**SANDIA REPORT**
SAND2001-1074
Unlimited Release
Printed April 2001

# Instructions and Changes to the NEWPEP Thermochemical Code

Jennifer L. Dobbs and Mark C. Grubelich

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.



Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.



Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865)576-8401
Facsimile: (865)576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.doe.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd
Springfield, VA 22161

Telephone: (800)553-6847
Facsimile: (703)605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/ordering.htm

SAND2001-1074
Unlimited Release
Printed April 2001

# Instructions and Changes to the NEWPEP Thermochemical Code

Jennifer L. Dobbs
Explosive Subsystems and Materials Department

Mark C. Grubelich
Explosive Projects/Diagnostics

Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185-1452

## Abstract

The NEWPEP thermochemical code is a computer program that has been developed to help predict the performance of a user generated propellant system. Sandia has used the program to model the use of different oxidizer/fuel combinations. The program has been adapted to fit Sandia's need by expanding the programs combustion species database and the ingredient list. This paper provides the user with a thorough set of operating instructions.

## Acknowledgments

Larry Williams (retired) and John Cunningham at the Lockheed Martin Electronics and Missiles Group in Florida for their contributed knowledge regarding the programs use and history and their help in combining all aspects of the NEWPEP program.

Chan Price (retired) and Alice Atwood of the Naval Weapons Center at China Lake for their help in providing many previous unknown and undocumented parts of the NEWPEP program.

# Contents



## Figures



## Tables

# Instructions and Changes to the NEWPEP Thermochemical Code

## Background

In 1960, the Naval Weapons Center at China Lake first started to develop a computer code to model thermodynamic reactions. Early versions of the code were originally called the NWC Thermochemical Program or the Propellant Evaluation Program. Later versions of the code have been named MICROPEP or NEWPEP. Many revisions have occurred to the code since the original program was developed. It was converted from a mainframe computer program to one for use on personal computers, other changes were made by individual users who adapted parts of the program to fit their needs. Past revisions have helped to increase the efficiency of the program and ease of program use. Due to drastic increases in computer technology, many factors, such as memory, are not primary concerns in program design.

Previous documentation of the code by Cruise[1] discusses the calculations that the program performs. It also discusses earlier history and development of the code. It includes a small introduction to use of the code, which will be expanded upon in this report.

## Sandia Interest

Sandia began using the code to model explosive reactions for use in research activities. It has been used extensively in the study of Hydrogen Peroxide as an oxidizer with different fuels. The version of PEP in use at Sandia is the VAX-8250, CODE 389 VERSION OF PEP, JAN 1988. This current version has been called NEWPEP. Many versions of the code exist. Many individual users have personalized the program to work for their own individual program needs. The NEWPEP version in use at Sandia is a complete version of the program including all contributing programs and source code.

# General Instructions

**Several files are included with the NEWPEP program, these are:**

| | |
|---|---|
| NEWPEP.EXE | Executable file for NEWPEP |
| PEPCODED.DAT | ASCII file of ingredients |
| JANNAF.DAT | JANNAF specific heat curve fit data in binary form |
| PEP.TXT | Short set of user instructions provided with original code |

**Other files included with NEWPEP are:**

| | |
|---|---|
| NEWPEP.FOR | FORTRAN source code for executable |
| PEPOST.FOR | FORTRAN source code for JANNAF curve fitting program |
| PEPOST.EXE | Executable from PEPOST.FOR |
| NEWPEPOS.DAT | ASCII form of JANNAF curve fit data |
| NEWJAN.FOR | FORTRAN source code for conversion of ASCII JANNAF curve fit data to binary form (converts NEWPEPOS.DAT to JANNAF.DAT) |
| NEWJAN.EXE | Executable from NEWJAN.FOR |
| LOXHYDRO.IN | Sample test case using the combustion of Liquid Oxygen with Cryogenic Hydrogen to practice or test use of the program |
| LOXHYDRO.OUT | NEWPEP results of LOXHYDRO.IN |

For general operation of the program NEWPEP.EXE, PEPCODED.DAT and JANNAF.DAT must be in the same folder.

