

## ChemRC 3.0



Ju's Group in Princeton university.

# Preface

## On the ChemRC 3.0 software

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*by Xiaolong Gou*

*ChemRC 3.0 is the updated software of ChemRC. This new release software can complete the whole chemistry reduction process automatically.*

## ChemRC 3.0

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### **Special thanks to:**

*All the people who contributed to this document, to Zheng Chen at peking univerisity and Wenting Sun at Georgia Tech.*

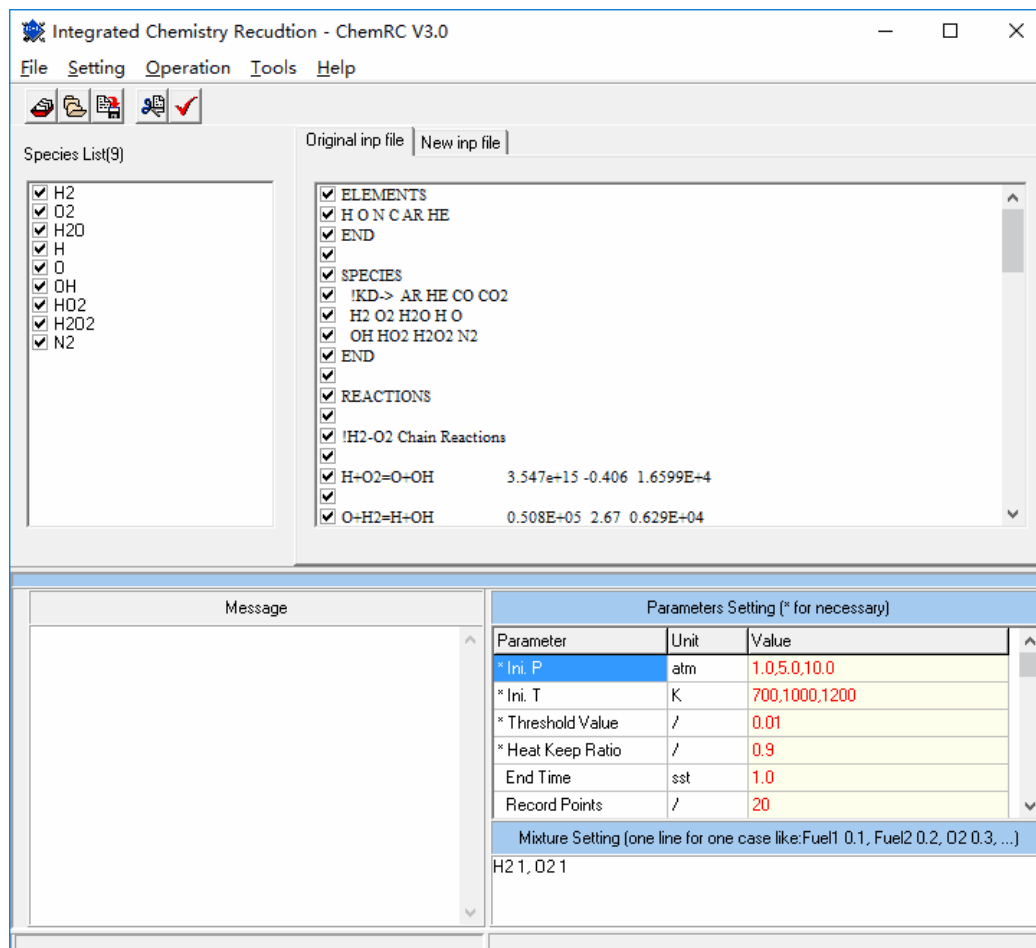
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# 1 About ChemRC

ChemRC is a software for chemistry reduction.



## Main functions and characteristics:

1. An integrated software for chemistry reduction.
2. The PFA (Path Flux Analysis) reduction method is used.
3. The heat release can be taken into account in the reduction process.

## Contact us:

EMAIL: yju@princeton.edu, simgxl@cqu.edu.cn

# 2 System Setting

There are following setting items, and the items with start are necessary.

1. Work directory
2. Initial pressure\*
3. Initial temperature\*
4. Threshold value\*
5. Mixture setting\*
6. Heat keep ratio
7. End time
8. Record points
9. Max. time

### 3 Work Modes

There two work modes for the reduction, one is the integrated mode, and the other one is running it step by step.


