

## Getting Started with QuickStart Folder

### Content of the QuickStart Folder

The information for quick start is stored in the folder  
<app\_dir>\Chemked50\QuickStart  
where <app\_dir> is the folder chosen for the program installation.

The QuickStart folder contains the following files:  
THERMO\_H2.mdb is a thermodynamic database,  
REAC\_H2.mdb is a reaction database,  
THERMO\_H2.txt, REAC\_H2.txt are text files in the CHEMKIN format,  
Chart.pg is an example of Chemked chart.

### Thermodynamic Database and Reaction Database

If you have not changed the delivery setting, the thermodynamic database THERMO\_H2.mdb will automatically open when starting Chemked. If the database does not open, close all child windows and then carry out the following steps.

1. Choose **File > THERMO Database > Connect**. The File dialog appears.
2. In the dialog, select the file path  
<app\_dir>\Chemked50\QuickStart\THERMO\_H2.mdb;  
click the Open button. The database will open.

To open the reaction database REAC\_H2.mdb, carry out the following steps.

1. Choose **File > Open**. The File dialog appears.
2. In the dialog, select the file path  
<app\_dir>\Chemked50\QuickStart\REAC\_H2.mdb;  
click the Open button. The database will open.

Now you can edit the data and create charts of thermodynamic functions and rate constants.

### Example for Chemical Kinetics Problem: Hydrogen Oxidation

Consider a steady one-dimensional gas flow in a tube (an idealized model of plug flow reactor). The inlet gas parameters are 0.5% H<sub>2</sub>+0.5% O<sub>2</sub> in N<sub>2</sub>, at 880 K and 0.3 atm. It is assumed that the tube walls are adiabatic and the gas pressure in the tube is constant. The aim is to find the gas composition versus residence

time. The thermodynamic data THERMO\_H2.mdb and the reaction mechanism REAC\_H2.mdb will be used in the calculation.

The solver runs directly from the database REAC\_H2.mdb.

1. Activate the database window (click on the window).
2. Choose **Reaction Kinetics > Run Solver**. The Solver dialog appears.
3. In the table and text boxes of the dialog, enter the inlet gas parameters (pressure, temperature and species mole fractions). Choose the Adiabatic option in the Temperature frame, and the Constant Pressure option. Enter the solver control parameters.

**Solver File SOLTMP.txt**

Starting Values | Options and Tips

Initial Mole Fractions

No.	Species Name	Fraction
1	AR	
2	H	
3	H2	5.E-01
4	H2O	
5	H2O2	
6	HO2	
7	N2	9.9E-01
8	O	
9	O2	5.E-01
10	OH	

Reaction mechanism consists of 21 valid reactions.

Options and Tips

☒ Constant Pressure  
☐ Constant Volume

Initial Pressure, atm: 0.3

Temperature  
☐ Constant ☒ Adiabatic  
Initial Value, K: 680

Solver Parameters

Initial Time, s: 0  
Final Time, s: 0.2  
Initial Step Size, s: 1.E-10  
Relative Tolerance: 1.E-06  
Absolute Tolerance: 1.E-15

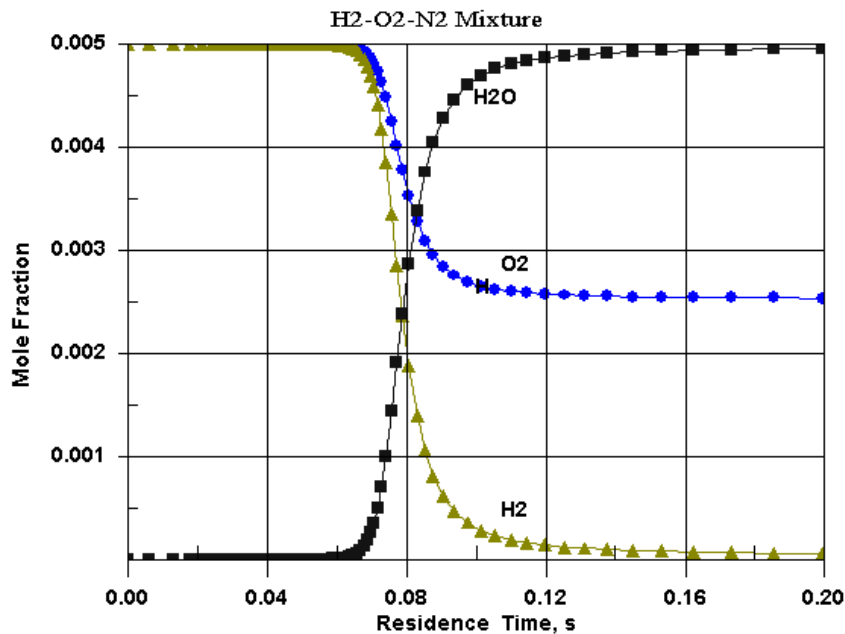
Settings  
Save Enter

Default Settings Run Solver  
Clear Fractions Cancel

4. Click the Run Solver button.

A console window appears where current information about the problem is displayed.

