposable.')
```

```
3 ... of which are not Moiety decomposable.
```

```
fprintf('%u%s\n',size(combinedModel.S,1),' combined model metabolites.')
```

```
3666 combined model metabolites.
```

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool &
~combinedModel.testMetBool),' ... of which are exclusively training
metabolites.')
```

```
672 ... of which are exclusively training metabolites.
```

```
fprintf('%u%s\n',nnz(combinedModel.trainingMetBool &
combinedModel.testMetBool),' ... of which are both training and test
metabolites.')
```

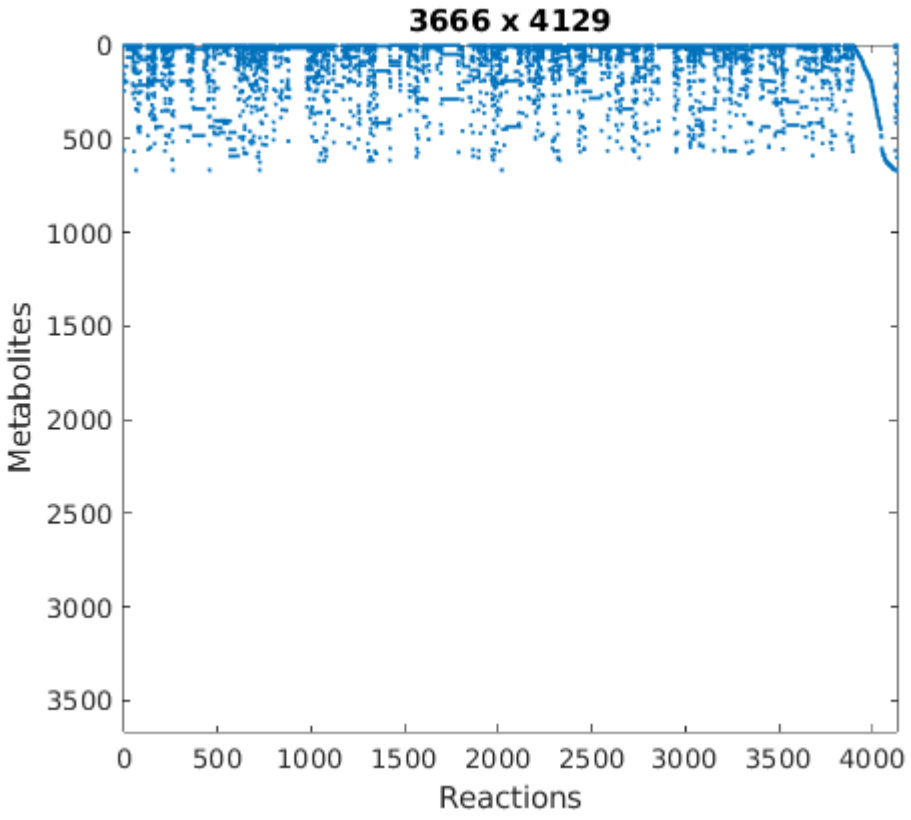
```
0 ... of which are both training and test metabolites.
```

```
fprintf('%u%s\n',nnz(~combinedModel.trainingMetBool &
combinedModel.testMetBool),' ... of which are exclusively test metabolites.')
```

