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CHEMSIMUL — a tool for simulating chemical reaction systems

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Abstract

CHEMSIMUL is a computer program system for numerical simulation of chemical reaction systems. It can be used for modeling complex kinetics in many different contexts. It contains a translator module and a module for solving the resulting coupled nonlinear ordinary differential equations. A number of special features are described, in particular a method for verifying the mass balance, and the computation af reaction heat and temperature rise by thermodynamic coupling to the kinetics. Graphical output is facilitated by so-called "plot expressions". The capabilities of CHEMSIMUL is illustrated by examples.

Introduction

Chemical transformations taking place in the natural environment as well as in industrial processes are in general very complex. Even in well designed laboratory experiments it is often difficult to study elementary chemical reactions without interference from simultaneous side reactions. Therefore computer simulation has become a powerful tool for the analysis of complex reactions, which are fundamental for understanding atmospheric chemistry, combustion chemistry and air pollution problems, and for the development of new technologies.

The program system CHEMSIMUL was developed at Risø National Laboratory as the result of a close co-operation between chemists and applied mathematicians. CHEMSIMUL is a computerized simulator of chemical kinetics with the following main components:

- Module for input of reaction equations in chemical notation
- Automatic translator from chemical equations to differential equations

- Solution of system of ordinary differential equations (ODEs)
- Output routines
- Miscellaneous facilities

The simulation results will be concentrations of the chemical species in the reaction system as functions of time. These can be given in tabular and graphical form. A detailed description of CHEMSIMUL can be found in [1].

Chemists at Risø and elsewhere have used CHEMSIMUL for many years as a simulation tool for supporting their experimental work. It was early realized that the construction of the ODEs from the reaction equations should be made fully automatic. This was accomplished in the translation module in CHEMSIMUL. It was a design criterion that the chemist could express the reaction processes to be studied in familiar chemical nomenclature. The program has been used in many simulations, particularly in radiation chemistry, where bursts of electron beams or γ-rays are modeled by rectangular source pulses of finite time duration, or trains of such pulses. Heat generation from the reactions is accounted for by a thermodynamic coupling to the rate constants. There are a number of other special features in the program, notably a method for checking the mass balance.

Chemical kinetics

CHEMSIMUL is constructed to simulate homogeneous kinetics in monophase. Only zero-, first-, and second-order reactions are allowed. Reactions of higher order must be emulated by suitable first- and second-order reactions.

When preparing input data for CHEMSIMUL, the reactions are written in normal chemical notation, e.g.

$$\mathrm{A} = \mathrm{B} + \mathrm{C}; \quad k_1$$

for a first-order reaction, and

$$\mathrm{A} + \mathrm{D} = \mathrm{E} + \mathrm{F}; \quad k_2$$

for a second-order reaction; k_1 and k_2 are the rate constants for these reactions.

An important example of a zero-order reaction is a radiolytic process. Here a species A is produced by radiation, say from electron beams or γ-rays. The rate of production is proportional to the dose rate $D(t)$:

$$\frac{d[\mathrm{A}]}{dt} = G(\mathrm{A})D(t).$$

where $G(\mathrm{A})$ is the yield value for production of the given species A with concentration [A]. CHEMSIMUL normally assumes that the dose rate $D(t)$ is a rectangular pulse:

$$D(t) = \begin{cases} D_0 & 0 < t < t_\mathrm{r} \\ 0 & \text{otherwise,} \end{cases}$$

where t_r is the time of radiation; this may be generalized to a train of equidistant rectangular pulses. It is also possible to handle cases with a sum of exponentially decaying dose rates.

The concept of G-values can be used for zero-order reactions in general, which admits other types of reactions to be simulated.

CHEMSIMUL allows a free choice of units in the computations.