NEWPEP can be run either through starting the computer in the DOS mode or running it through the MS-DOS prompt. An attempt will be made to note the commands relevant to use of this program.

1. Boot up computer in the MS-DOS mode or open the MS-DOS prompt.

2. Change to the directory in which the NEWPEP code is located.

```
C:\
C:\CD NEWPEP
C:\NEWPEP\
```

3. NEWPEP can be run through an interactive mode, with the user entering data as the prompts call for it, or it can be run by calling data from an input file which the user creates. The 11 lines for data entry are listed below.

***Table 1 NEWPEP Data Entry Lines***

| *Line Number* | *Variable* | *Format* | *Description* |
|---|---|---|---|
| 1 | FILNAME | A30 | File name for NEWPEP output<br>Include necessary information to specify file name<br>1. Defaults to "PEPOUT.DAT" |
| 2 | USER | A17 | Propellant title or users name<br>1. Used to include neccesary information for user |
| 3 | NIC,<br>NIU,<br><br>IRUN | 3I5 | Number of coded ingredients<br>Number of user defined ingredients<br>1. Total number of ingredients cannot exceed 10<br>Number of runs (defaults to 1) |
| 4 | DENEXP | F10.0 | Density Exponent used in calculation D-ISP, density ISP (defaults to 1.0).<br>NOTE: This calculation has not been characterized. It is allowed to run with its default values. |
| 5 | PROPTEMP | F10.0 | Temperature of ingredients in Kelvin (defaults to 298 K). Used for temperature conditioning effects. |
| 6 | CPA, CPB, CPC | 3F10.0 | Quadratic coefficients for solid specific heat. Used with temperature difference to adjust the system enthalpy for heating or cooling. (Defaults to 0.3 cal/gm K).<br>NOTE: This measurement has not been characterized. It is allowed to run with its default values. |
| 7 | <br>KR(1),<br>KR(2),<br>KR(3),<br>KR(4),<br>KR(5),<br><br>KR(6),<br>KR(7),<br><br>IDEBUG | 8I1 | Entry for this line is 1-yes, 0-no<br>Delete exit calculation<br>Include ionic species in calculations<br>Include boost velocities and nozzle design data<br>Input pressures in atmospheres instead of PSI<br>Sets the number of significant figures in results<br>1-1more sig. digit, 2-2 more sig. digit, etc.<br>Output a list of all combustion species considered<br>Fix chamber pressure, temperature is input in place of exit pressure on LINE 9<br>Debug options, 1-yes, 0-no. |

| *Line Number* | *Variable* | *Format* | *Description* |
|---|---|---|---|
| 8 | KR()<br>KR | 5I1 | Line 8 is not needed if IDEBUG in Line 7 is 0.<br>Thermo data at every guess<br>Values of J,M, VF, VB, PR, VA in subroutine TWITCH<br>Species composition every iteration<br>Log of equilibrium constant every guess<br>Classification of species each iteration, from TWITCH |
| 9 | ITAG(I) | 10I5 | Line 9 is not needed if NIC (number of coded ingredients) in Line 3 is 0.<br>Ingredient code numbers from PEPCODED.DAT ingredient code list |
| 10 | BLOK( I ),<br>JIE( I , L ),<br>JE( I , L ),<br><br>DH( I ),<br>RHO( I ) | A30,<br>6(I3, A2)<br><br><br>F5.0,<br>F6.0 | Line 10 is not needed if NIU (number of user ingredients) in Line 3 is 0.<br>Ingredient Name<br>Number of atoms of element in ingredient<br>Symbol of element<br>1. Total number of elements cannot exceed 6<br>Heat of formation, must be input in cal/gram<br>Density of ingredient, must be input in lb/cu-in |
| 11 | W1( 5 ),<br><br><br><br>W1( 6 ),<br>WING( I ) | 10E16.6 | Chamber pressure, PSI or ATM depending on input of KR(4) on Line 7.<br>1. Might also be used for temperature in K depending on input of KR(7) on Line 7<br>Exhaust pressure, PSI or ATM<br>Ingredient masses, ordered with respect to input from Line 9 and Line 10 |

*Adapted from D.R. Cruises Technical Report NWC TP 6037*[1]

## Running the Program

It is recommended that the program be run with input files to maintain a hard copy of the data used for runs.