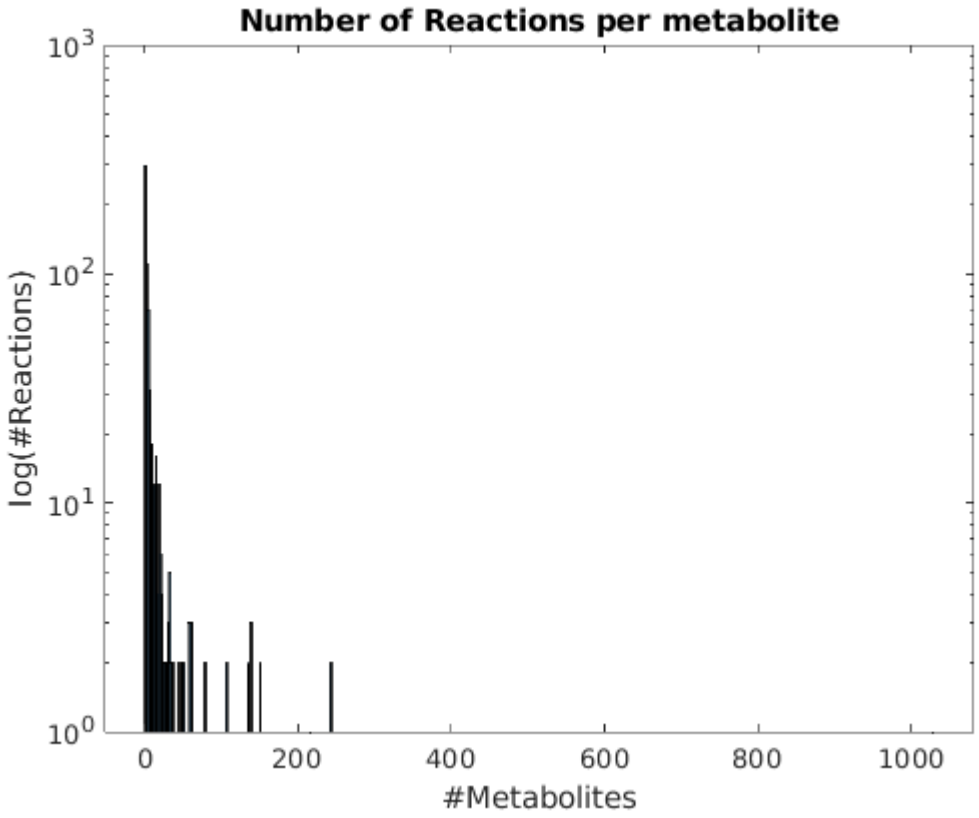
```
2994 ... of which are exclusively test metabolites.
```

Sparsity pattern of combinedModel.S

```
figure
spy(combinedModel.S);
title([int2str(size(combinedModel.S,1)) ' x '
int2str(size(combinedModel.S,2))])
xlabel('Reactions')
ylabel('Metabolites')
```



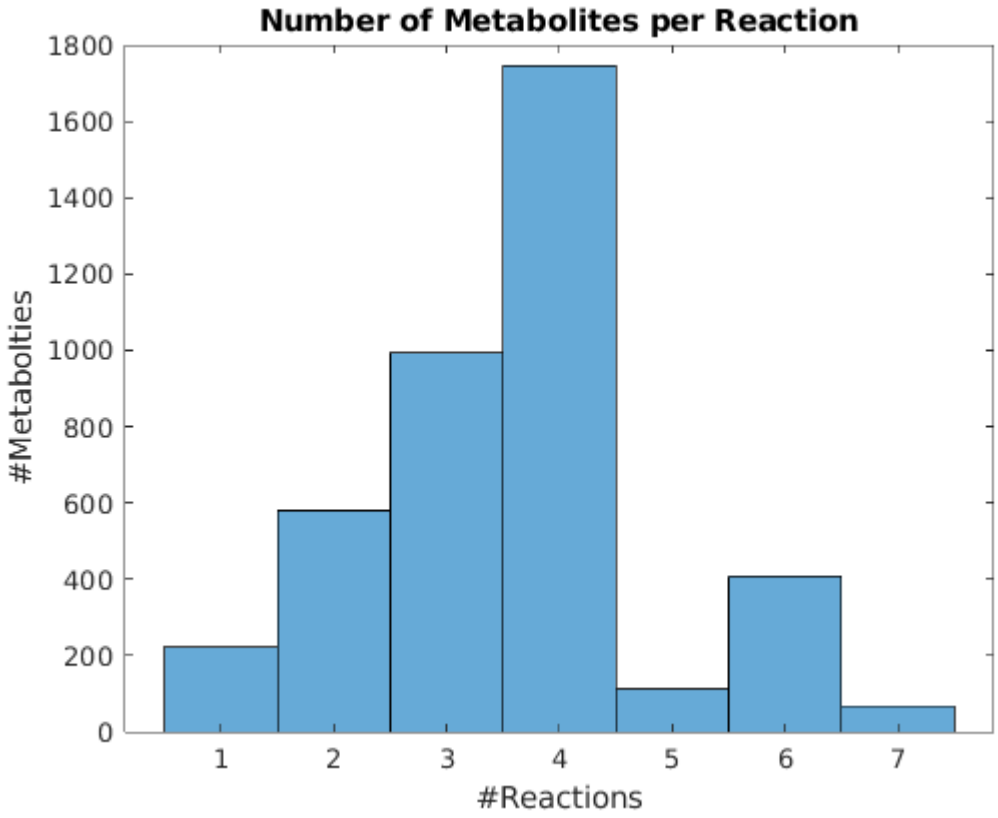

```
nReactionsPerMetabolite=full(sum(combinedModel.S~=0,2));
histogram(nReactionsPerMetabolite(nReactionsPerMetabolite~=0),'BinWidth',2)
title('Number of Reactions per metabolite')
xlabel('#Metabolites')
ylabel('log(#Reactions)')
set(gca,'YScale','log')
```




```
fprintf('%u%s\n',nnz(nReactionsPerMetabolite==0),' metabolites without
reactions.')
```