Translating reactions to differential equations

When explaining the translation in CHEMSIMUL from chemical reactions to differential equations we shall first use a very simple reaction scheme with only one reaction, and then a more realistic sample case from combustion. Consider the reaction

$$\mathrm{R1} + \mathrm{R2} \rightarrow \mathrm{R3} + \mathrm{R4}$$

with 4 *species* (2 *reactants* and 2 *products*). We assume that the reaction proceeds according to the law of mass action with the rate constant k. Suppose also that the chemical medium is irradiated either by an electronic beam or by γ-rays, such that the species R2 and R3 are produced by this radiation with yields determined by $G(\mathrm{R2})$ and $G(\mathrm{R3})$. Then the resulting differential equations for the concentrations are

$$\begin{aligned}
\frac{d[\mathrm{R1}]}{dt} &= -k[\mathrm{R1}][\mathrm{R2}] \\
\frac{d[\mathrm{R2}]}{dt} &= -k[\mathrm{R1}][\mathrm{R2}] + G(\mathrm{R2})D(t) \\
\frac{d[\mathrm{R3}]}{dt} &= k[\mathrm{R1}][\mathrm{R2}] + G(\mathrm{R3})D(t) \\
\frac{d[\mathrm{R4}]}{dt} &= k[\mathrm{R1}][\mathrm{R2}]
\end{aligned}$$

Here $[\cdot]$ denotes concentration and $D(t)$ is the external dose rate at time t.

The reaction between R1 and R2 is a second-order reaction, while the radiolytic production of R2 and R3 are zero-order reactions. CHEMSIMUL does not treat third-order reactions or higher directly, so these must be emulated by lower-order reactions. We see that a single chemical reaction equation is described by a system of Ordinary Differential Equations (ODEs), which are non-linear in the concentrations. Starting with the time $t = 0$ and the initial values of the reactant concentrations $[\mathrm{R1}]_0$, $[\mathrm{R2}]_0$, $[\mathrm{R3}]_0$ and $[\mathrm{R4}]_0$ we can integrate the system up to some final time $t = t_\mathrm{end}$.

Very small chemical systems such as this can be simulated by making a direct write-up of the ODE system, but for larger systems this would be tedious and error-prone. Therefore CHEMSIMUL has a module for automatic translation of the chemical reactions to differential equations.

Let us now consider a more realistic reaction system discussed in [2] for modeling a H_2–O_2 combustion process:

$$\begin{array}{lccl}
\text{(R1)} & \mathrm{H + H} & \rightarrow & \mathrm{H_2} \\
\text{(R2)} & \mathrm{H + O_2} & \rightarrow & \mathrm{HO_2} \\
\text{(R3)} & \mathrm{H + HO_2} & \rightarrow & \mathrm{OH + OH} \\
\text{(R4)} & \mathrm{HO_2 + HO_2} & \rightarrow & \mathrm{H_2O_2 + O_2} \\
\text{(R5)} & \mathrm{OH + OH} & \rightarrow & \mathrm{H_2O_2} \\
\text{(R6)} & \mathrm{H + OH} & \rightarrow & \mathrm{H_2O} \\
\text{(R7)} & \mathrm{OH + HO_2} & \rightarrow & \mathrm{H_2O + O_2} \\
\text{(R8)} & \mathrm{OH + H_2} & \rightarrow & \mathrm{H_2O + H}
\end{array}$$

The corresponding part of the CHEMSIMUL input file, with rate constants, reads:

```
RE1: H+H=H2; A=4.0E7
RE2: H+O2=HO2; A=4.5E8
RE3: H+HO2=OH+OH; A=6.5E10
RE4: HO2+HO2=H2O2+O2; A=2.0E9
RE5: OH+OH=H2O2; A=4.0E9
RE6: H+OH=H2O; A=1.0E10
RE7: OH+HO2=H2O+O2; A=6.0E10
RE8: OH+H2=H2O+H; A=4.0E3
```

We note the similarity with the chemical notation for this system. When processing a reaction system as this, CHEMSIMUL scans and "digests" all the kinetic equations, symbol by symbol. On encounter it tabulates every new species and includes its name in the current set of symbols. It also stores the reaction rates. After the scan phase an assembly phase is invoked. The technical details are discussed in [1,2]. Here we shall only show the outcome of the translation process, where we for illustration use CHEMSIMUL's ODE printout feature:

```
D[H]/DT   = - 2*K1*H*H - K2*H*O2 - K3*H*HO2 - K6*H*OH + K8*OH*H2
            + G(H)*CONST*DOSE
D[H2]/DT  =   K1*H*H - K8*OH*H2
D[O2]/DT  = - K2*H*O2 + K4*HO2*HO2 + K7*OH*HO2
D[HO2]/DT =   K2*H*O2 - K3*H*HO2 - 2*K4*HO2*HO2 - K7*OH*HO2
D[OH]/DT  =   K3*H*HO2 + K3*H*HO2 - 2*K5*OH*OH - K6*H*OH - K7*OH*HO2
            - K8*OH*H2
D[H2O2]/DT=   K4*HO2*HO2 + K5*OH*OH
D[H2O]/DT =   K6*H*OH + K7*OH*HO2 + K8*OH*H2
```

