

# Laboratory Products

## Updated Computer Program for Chemical Thermodynamic and Energy Release Evaluation

**An Interview with:** B. Keith Harrison, PhD, P.E., Developer, Emeritus Professor of Chemical Engineering, Emeritus Graduate Dean, Retired Associate Vice President of Academic Affairs, University of South Alabama, Mobile, Alabama 36688

and

Mr Dan Detman, Consultant and responsible for the transition of the historic Visual Basic application to a Microsoft Access® application. Responsible for creative design and implementation of new features in CHETAH 11.0

### 1. How many years in the making is this new version of CHETAH?

It's been four years since the last version of CHETAH.

Version 10.0 came out in 2016 with the main feature being moved from a CD product to a download to meet the needs of the secure labs and to move to a more current operating system. There were three service packs with various updates, the inclusion of SMILES, and minor bug fixes. It is highly recommended that buyers get the upgrade with the cumulative service packs included. Versions 9.0 and 10.0 will no longer be supported.

### 2. What are notable new additions to CHETAH 11.0?

a. Inclusion of NASA Lewis chemical equilibria calculations in a user-friendly way using the functionality of CHETAH.

New to CHETAH 11.0 is the ability to calculate chemical equilibrium. This is accomplished using the thermodynamically rigorous NASA Lewis CEA program which has been incorporated into CHETAH. The NASA CEA program was first developed for the space program. This same technology is now given a different use. Chemical equilibrium can be calculated for a number of different scenarios that are useful in assessing chemical reactive hazards. CHETAH also allows its extensive databases of chemicals and the use of the Benson group method to allow for a much greater number of possible reactive chemical hazards to be assessed using this new feature.

CHETAH can calculate the chemical equilibrium of a specified set of reactants in a specified set of conditions. The logic of the NASA Lewis program has been included within CHETAH but allows a much simpler interface and allows the input reactants to come from the large CHETAH databases of chemicals (over 1700) as well as allowing use of the Benson group contribution method to describe chemicals not in the databases. There is also a provision for the user to enter their own compounds in a special user database within CHETAH.

CHETAH Allows Three Types of Chemical Equilibrium Calculations:

1. Specified final temperature and pressure at chemical equilibrium. This option is especially useful to find the final product composition at equilibrium and the energy released in achieving the final conditions.

2. Specified final pressure and enthalpy. This option is especially useful for evaluating the final temperature and final product composition at equilibrium for an adiabatic reaction.

3. Specified internal energy and volume. This option is especially useful for evaluating the final pressure and final product composition at equilibrium for a constant volume reaction.

b. Ability to back up and restore Saved Sessions from CHETAH for reuse at a later time or with a future version of CHETAH.

c. Ability to save User-Defined Groups of chemicals and their properties and transfer such groups to later versions of CHETAH.

d. What critical information is found in this edition of the book that cannot be found elsewhere? This edition of CHETAH allows the user to evaluate potential reactive hazards by a number of methods not conveniently available elsewhere. This will help those professionals involved in preventing such hazardous situations.

### 3. How does this manual help an engineer (or other occupation) do his/her job better?

This software program is a valuable tool for allowing a sophisticated rigorous assessment of potential reactive and flammable hazards. Results from CHETAH can then lead to an experimental program that would allow a careful evaluation of hazards under the conditions envisioned by the user.

It should be noted that CHETAH is one element in a chemical safety program. It can rapidly evaluate a situation. However, CHETAH does not replace laboratory-based safety experimental programs. CHETAH is a valuable tool to help guide experimental investigations.

### 4. What type of person would benefit from CHETAH?

Professions that would heavily use CHETAH: Chemical Engineers, Chemists, Safety Engineers, and those involved in fire prevention. Also, users would include academic settings such as university chemistry and chemical engineering that have laboratory operations for teaching or research.

### 5. What are typical applications?

An industrial chemical production or research centre that needs to evaluate potential hazards from chemical reactions or flammability hazards.

A pharmaceutical firm that is synthesising new chemicals and/or pharmaceuticals as part of a research program would evaluate potential reactive hazards before doing or attempting a synthesis reaction to make a new chemical or pharmaceutical.

Firms that specialise in serving industry by providing reactive and flammability evaluations often use CHETAH to help customers ensure safe operations.

Often professionals in chemical related professions need to quantify the heat effects of proposed reactions. This is important to prevent hazards but also for routine reactor design. CHETAH can provide valuable information for these purposes.

### 6. Explain why/how/if this program would be a valuable resource in academia?

CHETAH has been used in chemistry, chemical engineering, environmental engineering/ sciences, and life sciences university programs involved in education and research. It is useful in instruction concerning energy consequences of reactions, an assessment of product distribution for reactions achieving chemical equilibrium, and in safety education involving chemicals. It is also useful for instruction concerning flammability parameters such as the lower flammable limit of mixtures and minimum ignition energy.

University research laboratories have the same concerns over safety as industrial labs and as such seek to avoid accidents. CHETAH can be a valuable tool to help prevent accidents involving chemical reactions and also to help prevent flammability related accidents.

### 7. What type of technical support is offered to users?

A user's manual of approximately 200 pages is furnished with the program. A PowerPoint tutorial on the use of the program is furnished as well. An extensive literature of scientific articles concerning CHETAH is available in the open literature. A listing of relevant articles is furnished with the program. Software support is offered by ASTM and by the authors of the program. Consultants are available to help clients in their use of the program and teach courses on the topic by WebEx or in person.

### 8. Are there publications that explain the use and experiences using the CHETAH functionality?

Yes, on the website we have a tab called References. There you can find almost 200 articles, books, and book chapters on the strategy, reactions, safety, etc. The reference list is also available in the user's manual. There is an extensive literature on the use of CHETAH covering about 50 years.

### 9. Is there an easy way to get up to speed on using CHETAH?

On the website, there is a tutorial page with an abbreviated version that allows you to use the functionality with a limited number of chemicals. There is a comprehensive PowerPoint presentation that covers all major features of CHETAH that users can review prior to any purchase. In addition to item a above, a long-time and experienced user of the program David Frurip, President of Frurip Consultancy, has taught courses on the use of CHETAH worldwide. He does this by one- and two-day courses on the site of the user. However, he also offers these courses in abbreviated form by the use of WebEx.

Dave Frurip prepared the 'how to' videos found on the Introduction page with an explanation and complete walk through of how to use the features. There are 4 videos:

- Introductory: A Short Overview Showing a Heat of Reaction Demo
- Energy Release Evaluation (ERE) Explosibility Potential of a Chemical Species or Mixture
- Flammability Calculations
- Chemical Equilibria Analysis using the NASA-Lewis Code