1. As mentioned, NEWPEP can be run in an interactive mode by entering the name of the executable file (NEWPEP). This will start a program that prompts the user for the same information in the format indicated and will output information to the named file as indicated by the user.
2. To create an input file, follow the input file format mentioned before to create a file using the DOS editor.
3. For ease in recognizing the input and output file, name the input file INPUT.IN, where INPUT can be replaced by information on the run as seen fit by the user. To recognize the output file associated with an input file, use the same file name with the extension ".OUT"
4. The command for running the program with a user created input is (at the DOS-Prompt)

   ```
   C:\NEWPEP\NEWPEP<INPUT.IN
   ```

   "C:\NEWPEP" is the path for the location of the NEWPEP program and NEWPEP <INPUT.IN is the executable code with the less than sign indicating the input file the user has created.
5. The results for running with an input file, will be output to the file name directed by the user on Line 1 of data input or will go to the default file PEPOUT.DAT

# Test Case

The following are instructions on how to practice use of the program using LOXHYDRO.IN, a test case using the combustion of Liquid Oxygen with Cryogenic Hydrogen to form Water.

1. Start the computer in either the MS-DOS mode or open the MS-DOS prompt.

2. Change to the directory containing the NEWPEP code.

   ```
   C:\
   C:\CD NEWPEP
   C:\NEWPEP\
   ```

3. Open the LOXHYDRO.IN file using the DOS editor. This command will open the file in the editor.

   ```
   C:\NEWPEP\EDIT LOXHYDRO.IN
   ```

The file is shown here with no changes.

```
LOXHYDRO.OUT
LOXYHYDRO
2,0,3



0,0,0,0,0,0,0,0
728,496
4500.,14.7,30.0,10.0
4500.,14.7,40.0,10.0
4500.,14.7,50.0,10.0
```

The same file is shown here, indicating line numbers and comments on the information provided on each line.

***Table 2 Test Case Indicating Line Numbers and Comments***

| **Line Number** | **File Contents** | **Comments** |
|---|---|---|
| Line 1 | `LOXHYDRO.OUT` | The output file name. The results generated by running the program will be found in an output file named LOXHYDRO.OUT |
| Line 2 | `LOXYHYDRO` | Generic information concerning the run that is printed in the output file. This will help a user include any information they need concerning the run. |
| Line 3 | `2,0,3` | The run here will use two coded ingredients indicated by the two in the first column. The zero corresponds to the number of user defined ingredients. The three corresponds to the number of runs. |
| Line 4 | | Left blank.<br>Density Exponent used in calculation D-ISP, density ISP (defaults to 1.0).<br>NOTE: This calculation has not been characterized. It is allowed to run with its default values. |
| Line 5 | | Left blank.<br>Temperature of ingredients in Kelvin (defaults to 298 K). Used for temperature conditioning effects. |

| Line Number | File Contents | Comments |
|---|---|---|
| Line 6 | | Left blank.<br>Quadratic coefficients for solid specific heat. Used with temperature difference to adjust the system enthalpy for heating or cooling. (Defaults to 0.3 cal/gm K). |
| Line 7 | `0,0,0,0,0,0,0,0` | On and off switches for different options available. All options here are zero to have the switches off. See above explanatory table to review each switch. |
| Line 8 | `728,496` | The ingredient line numbers taken from PEPCODED.DAT.<br>728 refers to liquid oxygen, and 496 to cryogenic hydrogen. |
| Line 9 | `4500.,14.7,30.0,10.0` | First NEWPEP run. The chamber pressure is set at 4500 atm and the backpressure is at 14.7 atm. There are 30.0 grams of liquid oxygen and 10.0 grams of cryogenic hydrogen. |
| Line 10 | `4500.,14.7,40.0,10.0` | Second NEWPEP run. The chamber pressure is set at 4500 atm and the backpressure is at 14.7 atm. There are 40.0 grams of liquid oxygen and 10.0 grams of cryogenic hydrogen. |
| Line 11 | `4500.,14.7,50.0,10.0` | Third NEWPEP run. The chamber pressure is set at 4500 atm and the backpressure is at 14.7 atm. There are 50.0 grams of liquid oxygen and 10.0 grams of cryogenic hydrogen. |