Checking mass balance and electro neutrality

The accurate solution of the differential equation system describing the chemical reactions requires an overall conservation of the chemical mass balance. The integration method belongs to a class with the implicit property of mass preservation, as shown by Rosenbaum [7,8], and so there is no need to check for mass balance continuously. We use instead a static consistency check. If the check fails, the simulation is halted before integration; this practice has proved useful for detecting input errors in the write-up of reaction equations. CHEMSIMUL recognizes each species as an entity with a name. This means that a formal stoichiometric balance does not imply an atom-to-atom balance. But it is possible to perform a *partial* consistency check based on the *stoichiometric matrix* $\mathbf{A}$, which enters the *balance equation*

$$\mathbf{A}\mathbf{v} = \mathbf{0},$$

For example, in our combustion case the balance equation reads

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & 1 & -2 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -2 & 1 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & -1 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 & -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathrm{H} \\ \mathrm{H2} \\ \mathrm{O2} \\ \mathrm{HO2} \\ \mathrm{OH} \\ \mathrm{H2O2} \\ \mathrm{H2O} \end{pmatrix} = \mathbf{0}$$

It must be possible to satisfy the matrix equation by a set of strictly positive values for the masses of all the elements of the species vector. Ridler *et al.* [9] proposed a heuristic checking method based on Gaussian elimination in integer arithmetics on $\mathbf{A}$. Later we have replaced this by a mathematically more stringent method: By the homogeneity of the balance equation we can replace the demand of positive values by a demand of all values be ≥ 1. Thus, if $\mathbf{A} = \{a_{ij}\}$, it must be possible to find solutions $y_j \geq 1$ to the equations

$$\sum_{j=1}^{N} a_{ij} y_j = 0, \quad i = 1, \ldots, M$$

which on writing $y_j = x_j + 1$ may be replaced by the system

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{x} \geq \mathbf{0}$$

where $\mathbf{x} = \{x_j\}$ and $\mathbf{b} = \{b_i\}$ with $b_i = -\sum_{j=1}^{N} a_{ij}$. To decide the feasibility of this system is a standard linear-programming problem. It can be solved efficiently by the simplex method.

CHEMSIMUL admits species names with charge designators as e.g. `FE[+++]` or `OH[-]`. Such a convention enables the program to check the electro neutrality both in the individual reactions and for the totality of G yield values. Like the mass balance check, this feature may be useful in catching errors in the input data file.

Names may also be qualified by a number in brackets, e.g. `FE[2]` or `FE[2][+]`.

Thermodynamic coupling to kinetics

It is possible for CHEMSIMUL to simulate an adiabatic reaction at constant volume. In particular this means that the total heat formation Q_{tot} and the temperature T can be simulated by two extra equations. To provide a thermodynamic coupling to the kinetics, CHEMSIMUL accepts rate coefficients in the modified Arrhenius form

$$k = AT^{\beta} \exp(-E_{\mathrm{a}}/(RT))$$

where T is the absolute temperature, E_{a} the activation energy, R the gas constant, and β an empirical exponent. The factor T^{β} is included for gas phase kinetics. The source of the heat may come from the chemical reactions as well as from irradiation. The specific heat capacity, $c_v(\mathrm{R}_s)$, must be known for each species R_s, and the specific heat of reaction, q_r, must be known for each reaction r. In this context q_r is defined as $-\Delta H$ (H = enthalpy), which means that q_r is positive for an exothermic reaction. The differential equations governing Q_{tot} and T are

$$\frac{dQ_{\mathrm{tot}}}{dt} = \sum_{r=1}^{M} k_r[\mathrm{R}_j][\mathrm{R}_k]\, q_r + \alpha D'(t)$$

