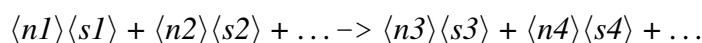


16.52 REACTEQN: Support for chemical reaction equation systems

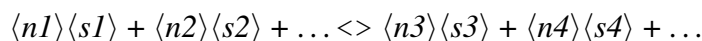
This package allows a user to transform chemical reaction systems into ordinary differential equation systems (ODE) corresponding to the laws of pure mass action.

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A single reaction equation is an expression of the form



or



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 \rightarrow 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 be 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:

```

reactode {  $\langle reaction \rangle$  [,  $\langle rate \rangle$  [,  $\langle rate \rangle$ ]] [,  $\langle reaction \rangle$  [,  $\langle rate \rangle$  [,  $\langle rate \rangle$ ]]] ....
};

```

where two rates are applicable only for $\langle \rangle$ reactions.

Result is a system of explicit ordinary differential equations with polynomial righthand 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 switch on REDUCE rounded mode for floating point numbers. That is

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: This input

```
% 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};
```

gives the output

$$\begin{aligned} \text{DF}(A1, T) &= \text{RHO} \cdot A1 \cdot A4 - \text{BETA} \cdot A1^2 - \text{GAMMA} \cdot A1 \cdot A2 + \text{EPSILON} \cdot A3, \\ \text{DF}(A2, T) &= -\text{GAMMA} \cdot A1 \cdot A2 + \text{EPSILON} \cdot A3 + \text{THETA} \cdot A3 - \text{MUE} \cdot A2 \cdot A5, \\ \text{DF}(A3, T) &= \text{GAMMA} \cdot A1 \cdot A2 - \text{EPSILON} \cdot A3 - \text{THETA} \cdot A3 + \text{MUE} \cdot A2 \cdot A5, \end{aligned}$$

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

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

The corresponding matrices are

```
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 := {};

react2ode { A1 + A4 <> 2A1,
           A1 + A2 <> A3,
           a3 <> A2 + A5};
```

```

new species: A1
new species: A4
new species: A3
new species: A2
new species: A5

```

$$\{DF(A1, T) = - A1^2 * RATE(2) + A1 * A4 * RATE(1) - A1 * A2 * RATE(3) + A3 * RATE(4),$$

$$DF(A4, T) = A1^2 * RATE(2) - A1 * A4 * RATE(1),$$

$$DF(A2, T) = - A1 * A2 * RATE(3) - A2 * A5 * RATE(6) + A3 * RATE(5) + A3 * RATE(4),$$

$$DF(A3, T) = A1 * A2 * RATE(3) + A2 * A5 * RATE(6) - A3 * RATE(5) - A3 * RATE(4),$$

$$DF(A5, T) = - A2 * A5 * RATE(6) + A3 * RATE(5) \}$$

```
% Example with rates computed from numerical expressions
```

```
species := {};
```

```

react2ode { A1 + A4 <> 2A1, 17.3* 22.4^1.5,
           0.04* 22.4^1.5 };

```

```

new species: A1
new species: A4

```

$$\{DF(A1, T) = - 4.24065 * A1^2 + 1834.08 * A1 * A4,$$

$$DF(A4, T) = 4.24065 * A1^2 - 1834.08 * A1 * A4\}$$