3. To practice running the program with this input file, it is recommended that the name of the output file be changed so as not to overwrite the output file LOXHYDRO.OUT that also comes with the test case.

**UNCHANGED LOXHYDRO.IN**

```
LOXHYDRO.OUT                <~CHANGE THIS NAME TO SOMETHING ELSE
LOXYHYDRO
2,0,3



0,0,0,0,0,0,0,0
728,496
4500.,14.7,30.0,10.0
4500.,14.7,40.0,10.0
4500.,14.7,50.0,10.0
```

**CHANGED LOXHYDRO.IN**
In this file, the output name has been changed to TEST.OUT

```
TEST.OUT
LOXYHYDRO
2,0,3



0,0,0,0,0,0,0,0
728,496
4500.,14.7,30.0,10.0
4500.,14.7,40.0,10.0
4500.,14.7,50.0,10.0
```

4. Save the file using the file command on the toolbar at the top of the editor.

5. Close the editor using the same toolbar, this returns to the MS-DOS prompt.

6. Run the NEWPEP executable code.

```
C:\NEWPEP\NEWPEP<LOXHYDRO.IN
```

This directs the executable program to look in the file LOXHYDRO.IN for the input information.

7. The program has completed its run and saved the results in the file indicated by the users choice on Line 1 of the input file. In the example, the output would have been saved in a file named TEST.OUT.

8. Use the MS-DOS editor to view the results.
```
C:\NEWPEP\EDIT TEST.OUT
```
The results can also be printed
```
C:\NEWPEP\PRINT TEST.OUT
```

Compare the TEST.OUT file to LOXHYDRO.OUT to make sure the program ran correctly.
The options on Line 7 should be tried, use the commands (0-no, 1-yes) to turn on or off the various switches.

# Ingredient List

The ingredient list is located in the file PEPCODED.DAT. This file can be edited in the DOS editor. It is a data base of chemicals commonly used as propellant ingredients. Ingredients can be used directly from the list or can be added as follows using the DOS editor.

1. When adding new ingredients, input them at the bottom of the file. This will help to prevent error in previously written input files by keeping the line numbers consistent.
2. The format for ingredient input is A30, 6(I3, A2), F5.0, F6.0

| | |
|---|---|
| A30 | The ingredient name input up to 30 characters |
| 6(I3, A2) | Six elements in the form of 3 integers and two alpha characters |
| F5.0 | Floating point with 5 integer places- Heat of formation in cal/gram |
| F6.0 | Floating point with 6 integer places- Density in lb/cu-in |

Ex:

```
ACAN  MAE CHAN                  9C  16H  10O   8N            -776 .1032
ACETAMIDE                       2C   5H   1O   1N           -1310 .0360
ACETONITRILE SOLID              2C   3H   1N                  309 .0283
ACETYL TRIETHYL CITRATE        22H  14C   8O                -1257 .0408
```

3. It is best if the user copies a line of previously written ingredient information and paste it at the bottom to use as a guide when adding own ingredients. This is to also help in keeping the rows and columns in order; FORTRAN is dependent on row and column placement.

4. The program does NOT need to be recompiled after addition of new ingredients.

5. To locate the line number of the ingredient, open the file PEPCODED.DAT in the MS-DOS editor. The line number in the bottom right hand corner will correspond to the line number that needs to be indicated for an ingredient in an input file.