and

$$\frac{dT}{dt} = \frac{dQ_{\mathrm{tot}}/dt}{\sum_{s=1}^{N} c_v(\mathrm{R}_s)\,[\mathrm{R}_s]} = \frac{\sum_{r=1}^{M} k_r[\mathrm{R}_j][\mathrm{R}_k]\, q_r + \alpha D'(t)}{\sum_{s=1}^{N} c_v(\mathrm{R}_s)\,[\mathrm{R}_s]}$$

respectively, where M is the number of reactions and N the number of species in the system; $D'(t)$ is the dose rate, and the *heat production coefficient* α converts dose to heat. R_j and R_k are the second-order reactants attached to the reaction r with rate constant k_r. For a first-order reaction we should set $[\mathrm{R}_k] = 1$.

The following example of an extended H2-O2 reaction mechanism is used to show this coupling. The input reactions are shown below. As it might be recognised by the reader, it is not necessary to number the reaction equations consecutively, which makes it possible to mark out single reactions as RE7, and to establish databases on certain reaction mechanisms.

```
RE1:H2+O2=H +HO2;A=2.400E-5,B=-1,EA=236960,Q=-4.367E-19
RE2:H2O2+M=OH+OH+M;A=2.140E+9,B=-4.86,EA=222780,Q=-3.629E-19
RE4:H+O2+M=HO2+M;A=1.760E-30,B=-1,EA=0,Q=3.350E-19
RE5:H+HO2=OH+OH;A=2.490E-10,B=0,EA=4200,Q=2.666E-19
RE6:HO2+HO2=H2O2+O2;A=3.000E-12,B=0,EA=0,Q=2.945E-19
*RE7:OH+OH+M=H2O2+M;A=1.600E-23,B=-3,EA=0,Q=3.629E-19
RE8: H2 + OH = H2O + H;A=1.060E-17,B=2,EA=12390,Q=1.067E-19
RE10: HO2+H=OH+OH;A=2.800E-10,B=0,EA=3660,Q=2.666E-19
RE11: H+OH+M=H2O+M;A=6.110E-26,B=-2,EA=0,Q=8.383E-19
RE14: HO2+OH=H2O+O2;A=2.400E-8,B=-1,EA=0,Q=5.033E-19
RE17: H2O2+OH=H2O+HO2;A=2.900E-12,B=0,EA=1330,Q=2.088E-19
```

In the following figure the results are shown.