Operation Tools Help

Integrated Reduction

- When the data is ready, you just click the menu item or the tool button

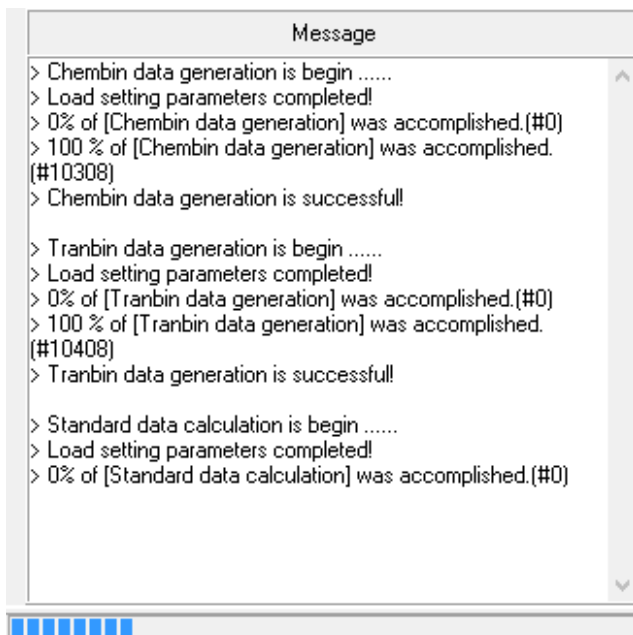


, the software will run until the process is end.

- And you also can click the items "Create Chem.bin", "Create Tran.bin", "Generate standard data", "Generate trimmed data", "Trim species and reactions" and "Create reduced inp file" one by one to complete the whole reduction process.
- Since the PFA function can be used many times, you can click the tool button  to run it.

During the running process, the important message will appear in the message box, and the progress bar will show the working progress.

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## 4 Work Process

The main work process of this software is as following:

- Set the work directory
- Open the data files
- Set the parameters
- Create Chem.bin
- Create Tran.bin
- Generate standard data
- Generate trimmed data
- Trim species and reactions
- Create reduced inp file

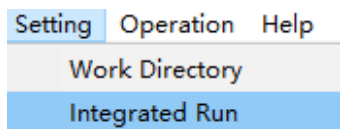
### 4.1 Set the work directory

When you begin to start a new reduction process, it is good to set a work directory for this work. When you set a work directory, all the input file like chemistry file, thermal data file and etc. need be copy to this directory, and all the output files like the new chemistry file and the message file will be saved in this directory.

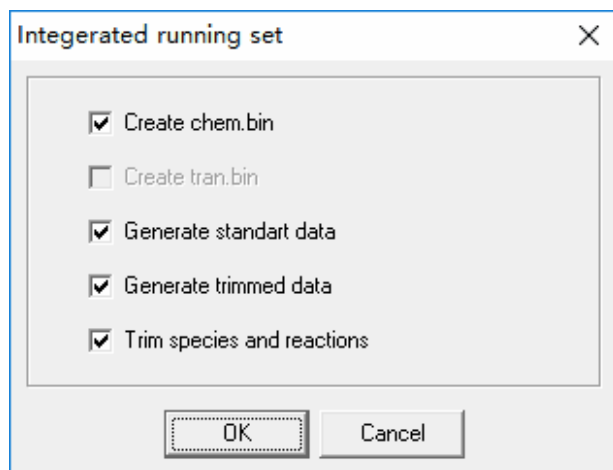
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## 4.2 Set the integrated running


The integrated running can include all the processes or some of them. You can use the menu item



and the blow window to define it.



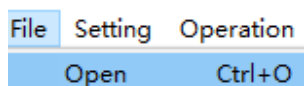
And the setting will not be saved, when the software is restart, the default setting will be used again.


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## 4.3 Open the data files



There are two modes to open the data file: open the chemistry and open the project.


- Open the chemistry file



You can use the menu item **Open** or the tool button  to open the data file.

- Open the project file

You can use the tool button  to open the project file. When open the project file, the parameters are loaded at the same time. And the current data and parameters can be saved into a project by click the tool button .

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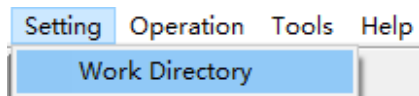


## 4.4 Set the parameters

There are following setting items, and the items with start are necessary.

1. Work directory

The directory for the input and output data files.

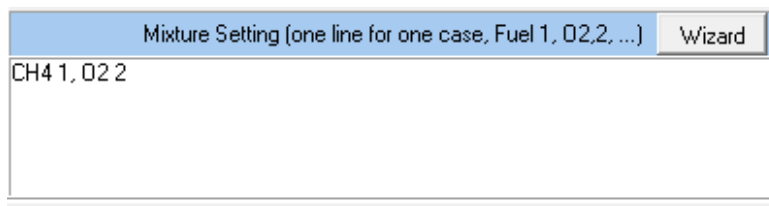


2. Initial pressure\*
3. Initial temperature\*
4. Threshold value\*

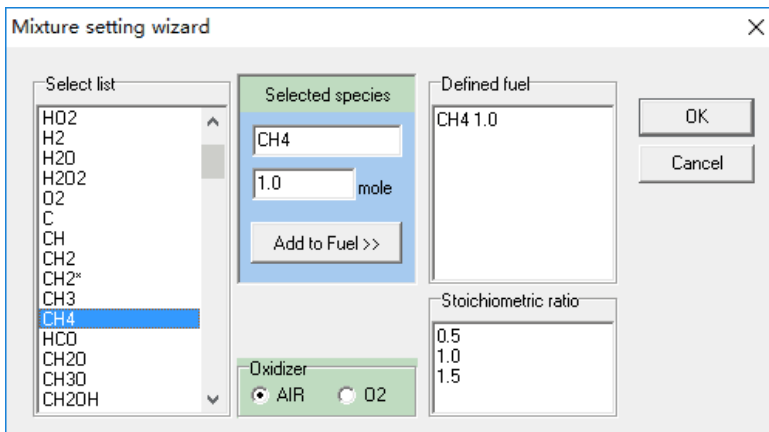
It's the threshold value for PFA reduction. When the relation rate between the species and the preselected one is bigger than this value, the species will be kept.