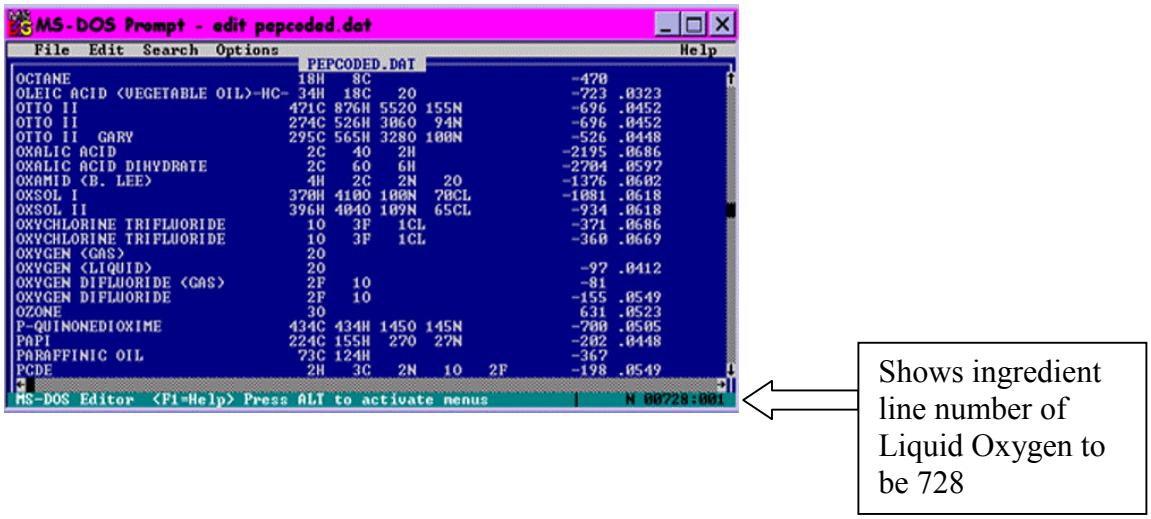


***Figure 1. PEPCODED.DAT Screen***

# Ingredient Errors

The heat of formation for varying concentrations of hydrogen peroxide was incorrect in PEPCODED.DAT. This error was found when runs using these concentrations came out incorrect. Hydrogen peroxide at concentrations of 50, 70 and 90 percent each had an incorrect heat of formation. These values were changed as follows:

| Concentration | Original (cal/gram) | Changed to(cal/gram) |
|---|---|---|
| 50% | -1927 | -2556 |
| 70% | -1684 | -2070 |
| 90% | -1439 | -1571 |

The incorrect values matched those found in the book written by Schumb[2]. Other sources[3] for concentrations of less than 100% had the same incorrect heats of formation, but it was observed that these books had referenced Schumb[2]. Values for the heat of formation were gathered from the *Hydrogen Peroxide Handbook*[4] and calculated with Hess' Law for comparison. Other concentrations of hydrogen peroxide were also added to the ingredient and information about these were found in the same source[4].

Estimated densities for various hydrogen peroxide concentrations were calculated by finding the average density of the two constituents, hydrogen peroxide and water. When adding 30% hydrogen peroxide to the ingredient list, the following calculation was done:

$1/\rho = \sum x_i / \rho_i$ Where $x_i$ = mass fraction of component and $\rho_i$ = density of same component

For 30% Hydrogen Peroxide:

$\rho(100\%\ H_2O_2, 25°C) = 0.0508$ lbs./ $in^3$ $0.3 = x_{H2O2}$
$\rho(H_2O, 25°C) = 0.0361$ lbs./ $in^3$ $0.7 = x_{H2O}$

$1/\rho = 0.3/0.0508 + 0.7/.0361$
$1/\rho = 28.290609\ in^3 / lb.$
$\rho = 0.0395$ lbs. / $in^3$

For addition of other ingredients, some common sources for chemical/physical properties of various compounds are listed below:

- Picatinny Arsenal. *Encyclopedia of Explosives and Related Items,* vol. 1-10. Dover: Compton Press, 1960.
- Lide, R., ed. *Handbook of Chemistry and Physics*. 79th Ed. Boca Raton: CRC Press LLC, 1998.
- National Technical Information Service, *Selected Values of Chemical Thermodynamic Properties.* Series from NBS Technical Note 270-8. Washington: U.S. Government Printing Office.
- Köhler, J. and Meyer, R. *Explosives*. 4th ed. Weinheim: VCH, 1993, translation.