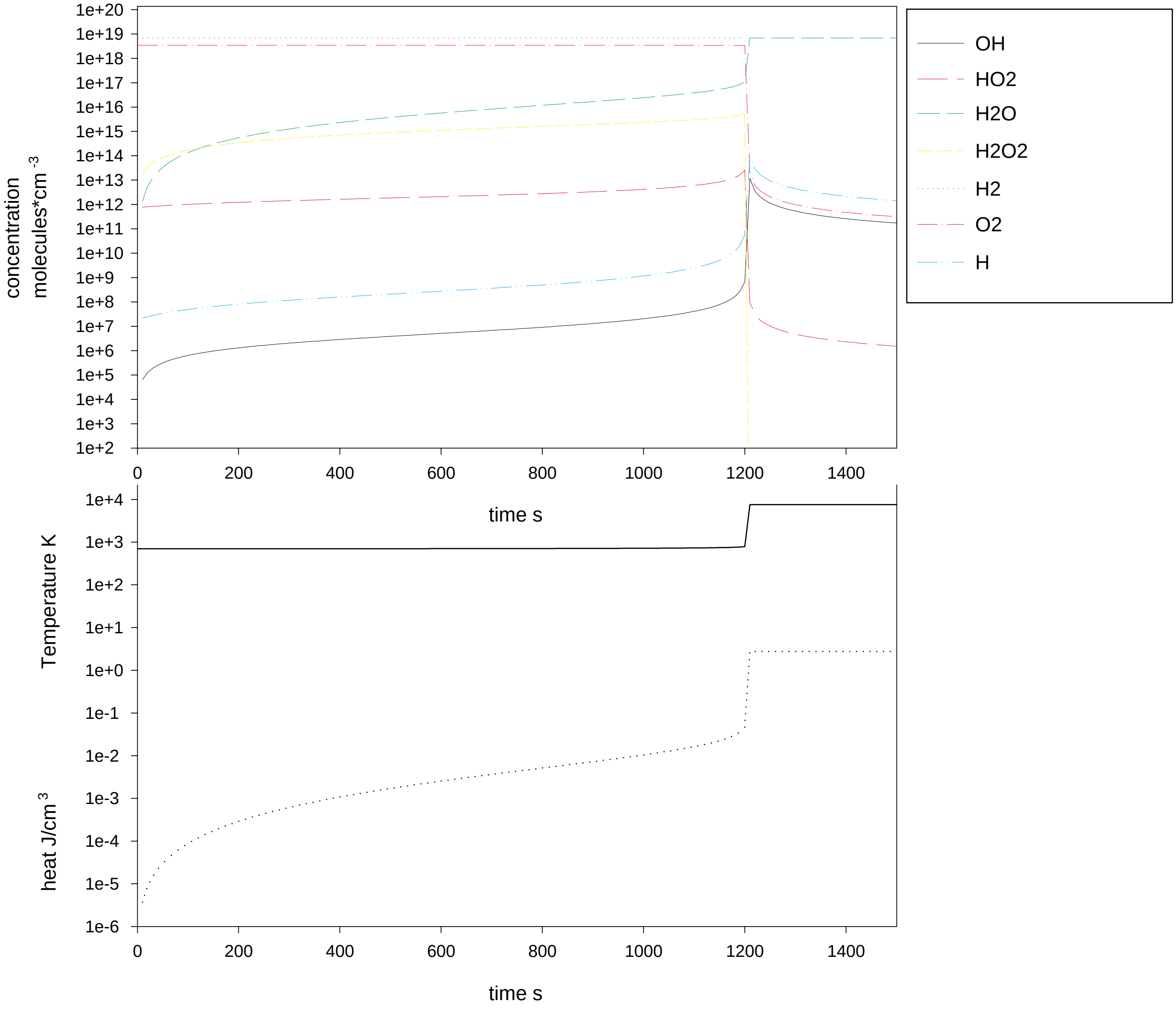


Figure 1: The figure is showing the output from the reaction mechanism. A run-away reaction starts at time 1200 s.

Special problems

Many special problems can be solved with CHEMSIMUL by resorting to a variety of "tricks". We give a few examples below.

How to mark a reaction:
If you want to know how much material is passing through a single reaction you can mark the reaction without sacrificing the material balance: The reaction

$$\texttt{RE1: A} + \texttt{B} = \texttt{C} + \texttt{D};\ \texttt{A} = k_1$$

is marked like this:

$$\texttt{RE1: A} + \texttt{B} = \texttt{AB};\ \texttt{A} = k_1$$

$$\texttt{RE2: AB} + \texttt{M} = \texttt{C} + \texttt{D} + \texttt{N};\ \texttt{A} = k_2$$

$$\texttt{CON(M)} = M$$

To ensure that `RE1` is rate determining during the whole simulation you must choose high values for [M] and k_2:

$$[\mathrm{M}] \times [\mathrm{AB}] \times k_2 \gg [\mathrm{A}] \times [\mathrm{B}] \times k_1$$

The simulated concentration [N] represents the yield of this reaction.

Maintaining a constant concentration of a solute:
An implicit way to ensure the constant concentration for some solute solute `S` is to use the *equilibrium method*, where you assign a high `DUMMY` concentration in equilibrium with `S`:

$$\texttt{CON(DUMMY)} = M$$

$$\texttt{RE1: DUMMY} = \texttt{S};\ \texttt{A} = a$$

$$\texttt{RE2: S} = \texttt{DUMMY};\ \texttt{A} = b$$

Then choose a value for the rate constant a (e.g. 100) and calculate b from the equation:

$$[\mathrm{DUMMY}] \times a = [\mathrm{S}] \times b$$

The concentration $\texttt{CON(DUMMY)} = M$ must be so high that the change in concentration during the simulation is insignificant.