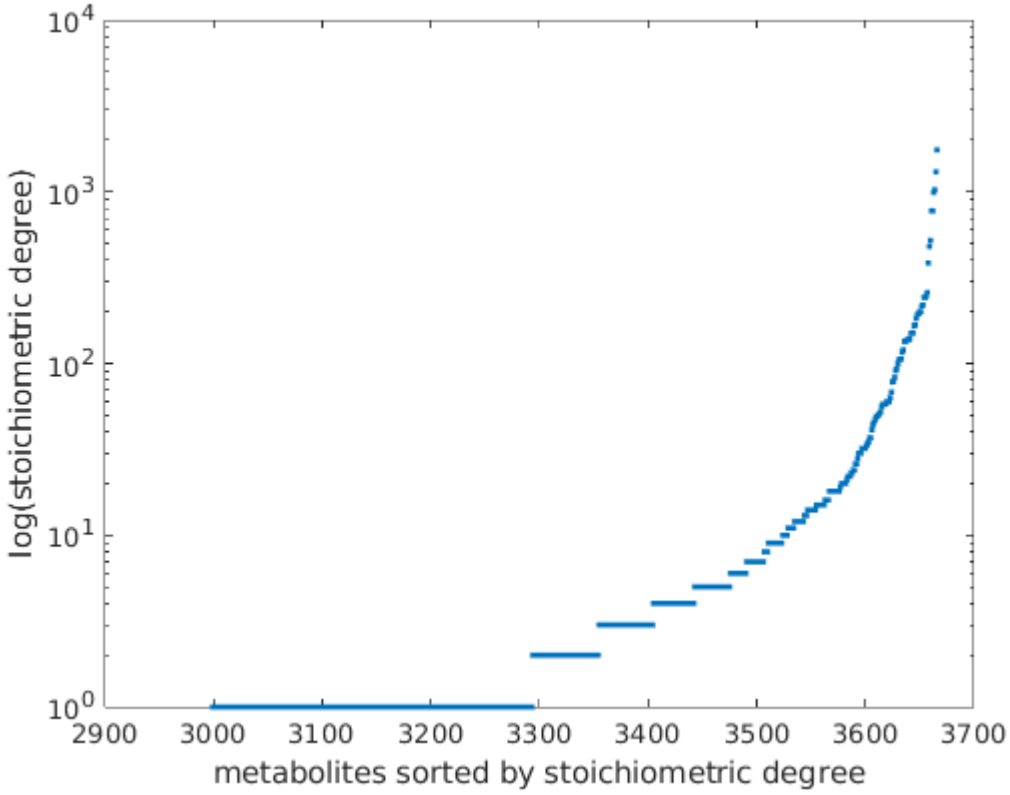
```
2998 metabolites without reactions.
```

```
nMetabolitesPerReaction=full(sum(combinedModel.S~=0,1)');
histogram(nMetabolitesPerReaction)
title('Number of Metabolites per Reaction')
xlabel('#Reactions')
ylabel('#Metabolties')
```




```
if any(nMetabolitesPerReaction==0)
    error('combinedModel.S reaction without a metabolite')
end
```

```
dX = diag(combinedModel.S*combinedModel.S');
figure
plot(sort(dX),'.')
set(gca,'YScale','log')
ylabel('log(stoichiometric degree)')
xlabel('metabolites sorted by stoichiometric degree')
```

