1. INTRODUCTION

OVERVIEW OF CHETAH PROGRAM

The CHETAH (Chemical Thermodynamic and Energy Release) program is a unique tool for predicting both thermochemical properties and certain “reactive chemicals” hazards associated with a pure chemical, a mixture of chemicals, or a chemical reaction. This is accomplished through a knowledge of only the molecular structure(s) of the components involved by an implementation of Benson’s method of group additivity. CHETAH is useful for classifying materials for their ability to decompose with violence, for estimating heats of reaction or combustion, and for predicting lower flammable limits.

For thermochemical estimations, CHETAH is designed to conveniently and accurately calculate several important properties as a function of temperature for pure materials, mixtures, and reactions. For hazard evaluation, CHETAH is designed to be a CONSERVATIVE screening tool for use during the early stages of compound synthesis or process development. Its use should be integrated within an experimental program for testing reactive chemical hazards. CHETAH WAS NOT DESIGNED TO REPLACE THE PHYSICAL TESTING OF MATERIALS. Rather, CHETAH’s computational results should be used to complement experimental results to help identify the need for further testing in the areas of impact sensitivity and/or flammability. Potential energy hazards associated with handling new chemicals will not, in general, be known a priori. Furthermore, experimentally determined thermochemical data for new chemicals used for process design and to predict hazards will often not be available. CHETAH exists largely to allow users to build compounds using group additivity methods, to predict thermochemical properties for compounds and reactions, and to use these predicted properties for energy hazard evaluation. Users may then use CHETAH’s predictions along with results from Accelerating Rate Calorimetric (ARC), Differential Scanning Calorimetry (DSC), flash point, dust explosion, drop-weight, or other tests to prepare, use, store, or dispose of new compounds safely. Personnel committed to ensuring the safe operations at sites where research, process development, or manufacturing occur should include CHETAH in their Reactive Chemicals evaluation programs. CHETAH also is of great utility for predicting ideal gas thermochemical properties of materials such as standard heats of formation, heat capacities, entropies, and free energies. Thermodynamic properties of user specified reactions could also be calculated. Extensive databases of thermodynamic properties for gas phase molecules, species in aqueous solution, and ionic solids are provided. CHETAH also allows the prediction of solid and liquid thermodynamic properties.

CAPABILITIES

CHETAH predicts potential hazards of compounds from thermochemical properties, most of which are estimated using Benson’s method of group additivity for gases. Even though CHETAH makes predictions for gas phase properties, energy release evaluations are valid for gas, liquid, or solid materials. Group additivity methods assume that each portion of a molecule contributes an increment to the heat capacity, heat of formation, and entropy of the molecule. When heat capacity data for groups are missing, CHETAH uses less accurate estimations methods (1, 2, 14).
CHETAH can be used to perform the following functions by simple menu selections:

- Classify a material or mixture with respect to its ability to decompose with violence when subjected to severe impact.
- Calculate the ENTHALPY OF COMBUSTION for a compound or mixture.
- Calculate THERMOCHEMICAL PROPERTIES for REACTIONS: \( \Delta C_{prxn}, \Delta H_{rxn}, \Delta S_{rxn}, \Delta G_{rxn}, \log K \)
- Calculate THERMOCHEMICAL PROPERTIES for COMPOUNDS: \( C_p, S, \Delta H_f, \Delta G_f, \log K_f \), Free Energy Function \((G-H)/T, H-T-H_{298}\)
- Estimate LOWER FLAMMABLE LIMITS, and other flammability properties.
- BUILD COMPOUNDS from library or user-entered groups for gases, liquids, or solid crystals.
- BUILD CRYSTALS from ionic groups.
- Enter PRIVATE THERMOCHEMICAL DATA (Benson groups, gases, solids, or liquids).
- View THERMOCHEMICAL DATA in CHETAH’s database.
- Modify previous CHETAH sessions.
- Generate reports.

Areas that are beyond the scope of this program include:

- **RADICALS**

- **CORRECTION OF IDEAL GAS VALUES TO LIQUID OR SOLID PHASES** This version of CHETAH can predict thermodynamic properties of solids and liquids using a predictive method based on Benson’s method. However the most general predictive method is based on ideal gas values. Many compounds can only have their properties predicted as ideal gases in CHETAH. This program cannot correct the ideal gas values back to condensed values. This can be an important consideration when calculating heats of reactions. Accurate heats require true representation of the states of reactants and products. In some cases, the gas phase heat of reaction may not differ significantly from the condensed phase value due to a cancellation of corrections. This is discussed in more detail in reference (17).