Maintenance of gas/liquid equilibrium:
If you have a gas phase (volume = g) in equilibrium with a liquid phase (volume = ℓ) and you want to maintain the equilibrium of for example oxygen during the simulation, this can be accomplished in the following way:

First determine the equilibrium concentration ratio of liquid oxygen O_2 and gas phase oxygen $O_{2,\mathrm{gas}}$:

$$\frac{[\mathrm{O}_2]}{[\mathrm{O}_{2,\mathrm{gas}}]} = r$$

Then calculate [DUMMY] as the oxygen concentration if the gas phase has the same volume as the liquid phase:

$$[\mathrm{DUMMY}] = [\mathrm{O}_2] \times \frac{g}{\ell}$$

Finally determine the rate constants a and b in the equilibrium reactions

$$\texttt{RE1: DUMMY} = \texttt{O2};\ \texttt{A} = a$$

$$\texttt{RE2: O2} = \texttt{DUMMY};\ \texttt{A} = b$$

Choose the value for a (e.g. 100) and calculate b from the equations:

$$[\mathrm{DUMMY}] \times a = [\mathrm{O}_2] \times b$$

and

$$\frac{[\mathrm{O}_2]}{[\mathrm{DUMMY}]} = r$$

CHEMSIMUL input and output

To give an impression of the user interface of CHEMSIMUL, we give here a complete listing of the input and result files for the sample case considered previously; illustration of the graphical facilities are given later.

Input file:

```
RE1: H+H=H2; A=4.0E7
RE2: H+O2=HO2; A=4.5E8
RE3: H+HO2=OH+OH; A=6.5E10
RE4: HO2+HO2=H2O2+O2; A=2.0E9
RE5: OH+OH=H2O2; A=4.0E9
RE6: H+OH=H2O; A=1.0E10
RE7: OH+HO2=H2O+O2; A=6.0E10
RE8: OH+H2=H2O+H; A=4.0E3
G(H)=1.0
TOTALDOSE=0.9
CON(O2)=2.0E-4
CON(H2)=4.0E-3
RADTIME=5.0E-9
PRINTS=8
RADPRS=2
TEND=1.0E-3
PE1:HO2
CASE: 5 mbar O2 + 100 mbar H2 + Ar to 1 atm. k8=4E3
ENDDATA
```

Result file:

```
             ###############################
             CHEMSIMUL COMPILED:    DEC 1999
             ###############################

 INPUT DATA FILE: h2-o2
 DATE OF COMPUTATION:  27-JAN-2000 16:39
```

```
---------------------------------------
CASE: 5 mbar O2 + 100 mbar H2 + Ar to 1 atm. k8=4E3

NO. OF REACTION EQUATIONS =   8
NO. OF G-VALUES           =   1
NO. OF CONCENTRATIONS     =   2

REACTION EQUATION SYSTEM
------------------------
RE1:H+H=H2;A=4.0E7
RE2:H+O2=HO2;A=4.5E8
RE3:H+HO2=OH+OH;A=6.5E10
RE4:HO2+HO2=H2O2+O2;A=2.0E9
RE5:OH+OH=H2O2;A=4.0E9
RE6:H+OH=H2O;A=1.0E10
RE7:OH+HO2=H2O+O2;A=6.0E10
RE8:OH+H2=H2O+H;A=4.0E3

PLOT EXPRESSIONS
----------------
PE1:HO2

G - VALUES
----------
G(H)=1.0

START CONCENTRATIONS
--------------------
CON(O2)=2.0E-4
CON(H2)=4.0E-3

NO. OF TERMS IN DIFFERENTIAL SYSTEM =  25
NO. OF SPECIES                      =   7

NO. OF RADIATION PERIODS.........=        1
TOTAL DOSE.......................= 9.00E-01
RADIATION TIME FOR EACH PERIOD...= 5.00E-09
NO. OF RESULTS DURING RADIATION..=        2

TOTAL NO. OF RESULTS.............=        8
MAXIMUM INTEGRATION TIME.........= 1.00E-03
RELATIVE INTEGRATION TOLERANCE...= 1.00E-03

                              RESULT TABLE
------------------------------------------------------------------------
   TIME       H          H2         O2        HO2         OH        H2O2
 0.00E+00  0.00E+00  4.00E-03  2.00E-04  0.00E+00  0.00E+00  0.00E+00
 2.50E-09  4.66E-07  4.00E-03  2.00E-04  5.25E-11  2.75E-15  4.45E-21
 5.00E-09  9.32E-07  4.00E-03  2.00E-04  2.10E-10  3.43E-14  9.92E-20
 1.67E-04  2.76E-12  4.00E-03  2.00E-04  2.35E-07  1.57E-08  4.18E-08
 3.33E-04  3.35E-13  4.00E-03  2.00E-04  1.92E-07  1.90E-09  5.66E-08
 5.00E-04  5.53E-14  4.00E-03  2.00E-04  1.69E-07  3.14E-10  6.73E-08
 6.67E-04  1.11E-14  4.00E-03  2.00E-04  1.51E-07  6.35E-11  7.58E-08
 8.33E-04  2.81E-15  4.00E-03  2.00E-04  1.38E-07  1.50E-11  8.28E-08
 1.00E-03 -4.28E-17  4.00E-03  2.00E-04  1.26E-07  4.01E-12  8.86E-08

                              RESULT TABLE
------------------------------------------------------------------------
   TIME      H2O
 0.00E+00  0.00E+00
 2.50E-09  1.06E-20
 5.00E-09  3.28E-19
 1.67E-04  2.99E-07
 3.33E-04  3.13E-07
```

```
  5.00E-04  3.15E-07
  6.67E-04  3.15E-07
  8.33E-04  3.15E-07
  1.00E-03  3.15E-07

 EXECUTION TIMES FOR CHEMSIMUL (SECS)
 INPUT       SETUP    INTEGRATION    OUTPUT             TOTAL
  0.01        0.02        0.04        0.05               0.12
```