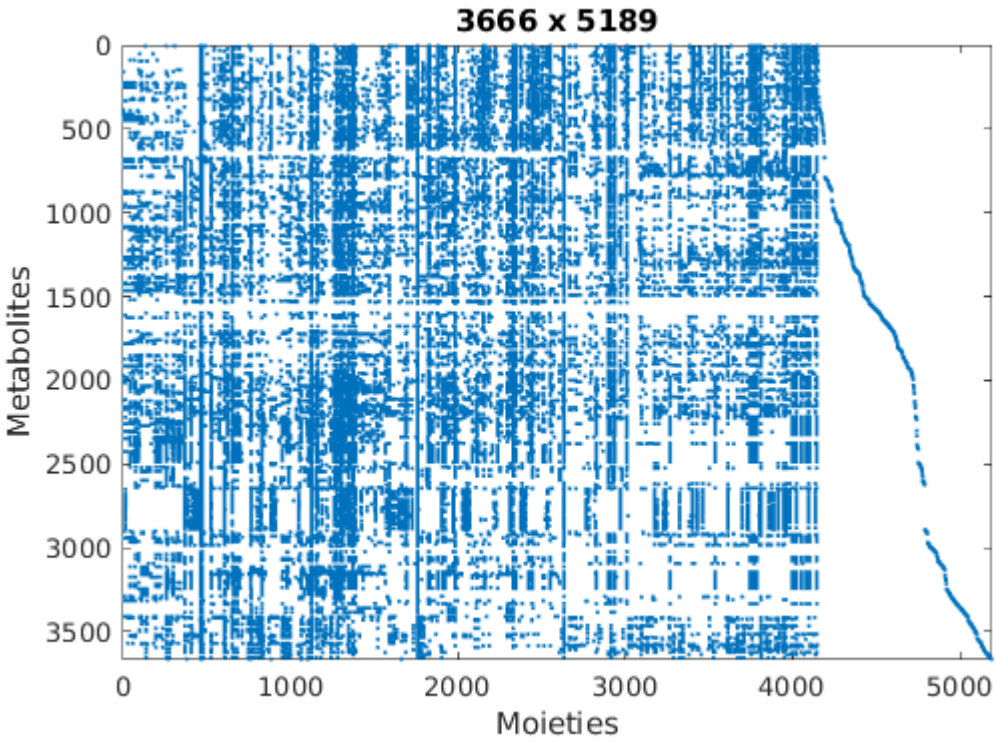



```
nnz(dX==0)
```

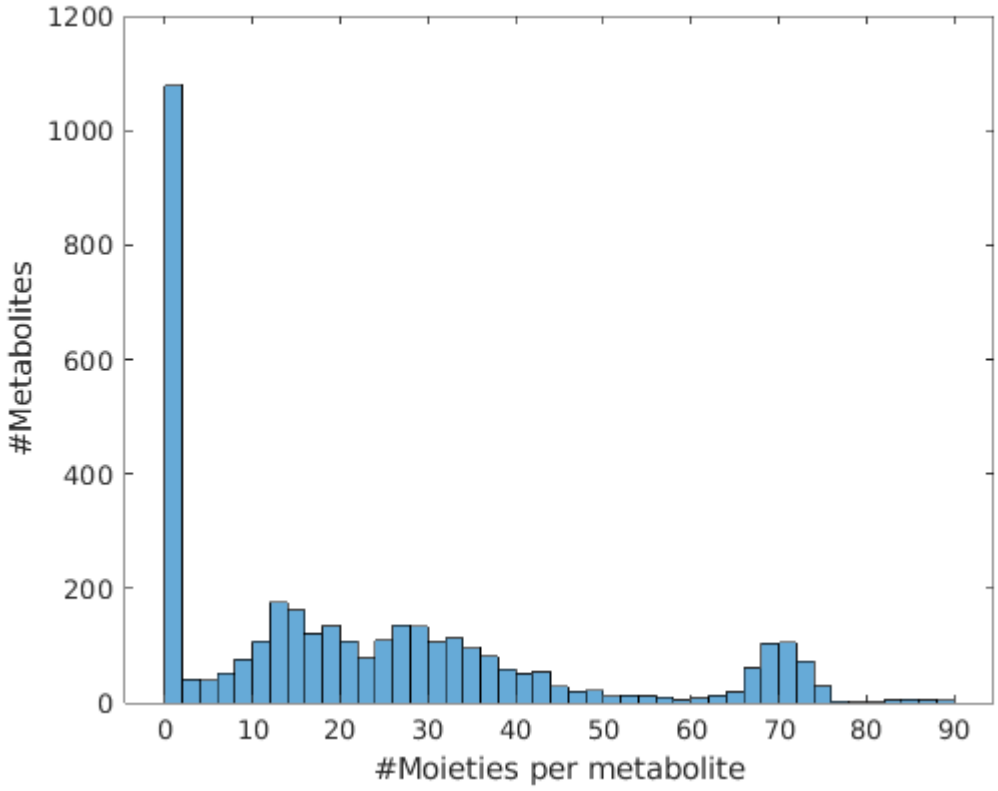
```
ans = 2998
```

Sparsity pattern of combinedModel.G

```
figure
spy(combinedModel.G)
title([int2str(size(combinedModel.G,1)) ' x '
int2str(size(combinedModel.G,2))])
xlabel('Moieties')
ylabel('Metabolites')