When the solver finishes successfully the program will display a prompt: 'Show Output?' If Yes is chosen a solver file will open and the Solver Output dialog will appear. Using features of the dialog you can plot functions and view numeric data for species and average gas parameters; an example is presented here.



Hydrogen oxidation: species mole fractions versus residence time

## Starting a New Project

### Data Sources

In Chemked there are no information on thermodynamics and reaction rates; you must use external sources for this data. Here we will employ the data on hydrogen oxidation from

Marcus Ó Conaire, Henry J. Curran, John M. Simmie, William J. Pitz, Charles K. Westbrook. "A comprehensive modeling study of hydrogen oxidation", Int. J. Chem. Kinet., 36:603-622, 2004.

[https://www-pls.llnl.gov/?url=science\\_and\\_technology-chemistry-combustion-hydrogen](https://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion-hydrogen)

The data is stored in text files

<app\_dir>\Chemked50\QuickStart\THERMO\_H2.txt (thermodynamic data) and <app\_dir>\Chemked50\QuickStart\REAC\_H2.txt (reaction mechanism.) where <app\_dir> is the folder chosen for the program installation.

It is convenient to gather all files of the project in a single folder; let this folder be called <project\_dir>.

- 1 Create the folder <project\_dir>.
- 2 In the folder <app\_dir>\Chemked50\QuickStart, copy the files THERMO\_H2.txt and REAC\_H2.txt
- 3 Paste these files to the folder <project\_dir>.

## Creating a New Thermodynamic Database

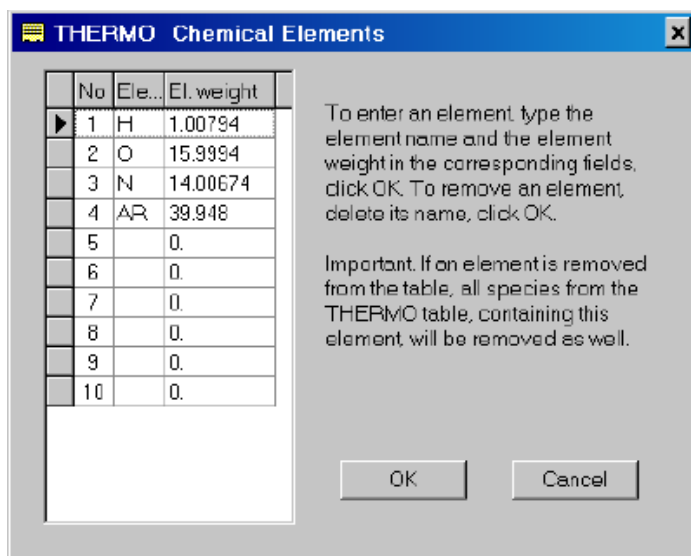
- 1 Run Chemked.
  - 2 Close all child windows.
  3. Choose **File > THERMO Database > New**. The File dialog appears.
  4. In the dialog, choose the path of the folder <project\_dir> and specify the database name Thermo\_H2.mdb. Click the Open button.
- The program will connect to the new database and the THERMO window with an empty table for thermodynamic data will open. In addition a window with an empty Chemical Elements table appears.

Remark -----

If the chemical elements window does not appear, then choose **Edit > Chemical Elements** or on the toolbar, click the **Chemical Elements** button. The window will open.

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In the fields of Chemical Elements table, enter the element names H, O, N, AR. The atomic weights of these elements appear automatically in the corresponding fields; you can change these values.



Click OK; the Chemical Elements window closes. The element names will appear as column headers of the THERMO table.

## Entering Data in the THERMO table

1. Choose **File > Open**. The File dialog appears.
2. In the dialog, select the file path <project\_dir>\THERMO\_H2.txt; click the Open button.