Moreover, we have already seen that the program can give a formal print-out of the differential equation system to be solved. This may be a useful tutorial facility for understanding reaction kinetics.

Plot expressions

CHEMSIMUL produces a plot table file that can be interfaced with many graphics systems. By default CHEMSIMUL assumes that the plotting is carried out by the public-domain bannerware program GNUPLOT [10].

Expressions derived from the output concentrations can be plotted by using *plot expressions*. A plot expression may be just a single species concentration, as in our sample input file. However, the concept is much more versatile, as it supports all the 5 operations $+$, $-$, $\times$, $/$, and ˆ (exponentiation), together with the common mathematical functions. This is a useful facility, when a researcher wants to plot a curve which is directly comparable with certain experimental results. An example is the measurement of extinction

$$E = (\varepsilon_A[\mathrm{A}] + \varepsilon_B[\mathrm{B}])\ell$$

where ε_A and ε_B are the extinction coefficients for species A and B, respectively, ℓ is the optical path length, and $[\cdot]$ denotes concentration.

Two examples of plots produced by CHEMSIMUL/GNUPLOT will be given later.

Solution of the ODE system

The differential equations in chemical kinetics are non-linear and of the "stiff" type. In the chemists' language stiffness means that the kinetic system has a wide range of relaxation times for perturbations. It is important to use numerical methods that admit fast and accurate integration of such equations. Stiff methods for ODEs in kinetics came in widespread use after the work of Gear [3]. His DIFSUB code replaced the classical fifth-order Runge-Kutta methods. Eventually, DIFSUB was refined by Hindmarsh and Byrne [4], leading to the EPISODE code, and still later Hindmarsh [5] and Petzold [6] constructed the ODE solver LSODA which is used today in CHEMSIMUL.

Computer requirements — MINICHEM

Since 1992 CHEMSIMUL has been entirely Fortran based and should be able to run on many different computer systems. In 1997 it was converted to Fortran 90 with the result that most of the restrictions on problem size were alleviated: In principle, there are no limits on the number reactions, species, etc., although the specific hardware you are using might put its own restriction on problem size by limiting the total amount of allocatable data storage.

The PC is the most important computer platform for running CHEMSIMUL at Risø and elsewhere; however, the program may run under any system that supports Fortran 90, as for example IBM or HP workstations under Unix, or Digital/Compaq VMS.

If you are interested in acquiring CHEMSIMUL, you should contact the authors.