# Program Changes and Additions

Due to the nature of Sandia's interest in studying explosive reactions, it was beneficial to study the addition of new combustion species to JANNAF.DAT. An energetic reaction using silver oxide needed to be studied. Use of the program was not idea because of the lack of silver combustion species. When the program was run with silver containing reactants an error message stating that there were "NO COMBUSTION SPECIES FOR AG REVISE JANNAF.DAT" appeared in the output file. To be able to run the program with silver containing compounds, the method of adding combustion species to JANNAF.DAT had to be investigated.

JANNAF.DAT is the binary file that the NEWPEP program directly uses for combustion species. Complete instructions regarding additions to JANNAF.DAT will be noted. A brief explanation is as follows: Thermochemical data generally found in tables is used to form the curve fits used for JANNAF.DAT. This data is entered in table form and converted using PEPOST.EXE. The source code for this program was received from Chan Price at the China Lake Naval Weapons center. PEPOST.EXE will produce a seven coefficient curve fit. This curve fit is entered into the ASCII file NEWPEPOS.DAT and converted into the binary file JANNAF.DAT using NEWJAN.EXE. The following are detailed instructions to complete the process.

1. Obtain thermochemical tables for the species to be added. The primary source of these are the NIST-JANAF Thermochemical Tables[5], other sources[6,7] were also found for the tables.

2. The information needed from these tables is the temperature, heat capacity, enthalpy (heat) of formation, and the entropy. Units are as follows:
   Temperature [=] degree K

Heat Capacity [=] cal/kmol
Heat of Formation [=] kcal/mol
Entropy [=] cal/kmol

3. Use input and output files to maintain a hard copy of data.
   The following is a sample input file for silver in the solid state. This data was manually input into the DOS editor.

```
298.,6.073,0.000,10.200
300.,6.073,0.000,10.238
400.,6.163,0.000,11.996
500.,6.294,0.000,13.384
600.,6.441,0.000,14.545
700.,6.596,0.000,15.545
800.,6.755,0.000,16.440
900.,6.936,0.000,17.246
1000.,7.136,0.000,17.987
0.0
```

   NOTE: The temperature ranges for species are done in intervals, primarily by physical state or by 500 K or 1000 K temperature ranges. Study the temperature ranges in NEWPEPOS.DAT for clarification. The solid state of silver was done in the range of 298 – 1000K and then from 1000 - 1234 K.

4. Use the PEPOST executable to create the curve fit coefficients. Direct the output to a file.
   `C:\NEWPEP\PEPOST<AGSOLID.IN>AGSOLID.OUT`

5. The curve fit coefficients are generated and info is placed into the output file indicated. In this case the input file was AGSOLID.IN and the output file AGSOLID.OUT. The contents of AGSOLID.OUT are shown here:

```
ENTER TABULAR VALUES OF TEMP,CP,H, AND S
  ENTRY OF 0.0 FINISHES INPUT
  RMS FIT FOR SPECIFIC HEAT =      0.0002
   298.     6.073     6.073     0.000    -1.997    10.200    10.197
   300.     6.073     6.073     0.000    -1.985    10.238    10.238
   400.     6.163     6.162     0.000    -1.374    11.996    11.995
   500.     6.294     6.295     0.000    -0.751    13.384    13.384
   600.     6.441     6.441     0.000    -0.115    14.545    14.545
   700.     6.596     6.594     0.000     0.537    15.545    15.549
   800.     6.755     6.757     0.000     1.204    16.440    16.440
   900.     6.936     6.935     0.000     1.889    17.246    17.246
  1000.     7.136     7.136     0.000     2.592    17.98717.987

  FIT CONSTANTS
    0.494773E+01    0.351538E+01   -0.273505E+01    0.138280E+01
    0.251923E-01   -0.199737E+01    0.101971E+02
```