```

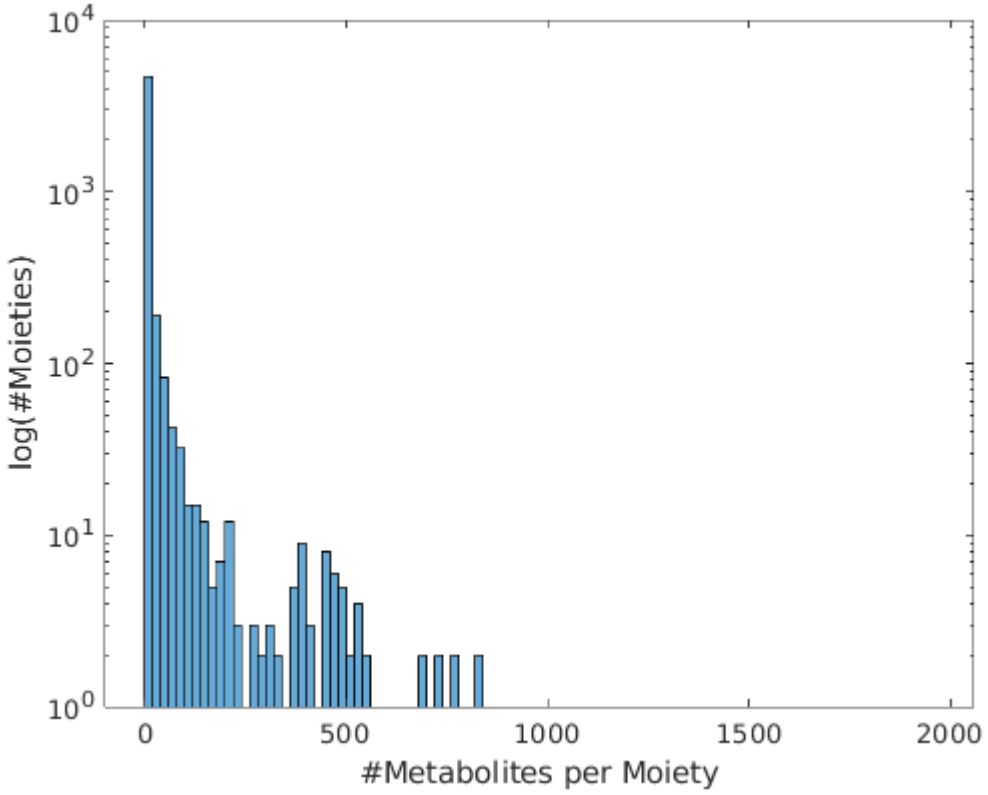



```
nGroupPerMetabolite = full(sum(combinedModel.G~=0,2));
histogram(nGroupPerMetabolite,'BinWidth',2)
xlabel('#Moieties per metabolite')
ylabel('#Metabolites')
```




```
if any(nGroupPerMetabolite==0)
    error('Metabolite without any Moiety')
end
```