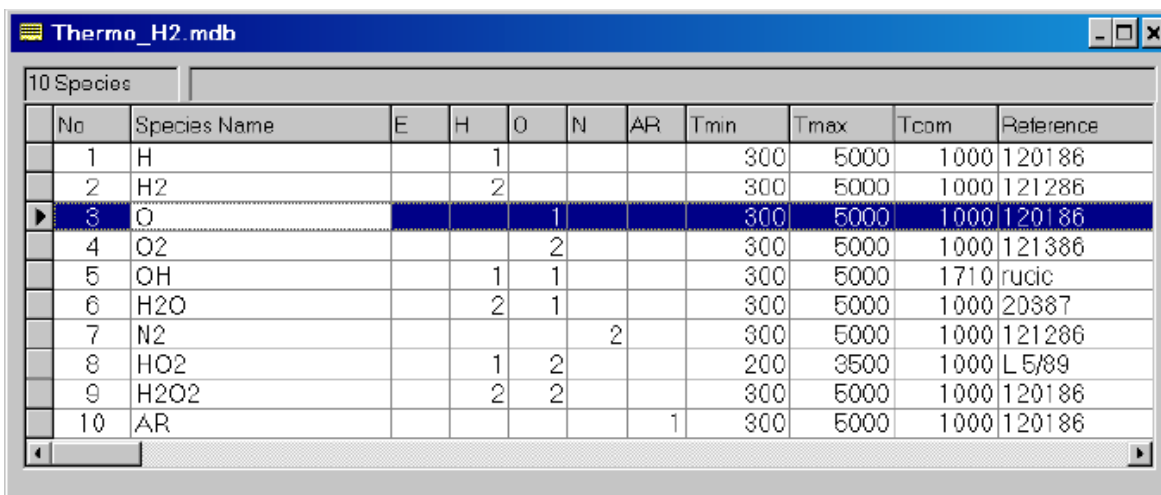
A window with thermodynamic data in CHEMKIN text format opens.

3. Choose **Edit > Select All**.

4. Choose **Edit > Copy**. The thermodynamic data in the text format will be stored in the clipboard.

5. Activate the THERMO window (click on the window); menu of the thermodynamic database appears.

6. Chose **Edit > Paste**; the data will be pasted to the THERMO table.



No	Species Name	E	H	O	N	AR	Tmin	Tmax	Tcom	Reference
1	H			1			300	5000	1000	120186
2	H2			2			300	5000	1000	121286
3	O				1		300	5000	1000	120186
4	O2				2		300	5000	1000	121386
5	OH			1	1		300	5000	1710	rucic
6	H2O			2	1		300	5000	1000	20387
7	N2					2	300	5000	1000	121286
8	HO2			1	2		200	3500	1000	L5/89
9	H2O2			2	2		300	5000	1000	120186
10	AR					1	300	5000	1000	120186

The database is ready for use. You can edit the data, add new chemical elements and species, create charts and view numeric values of the thermodynamic functions.

## Creating a New Reaction Database

1. Choose **File > New > Reaction Database**. The File dialog appears.

2. In the dialog, choose the path of the folder <project\_dir> and specify the database name Reac\_H2.mdb. Click the Open button.

A window with an empty reaction table will appear.

To enter the data in the database you should carry out the following steps.

1. Choose **File > Open**. The File dialog appears.

2. In the dialog, select the file path <project\_dir>\REAC\_H2.txt; click the Open button.

A window with reaction data in CHEMKIN text format opens.

3. Choose **Edit > Select All**.

4. Choose **Edit > Copy**. The reaction data in the text format will be stored in the clipboard.

5. Activate the reaction window (click on the window); menu of the reaction database appears.

6. Chose **Edit > Paste**; the data will be pasted to the reaction table.

Reac_H2.mdb							
21 reactions							
No	Reaction	A	n	E	Type	Refs	
1	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$1.92\text{E}+14$	0.00	16440	Rev		
2	$\text{O} + \text{H}_2 \rightleftharpoons \text{H} + \text{OH}$	$5.08\text{E}+04$	2.67	6292	Rev		
3	$\text{OH} + \text{H}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}$	$2.16\text{E}+08$	1.51	3430	Rev		
4	$\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{OH} + \text{OH}$	$2.97\text{E}+06$	2.02	13400	Rev		
5	$\text{H}_2 + \text{M} \rightleftharpoons \text{H} + \text{H} + \text{M}$	$4.58\text{E}+19$	-1.40	104400	Rev		
6	$\text{O}_2 + \text{M} \rightleftharpoons \text{O} + \text{O} + \text{M}$	$4.52\text{E}+17$	-0.64	118900	Rev		
7	$\text{OH} + \text{M} \rightleftharpoons \text{O} + \text{H} + \text{M}$	$9.88\text{E}+17$	-0.74	102100	Rev		
8	$\text{H}_2\text{O} + \text{M} \rightleftharpoons \text{H} + \text{OH} + \text{M}$	$1.91\text{E}+23$	-1.83	118500	Rev		
9	$\text{H} + \text{O}_2 + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$	$1.49\text{E}+10$	0.00	0	Low Temp		

The database is ready for use. You can edit the data, add new reactions, create charts and view numeric values of reaction rate constants. From the reaction database you can run the Chemked solver to solve problems of chemical kinetics (see other help topics, for example, 'Getting Started with QuickStart Folder')