

%% %% VARIABLES: N: (compressed) stoichiometric matrix; q: number of columns (reactions) in N
 %% rev: indices of reversible reactions (columns in N); irrev: indices of irreversible reactions (columns in N)

%% %% PRE-PROCESSING %% %%

%% reconfiguration: we only need to store here the number of reactions in the reconfigured network

qsplit=q+length(rev);

%% sub-routine *initializeR*: initializes matrix R by computing a proper null space matrix of Nsplit (see remarks in text and Methods section)

R=*initializeR*(N, rev); % dimension of the returned matrix R is: qsplit rows; qsplit-m columns

%% splitting R in binary (R1) and real number part (R2)

R1=*makeBitmap*(R(1:(qsplit-m), :));

% *makeBitmap* returns the bit mask of a matrix

R2=R((qsplit-m+1):qsplit, :);

numr=qsplit-m;

%% %% MAIN PART %% %%

for p=(q-m+1):q % m loops from p=(q-m+1) TO q

new_numr=numr;

jneg=*find*(R2(1,:)<0);

jpos=*find*(R2(1,:)>0);

for k=1:length(jneg)

for l=1:length(jpos)

newr=*or*(R1(:,k),R1(:,l)); % element-wise OR

% check for minimum number of zeros; see remarks in text

if(*numberOfNullBits*(newr)+1<qsplit-m-1)

continue;

end

%Adjacency test

adj=1; r=0;

while(adj & r<=numr)

r=r+1;

testr=*or*(newr, R1(:,r));

if(r~=l & r~=k & *all*(testr == newr)) % ~= means "unequal to"

adj = 0;

end

end

if(adj) %If adjacent then combine

new_numr=new_numr+1;

R1(:,new_numr)=newr;

R2(:,new_numr)=R2(1,l)*R2(:,k) - R2(1,k)*R2(:,l);

end

end

end

%deletion of negative rays

R1(:,jneg)=[];

R2(:,jneg)=[];

numr=new_numr - length(jneg);

% transfer current (i.e. the first) row of R2 as Bitmap into R1; then delete this row in R2

R1(p,:)=*makeBitmap*(R2(1,:));

R2(1,:)=[];

end

%% first result: the columns of R1 are the bitmaps of the EMs from the reconfigured network

%% %% POST-PROCESSING %% %%

%% Post-processing step 1: EMs(binary) of S^* $\rightarrow$ EMs(binary) of S

remove2cycles(R1);

% this sub-routine removes the 2-cycles obtained from splitting rev. reactions

numr=numr-rev;

R1(rev,:)=*or*(R1(rev,:), R1(q+1:qsplit,:));

% the rules for back-configuration

R1(q+1:qsplit,:)=[];

% deletes backward directions

%% Post-processing step 2 (optionally): EMs(binary) of $S \rightarrow$ EMs(real) of S (Determination of the (rate) coefficients in each EM)

fullEM=*zeros*(q,numr);

for i=1:numr

preacs=*findOneBits*(R1(:,i));

% this sub-routine delivers the positions in EM i whose bit is 1

Ne=N(:,preacs);

v=*null*(Ne);

% from eq. (14)

temp=*intersect*(preacs,irrev);

% first participating irreversible component

if isempty(temp))

% reversible EM

findAndDeleteDuplicate(R1,i);

% deletes the reverse direction of this EM

numr=numr-1;

% (here, reversible EMs are considered only once)

fullEM(preacs,i)=v/abs(v(1));

% normalization of the reversible EM

else

% irreversible EM

fullEM(preacs,i)=v/v(temp(1));

% Normalization to the

end

% first irreversible component

end

%% result: columns of fullEM are the EMs; post-processing step 3 can be appended for expanding the EMs for the uncompressed network