REDUCE Support for Reaction Equation Systems

Herbert Melenk
Konrad-Zuse-Zentrum für Informationstechnik Berlin
Takustraße 7
D–14195 Berlin–Dahlem
Germany
e-mail: melenk@zib.de

January 1991

The REDUCE package REACTEQN allows one to transform chemical reaction systems into ordinary differential equation systems (ode) corresponding to the laws of pure mass action.
A single reaction equation is an expression of the form

$\langle n1\rangle\langle s1\rangle + \langle n2\rangle\langle s2\rangle + \ldots - > \langle n3\rangle\langle s3\rangle + \langle n4\rangle\langle s4\rangle + \ldots$

or

$\langle n1\rangle\langle s1\rangle + \langle n2\rangle\langle s2\rangle + \ldots \langle\rangle\ \langle n3\rangle\langle s3\rangle + \langle n4\rangle\langle s4\rangle + \ldots$

where the $\langle si\rangle$ are arbitrary names of species (REDUCE symbols) and the $\langle ni\rangle$ are positive integer numbers. The number 1 can be omitted. The connector $- >$ describes a one way reaction, while $\langle\ \rangle$ describes a forward and backward reaction.

A reaction system is a list of reaction equations, each of them optionally followed by one or two expressions for the rate constants. A rate constant can a number, a symbol or an arbitrary REDUCE expression. If a rate constant is missing, an automatic constant of the form RATE(n) (where n is an integer counter) is generated. For double reactions the first constant is used for the forward direction, the second one for the backward direction.

The names of the species are collected in a list bound to the REDUCE variable

SPECIES. This list is automatically filled during the processing of a reaction system. The species enter in an order corresponding to their appearance in the reaction system and the resulting ode's will be ordered in the same manner.

If a list of species is preassigned to the variable SPECIES either explicitly or from previous operations, the given order will be maintained and will dominate the formatting process. So the ordering of the result can be easily influenced by the user.

Syntax:

reac2ode { ⟨*reaction*⟩ [,⟨*rate*⟩ [,⟨*rate*⟩]]

[,⟨*reaction*⟩ [,⟨*rate*⟩ [,⟨*rate*⟩]]]

....

};

where two rates are applicable only for ⟨⟩ reactions.

Result is a system of explicit ordinary differential equations with polynomial right-hand sides. As side effect the following variables are set:

lists:

rates: list of the rates in the system

species: list of the species in the system

matrices:

inputmat: matrix of the input coefficients

outputmat: matrix of the output coefficients

In the matrices the row number corresponds to the input reaction number, while the column number corresponds to the species index. Note: if the rates are numerical values, it will be in most cases appropriate to select a REDUCE evaluation mode for floating point numbers. That is

REDUCE 3.3: on float,numval;

REDUCE 3.4: on rounded;

Inputmat and outputmat can be used for linear algebra type investigations of the reaction system. The classical reaction matrix is the difference of these matrices; however, the two matrices contain more information than their differences because the appearance of a species on both sides is not reflected by the reaction matrix.

EXAMPLES:

```
% Example taken from Feinberg (Chemical Engineering):

species := {A1,A2,A3,A4,A5};

reac2ode { A1 + A4 <> 2A1, rho, beta,

A1 + A2 <> A3, gamma, epsilon,

A3 <> A2 + A5, theta, mue};

2

{DF(A1,T)=RHO*A1*A4 - BETA*A1 - GAMMA*A1*A2 + EPSILON*A3,

DF(A2,T)= - GAMMA*A1*A2 + EPSILON*A3 + THETA*A3 - MUE*A2*A5,

DF(A3,T)=GAMMA*A1*A2 - EPSILON*A3 - THETA*A3 + MUE*A2*A5,

2

DF(A4,T)= - RHO*A1*A4 + BETA*A1 ,

DF(A5,T)=THETA*A3 - MUE*A2*A5}

% the corresponding matrices:

inputmat;

        [ 1 0 0 1 0 ]
        [           ]
        [ 1 1 0 0 0 ]
        [           ]
        [ 0 0 1 0 0 ]
```

```
outputmat;

                    [ 2 0 0 0 0 ]
                    [           ]
                    [ 0 0 1 0 0 ]
                    [           ]
                    [ 0 1 0 0 1 ]
```

```
% computation of the classical reaction matrix as difference
% of output and input matrix:
reactmat := outputmat-inputmat;

                [ 1    0    0    -1   0 ]
                [                       ]
REACTMAT :=     [ -1   -1   1    0    0 ]
                [                       ]
                [ 0    1    -1   0    1 ]
```

```
% Example with automatic generation of rate constants
% and automatic extraction of species
species := {};
reac2ode { A1 + A4 <> 2A1,
A1 + A2 <> A3,
a3 <> A2 + A5};
```

```
new species: A1
new species: A4
new species: A3
new species: A2
new species: A5
2
{DF(A1,T)= - A1 *RATE(2) + A1*A4*RATE(1) - A1*A2*RATE(3) +
A3*RATE(4),
2
DF(A4,T)=A1 *RATE(2) - A1*A4*RATE(1),
DF(A2,T)= - A1*A2*RATE(3) - A2*A5*RATE(6) + A3*RATE(5) + A3*RATE(4),
DF(A3,T)=A1*A2*RATE(3) + A2*A5*RATE(6) - A3*RATE(5) - A3*RATE(4),
DF(A5,T)= - A2*A5*RATE(6) + A3*RATE(5)}
% Example with rates computed from numerical expressions
species := {};
reac2ode { A1 + A4 <> 2A1, 17.3* 22.4^1.5,
0.04* 22.4^1.5 };
new species: A1
new species: A4
2
{DF(A1,T)= - 4.24065*A1 + 1834.08*A1*A4,
2
DF(A4,T)=4.24065*A1 - 1834.08*A1*A4}
```