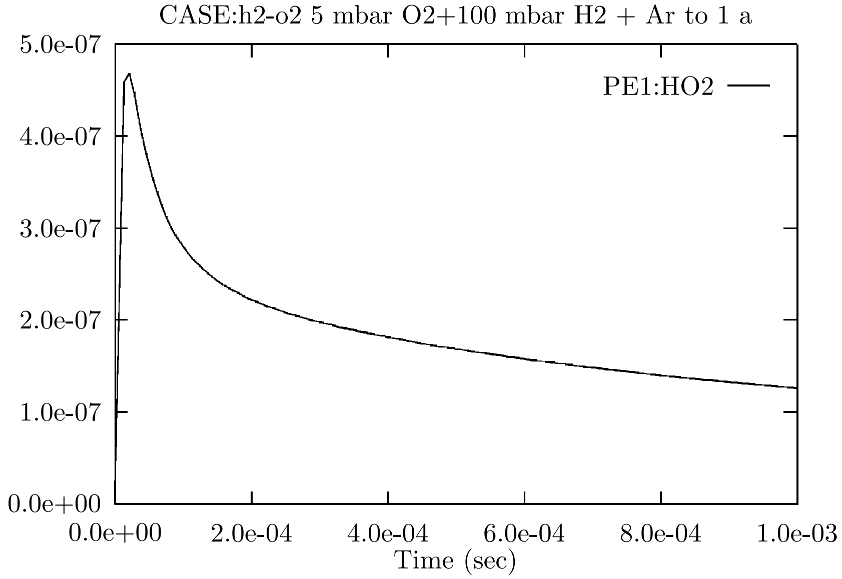
MINICHEM is a demonstration version of CHEMSIMUL for PC. It is freely available on request from the authors, and it may be freely redistributed. MINICHEM has the same features as CHEMSIMUL, but problem size parameters are restricted in the following way:

Maximum number of reactions	10
Maximum number of species	20
Maximum number of isotopes	1

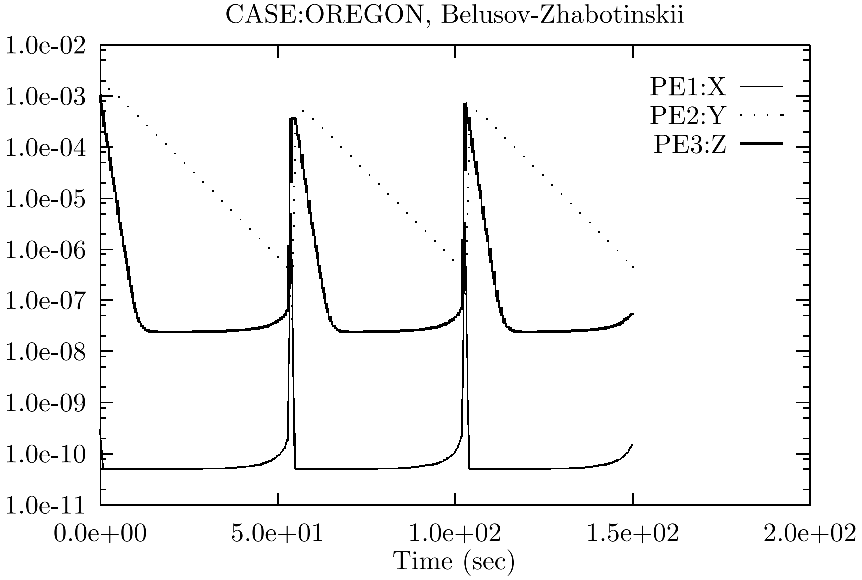
Otherwise MINICHEM runs precisely as CHEMSIMUL does, and the CHEMSIMUL documentation [1] therefore applies to MINICHEM, too.

More simulation examples

Below we present some examples of simulations with CHEMSIMUL in graphical form. We begin with our previously discussed combustion case, where we show the time evolution of the HO_2 concentration:



Our next example is the classical Belusov-Zhabotinskij oscillating reaction, which has gained renewed interest as a chemical example of a dynamic system with the typical nonlinear features of limit cycles, period doubling, and eventually chaos:



Possible future extensions

CHEMSIMUL is a program system under continual development. In the near future we foresee a number of enhancements of its capabilities. Some of these will probably be:

- Optional choice among several consistent unit systems, notably the SI system.
- As a supplement to purely adiabatic or isothermal conditions, it should be possible to consider "intermediate" states too.
- A more flexible representation of temperature dependence of reaction constants and other quantities.
- Improved balance check for yields ("*G*-values").

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