6. The seven constants along the bottom are those to be entered in NEWPEPOS.DAT. The format is slightly different.
   EX: The first coefficient for silver in the solid state generated by PEPOST is `0.494773E+01`. The format required for NEWPEPOS.DAT is an 8 digit number.
   The fit generated by PEPOST is

```
0.494773E+01    0.351538E+01   -0.273505E+01    0.138280E+01
0.251923E-01   -0.199737E+01    0.101971E+02
```

These numbers need to be entered in NEWPEPOS.DAT. This was done manually.

```
Silver                          (C)          AG 1                          4453-A
0.4977730E+010.3515380E+01-.2735050E+010.1382800E+01  298 TO 1000         4453-B
0.2519230E-01-.1997370E+010.1019710E+020.0000000E+00  298 TO 1000         4453-C
```

The first line of input indicates the species name, in this case silver. The next notation on the first line indicates the state of the material, (C) representing crystalline state or solid. The notation for other states are (L) for liquid and (G) for gas. The number at the end of the line indicates the species number. In this case, silver is the 4453 species and the letters following indicate all the lines that correspond to that species. For the second temperature range of silver in the solid state a user would use the same species number but continue on with the lettering, using D, E, and F for the next entry. The coefficients entered are those generated by PEPOST. There is a change in the number of significant figures entered and the spacing. There must be eight significant figures in the coefficients and there is no spacing. The eighth spot for a coefficient is the average heat of formation of the species over the temperature range. For silver, the heat of formation in the solid state is 0 so 0.0000000E+00 is entered in the eighth place. The continuation of the curve fit coefficients correspond to the temperature range of that curve fit. Since the coefficients were done for the range of 298 K to 1000 K, it is indicated both on the second and third lines.

7. More than one combustion species can be added at once. However, because FORTRAN is line and column dependent, insert new combustion species only at the end of the file. Also, to ensure correct placement of information, follow the format of the lines above in the file.

8. The ASCII form in the file NEWPEPOS.DAT now needs to be converted to the binary form JANNAF.DAT. This is done using NEWJAN.EXE, the executable file formed from compiling NEWJAN.FOR. NEWJAN.EXE will write the binary conversion of NEWPEPOS.DAT to JANNAF.DAT.
   The command for this is:
   `C:\NEWPEP\NEWJAN`
   After the program has completed converting the data, it will output a message saying

```
JANCREATE WORKED SUCCESSFULLY
```

JANNAF.DAT has now been created with all of the species in the NEWPEPOS.DAT file

9. The information at the very beginning of NEWPEPOS.DAT before the curve fit information begins appears to be some sort of identification for the elements of the periodic table. Most elements tend to support this idea, although a few vary from the expected trend. There is no need to change this data.

10. After the last element curve fit, there is a FORTRAN end statement, DONE, which should indicate that no more data will be read from the file. There is data following this statement in the original file, which has been maintained. None of this data was changed and it remains in the file.

11. **NOTE:** The program NEWPEP does not need to be recompiled after the creation of a new JANNAF.DAT.

Upon completion of the above steps, a reaction containing silver compounds was able to run correctly. No error messages were created in the output and the NEWPEP program was able to successfully identify the newly added combustion species.

# Applications

After the addition of new combustion species, NEWPEP's application toward modeling of specific energetic reactions improved. Much of the work done included the use of hydrogen peroxide with variances on the fuel, such as RP-1, Ammonia, or Methanol. This work was documented through graphs. A sample of which follows:

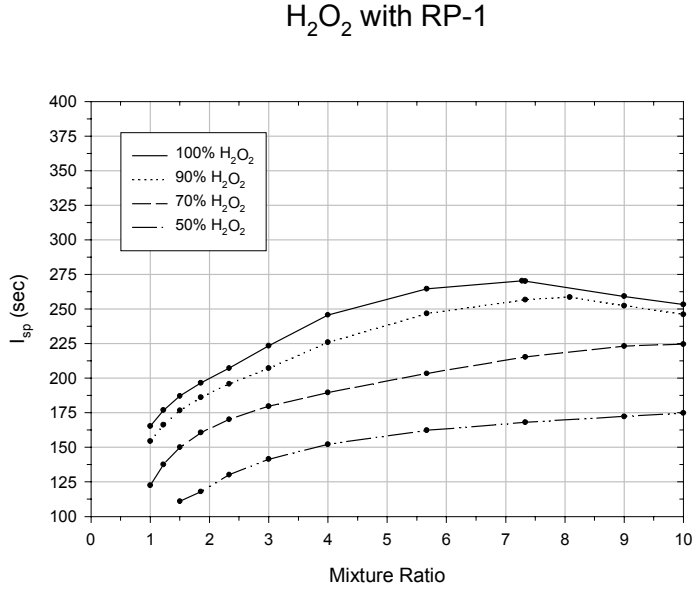


***Figure 2. Sample Graph***

All work done and all graphs created pertaining to the study of hydrogen peroxide will be combined in a future report. The above is a sample to show the information that can be provided by NEWPEP. Using several different input files, a user can create multiple sets of data for a research project. For this case, four input files were used, each with different concentrations of hydrogen peroxide. In each of these runs, varying mixture ratios were used and then the output files printed. The data was manually entered into SIGMA Plot 2000 and the graphs created.

# Conclusion

The work done on the NEWPEP code has helped to improve the contributions the code can make to Sandia's work. The addition of new combustion species to the database will benefit future users as they will have more propellant components to choose from. This documentation will serve as a reference to all users of the code and facilitate use of NEWPEP. Future work could include creation of a more user-friendly program interface, and a more simple method for inputting data for combustion species. Using this document as an example, it is hoped that future work on the code will also be documented.

# References


1. Cruise, D.R., *Theoretical Computations of Equilibrium Composition, Thermodynamic Properties, and Performance Characteristics of Propellant Systems,* NWC TP 6037. Naval Weapons Center, China Lake, 1979, 1991 (revision 1).

2. Schumb, W.C., Satterfield, C.N., and Wentworth, R.L., American Chemical Society's Series of Chemical Monographs, *Hydrogen Peroxide*, pg. 189-309, Reinhold Publishing Corporation, 1955.

3. FMC, *Hydrogen Peroxide Physical Properties Data Book*, pg. 8-11 and 46-47, Tables 2-5 and 62-63, Fig. 2-5. 1969.

4. Cain, E.F.C. and Constantine, M.T., Air Force Rocket Propulsion Laboratory, *Hydrogen Peroxide Handbook*, Report No. R-6931, pg. 19, 24, Tables 2.3-2.8, Fig. 2.12 – 2.12a, Edwards Air Force Base: California,1967.

5. National Institute of Standards and Technology,. Chase, M. ed. *Journal of Physical and Chemical Reference Data: NIST-JANAF Thermochemical Tables*, 4th ed.. Part I-II. New York: American Chemical Society and the American Institute of Physics, 1998.

6. Barin, I., Saurt, F., Schultze-Rhonhof, F., and Shu Sheng, W., *Thermochemical Data of Pure Substances,* British Library Cataloguing, 1989, translation.

7. Barin, I., Knack, O., and Kubachewski, O., , *Thermochemical Properties of Inorganic Substances*, Springer-Verlag Berlin Heidelberg New York,1977, translation.

# Distribution

| | | |
|---|---|---|
| | MS 1351 | Sharon Ortiz, 3535 |
| | MS 1452 | John A. Merson, 2552 |
| 10 | MS 1452 | Jennifer L. Dobbs, 2552 |
| | MS 1452 | Thomas M. Massis, 2552 |
| | MS 1453 | Greg Scharrer, 2553 |
| | MS 1454 | Lloyd L. Bonzon, 2554 |
| | MS 1454 | Mark C. Grubelich, 2554 |
| | MS 1454 | Brian Melof, 2554 |
| 1 | MS-9018 | Central Technical Files, 8945-1 |
| 2 | MS 0899 | Technical Library, 9616 |
| 1 | MS 0612 | Review & Approval Desk, 09612<br>for DOE/OSTI |