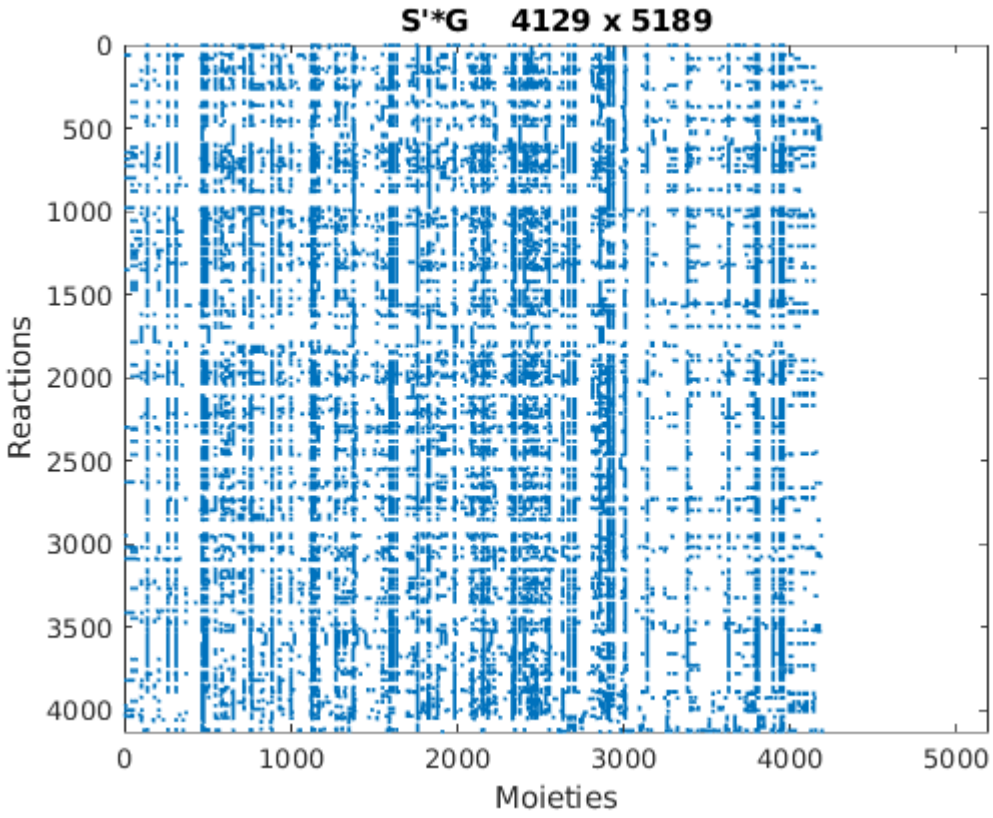
```
nMetabolitePerGroup = sum(combinedModel.G~=0,1)';
if 0
    histogram(nMetabolitePerGroup);
    %set(gca,'YScale','log')
    ylim([0, 10]);
else
    histogram(nMetabolitePerGroup);
    set(gca,'YScale','log')
end
xlabel('#Metabolites per Moiety')
ylabel('log(#Moieties)')
```