5. Mixture setting\*

Before reduction, the mixture needs to be set. You can directly set it in the mixture setting edit block, using the formation of species name followed by its mole number.



And you can also use the wizard to create the mixture easily.



6. Heat keep ratio

It's the value to judge whether a species will be kept or not based on its heat release. Select the species according to the heat release from large to small, until the cumulative heat release is equal or above this value.

7. End time

It's the end time of the calculation in the standard data generation. There are three modes to define the

end time: sst-running to the steady state, s- seconds, Tau- the multiple of ignition delay time. When the mode sst is choose, the value is not necessary.

#### 8. Record points

It is the recording number of standard calculation for one working condition. The default value is 20.

#### 9. Max. time

It's the maximum time in the standard calculation, be a large number, to avoid the simulation process cannot end.

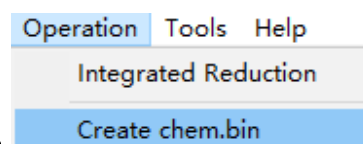
Parameters Setting (* for necessary)		
Parameter	Unit	Value
* Ini. P	atm	1
* Ini. T	K	1000
* Threshold Value	/	3
* Heat Keep Ratio	/	0
End Time	sst	1.0
Record Points	/	20
Max. Time	s	1.0E+10


 Return to the upper level

## 4.5 Create Chem.bin

For the reduction, only the inp chemistry file is needed, and this software can translate it into binary

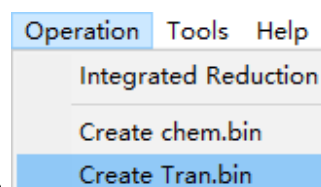
file, and if the binary file is exists this step can skip. By click the item to run this model.




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## 4.6 Create Tran.bin

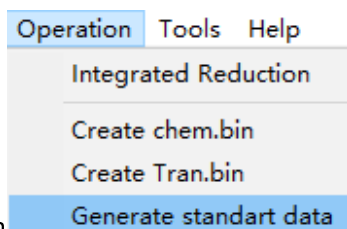
When the transport data is needed, you can click the menu item to run this function.




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## 4.7 Generate standard data

Through this function, the standard data used for path flux analysis under all the working conditions will be generated.

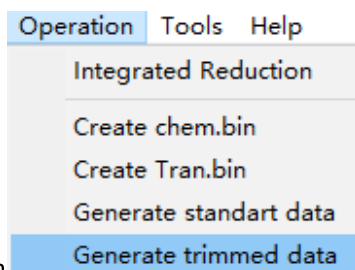


By click the menu item **Generate standart data** to run this fucniton.


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## 4.8 Generate trimmed data

Through this function, the trimmed species file will be generated by the path flux analysis.

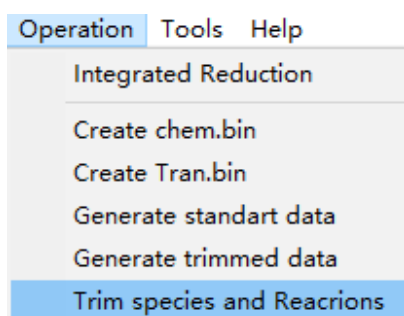


By click the menu item **Generate trimmed data** to run this fucniton.


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## 4.9 Trim species and reactions

Through this function, this system will get the final kept specie and reactions based

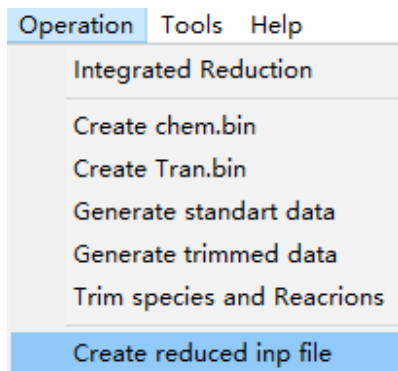


on the trimmed data. By click the menu item to run this function.


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## 4.10 Create reduced inp file

Through this function, the reduction chemistry will be generated. By click the menu item



to run this function.

 Return to the upper level

## 5 Citation

Using this software please cite the following paper:

Wenting Sun, Zheng Chen, Xiaolong Gou and Yiguang. Ju. A Path Flux Analysis Method for the Reduction of Detailed Chemical Kinetic Mechanisms. Combustion and Flame, 2010,157(7) : 1298-1307.

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