**NOTE:** The hazard evaluation portion of CHETAH (ERE option) classifies materials in the condensed state based on gas phase thermodynamic properties. This is feasible because the correlations used by CHETAH were developed using data that were measured for condensed phase materials and because phase transition energies are small with respect to the amount of energy that is required to generate a violent explosion. CHETAH uses gas state thermodynamics to classify materials that are in any of the gas, liquid, or solid states.

- **KINETICS.** CHETAH cannot predict rates of chemical reactions in the classic sense of determination of Arrhenius parameters.
• Version 10.0 has a new interface to improve ease of use.

• Database for Ideal Gas Benson groups is expanded. This database now contains 1060 groups and is the largest Benson group database known to exist. 148 groups were added since version 9.0 of CHETAH.

• Updated thermodynamic values provided for 20 Benson groups based on latest best values in the literature.

• Entropy values were predicted and added to the database for many ideal gas Benson groups that were missing such values.

• Various property databases reviewed for consistency and accuracy.

• Mixture flammability calculations were improved in accuracy to reflect latest technology.

• Program now uses the Microsoft Access® Database for database management and to manage the user interface. The calculation details are now accomplished in the VBA structure of Access and in C language. This change in programming language for CHETAH makes the program more compatible and seamless with the current versions of the Microsoft Windows® operating system.

• Output reports have been improved for clarity of presentation. It is now possible to generate pdf format reports direct from the interface.

• The program now maintains a clear record of use with details of past sessions. Past sessions can easily be modified and recalculated.

• It is now much easier to establish and maintain a user database of proprietary data to enhance the usefulness of CHETAH. The user database is portable to future versions or service packs.
PROGRAM REQUIREMENTS

You must have one of the following to install CHETAH:

- Windows 7® with Service Pack 1, Windows 8®, Windows 8.1®, Windows 8.1® with Update 1. Installation on Windows XP or earlier versions is not supported. Limited testing on Windows 10 would indicate compatibility, but Windows 10 is not supported at the present time.
- A hard disk with at least 400 megabytes of available space.
- Note that CHETAH is a complex scientific database program. Depending on the speed and condition of your computer, calculations may take some time. For example a typical time for a five component mixture flammability calculation on a midrange 32-bit computer is 40 seconds. Simpler calculations on the same computer may appear to be instantaneous. Efforts are being made to speed up calculations and as progress is made a service pack will be issued.

INSTALLATION (32-BIT PC & 32-BIT MS OFFICE®)

CHETAH 10.0 has an installation program built in on the program disk. Inserting the disk into the drive would automatically initiate the installation process. However this would happen only if the auto installation setting on the computer is set to ON. If the machine does not have this option the user would have to access the drive and click on the SETUP.EXE file. This would then initiate the installation process. Care should be taken to insure that existing CHETAH files are deleted before carrying out the installation of the CHETAH 10.0 version.

CHETAH makes use of Microsoft Access®. However it is not necessary to have Microsoft Access® installed on the PC, as a runtime version of Access is incorporated within CHETAH.

INSTALLATION (64-BIT MS OFFICE®)

The CHETAH 10.0 installation routine shown above must be completed first. Users of 64-bit MS Office® or 64-bit MS Access® must then run the update program found on the disk: “update-x64.exe”

TECHNICAL SUPPORT

You may contact ASTM at the following address: ASTM
100 Barr Harbor Drive
West Conshohocken, PA 19428-2959

Email: SERVICE@LOCAL.ASTM.ORG Phone: (610) 832-9500
Fax: (610) 832-9555
If you have questions regarding the use of CHETAH, please contact:

B. Keith Harrison University of South Alabama AD 300
Mobile AL 36608
Or:
7386 Adamoor Court, Mobile, AL 36695
Email: kharrison@southalabama.edu
Phone: (251) 460-6261 (office) or (251) 635-1795 (home) or (251) 251-455-1014 (cell)
Fax: (251) 460-6575 (office)

If you have technical questions relating to the data or interpretation of results, contact:

Dr. David J. Frurip
Michigan Molecular Institute
1910 St Andrews St
Midland, MI 48640
Email: DFrurip@charter.net
Phone: (989) 832-5555