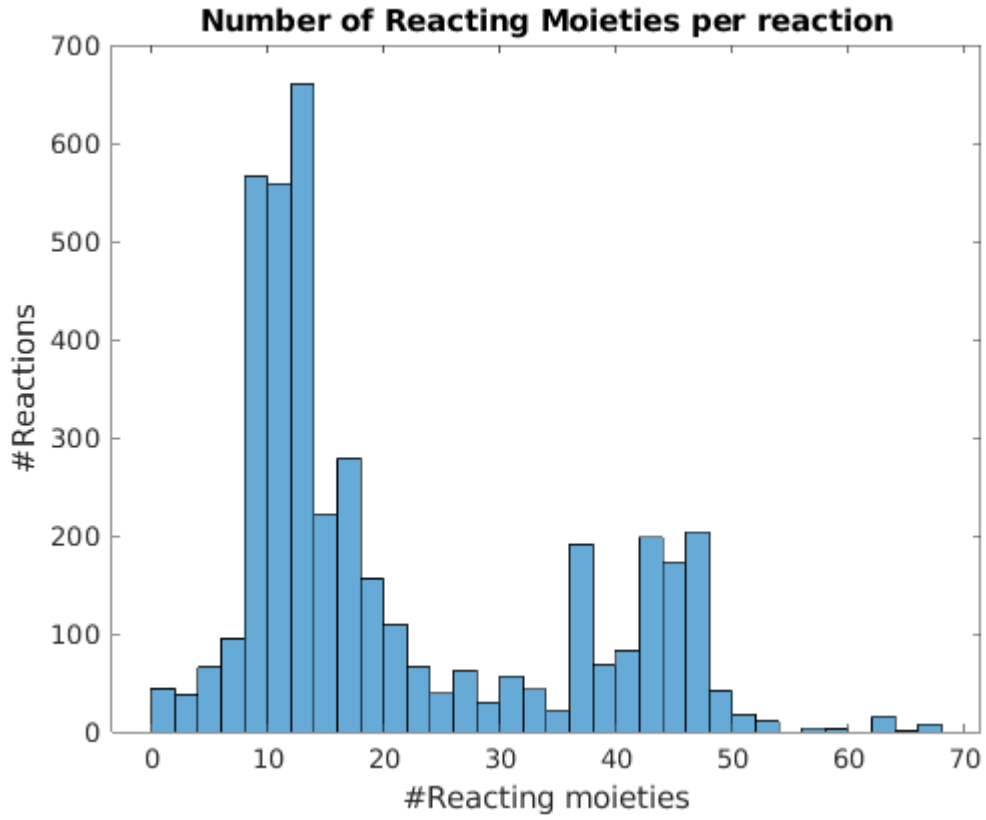

```
if any(nMetabolitePerGroup==0)
    error('Moiety without metabolite')
end
```

Sparsity pattern of combinedModel.StG

```
StG=combinedModel.S'*combinedModel.G;
figure
spy(StG)
title(['S''*G    ' int2str(size(StG,1)) ' x ' int2str(size(StG,2))])
xlabel('Moieties')
ylabel('Reactions')
```




```
nReactingMoieties=full(sum(StG~=0,2));
histogram(nReactingMoieties,'BinWidth',2)
title('Number of Reacting Moieties per reaction')
xlabel('#Reacting moieties')
ylabel('#Reactions')
```




```
fprintf('%u%s\n',nnz(nReactingMoieties==0),' reactions without reacting moieties.')
```

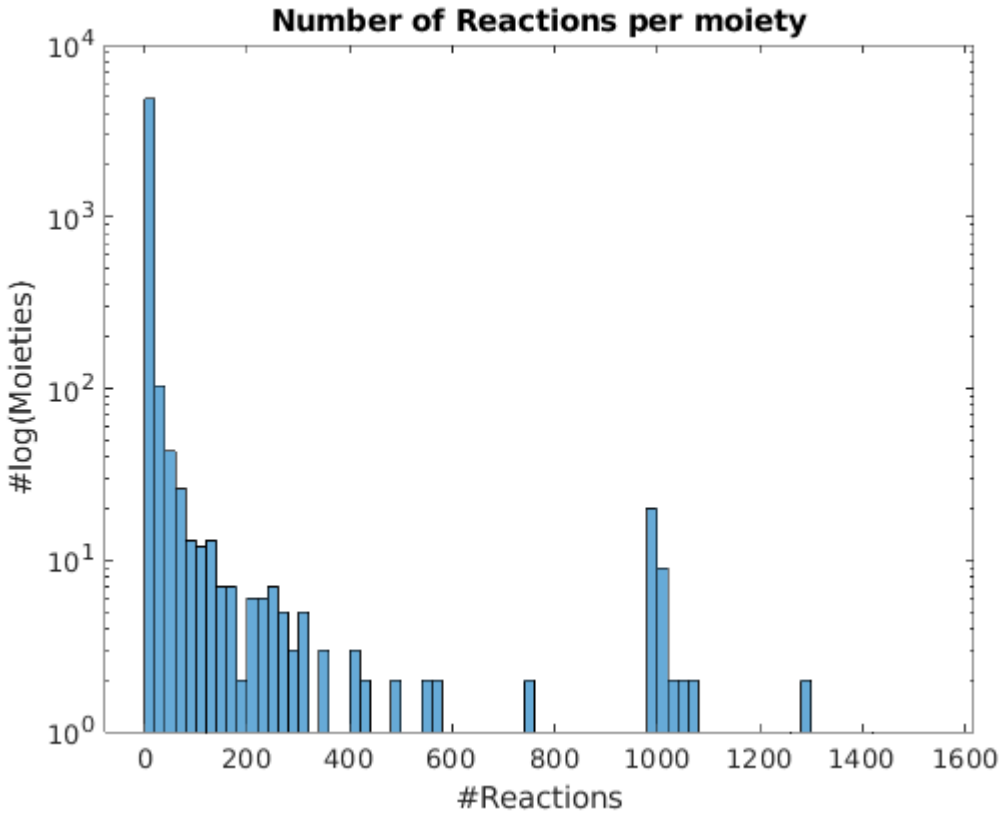
```
19 reactions without reacting moieties.
```

```
printRxnFormula(combinedModel,combinedModel.rxns(nReactingMoieties==0));
```

```
TECRDB_373    C00002 + C00015     ->    C00008 + C00075
TECRDB_764    C00004 + C00006     ->    C00003 + C00005
TECRDB_765    C00004 + C00006     ->    C00003 + C00005
TECRDB_766    C00004 + C00006     ->    C00003 + C00005
TECRDB_767    C00004 + C00006     ->    C00003 + C00005
TECRDB_768    C00004 + C00006     ->    C00003 + C00005
TECRDB_769    C00004 + C00006     ->    C00003 + C00005
TECRDB_770    C00004 + C00006     ->    C00003 + C00005
TECRDB_771    C00004 + C00006     ->    C00003 + C00005
TECRDB_772    C00004 + C00006     ->    C00003 + C00005
TECRDB_773    C00004 + C00006     ->    C00003 + C00005
TECRDB_822    C00003 + C00005     ->    C00004 + C00006
TECRDB_823    C00003 + C00005     ->    C00004 + C00006
TECRDB_824    C00003 + C00005     ->    C00004 + C00006
TECRDB_2364    C00002 + C00015     ->    C00008 + C00075
TECRDB_2521    C00002 + C00035     ->    C00008 + C00044
TECRDB_2639    C00002 + C00104     ->    C00008 + C00081
TECRDB_2870    C00166     ->    C02763
TECRDB_3904    C00036     ->    C03981
```

```
nReactionsPerMoiety=full(sum(StG~=0,1)');
histogram(nReactionsPerMoiety)
set(gca,'YScale','log')
```

```
title('Number of Reactions per moiety')
xlabel('#Reactions')
ylabel('#log(Moieties)')
```




```
fprintf('%u%s%u%s\n',nnz(nReactionsPerMoiety==0),' of the ',
length(nReactionsPerMoiety), ' moieties do not react in any training
reaction.')
```

```
3789 of the 5189 moieties do not react in any training reaction.
```