## Input Data Files

**Kinetics2015** can analyze a maximum of 51 data files simultaneously. One data file is usually used for each experiment, although a series of experiments following the same thermal history and having limited data per experiment (e.g., product yield only at the end of each experiment) can be combined into one file. The total of all data points in all files used in a given analysis cannot exceed 20000, although data files as large as 32000 points can be preprocessed and thinned using the Data Module. An example of an input data file with standard format is:

```
Example of standard format for Kinetics05
  Time(m)      Temp(C)      Rate
  1.65000E+00  2.88683E+02  3.43000E+00
  1.81000E+00  2.90693E+02  4.02000E+00
  1.97000E+00  2.92723E+02  4.84000E+00
  2.13000E+00  2.94783E+02  5.80000E+00
  2.29000E+00  2.96963E+02  6.69000E+00
  2.45000E+00  2.98973E+02  7.58000E+00
  2.61000E+00  3.01103E+02  8.70000E+00
  2.77000E+00  3.03223E+02  9.59000E+00
  2.93000E+00  3.05293E+02  1.07000E+01
  3.09000E+00  3.07393E+02  1.19600E+01
  3.25000E+00  3.09513E+02  1.30000E+01
  3.41000E+00  3.11863E+02  1.37400E+01
  3.57000E+00  3.13743E+02  1.44800E+01
  3.73000E+00  3.15903E+02  1.54500E+01
  3.89000E+00  3.18273E+02  1.61100E+01
  4.05000E+00  3.20183E+02  1.73000E+01
  4.21000E+00  3.22303E+02  1.83400E+01
  4.37000E+00  3.24433E+02  1.90800E+01
  4.53000E+00  3.26743E+02  1.99700E+01
  4.69000E+00  3.28873E+02  2.09400E+01
  4.85000E+00  3.31193E+02  2.19700E+01
  5.01000E+00  3.33533E+02  2.33100E+01
  5.17000E+00  3.35813E+02  2.46500E+01
  5.33000E+00  3.38033E+02  2.60500E+01
  5.49000E+00  3.40213E+02  2.71700E+01
  5.65000E+00  3.42453E+02  2.83500E+01
  5.81000E+00  3.44613E+02  2.96900E+01
  5.97000E+00  3.46773E+02  3.11700E+01
  6.13000E+00  3.48903E+02  3.28100E+01
  6.29000E+00  3.51013E+02  3.45900E+01
  6.45000E+00  3.53123E+02  3.64400E+01
  6.61000E+00  3.55283E+02  3.83700E+01
  6.77000E+00  3.57423E+02  4.05200E+01
  6.93000E+00  3.59573E+02  4.29700E+01
  7.09000E+00  3.61773E+02  4.55700E+01
  7.25000E+00  3.63993E+02  4.87600E+01
  7.41000E+00  3.66213E+02  5.19500E+01
  7.57000E+00  3.68353E+02  5.53600E+01
  7.73000E+00  3.70493E+02  5.86200E+01
  7.89000E+00  3.72653E+02  6.23300E+01
  8.05000E+00  3.74793E+02  6.63400E+01
  8.21000E+00  3.76943E+02  7.07100E+01
  8.37000E+00  3.79093E+02  7.57600E+01
  8.53000E+00  3.81263E+02  8.10300E+01
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8.69000E+00  3.83443E+02  8.66600E+01
8.85000E+00  3.85583E+02  9.23800E+01
9.01000E+00  3.87773E+02  9.89800E+01
9.17000E+00  3.89883E+02  1.06100E+02
9.33000E+00  3.92113E+02  1.14040E+02
9.49000E+00  3.94333E+02  1.22860E+02
9.65000E+00  3.96503E+02  1.32140E+02
9.81000E+00  3.98683E+02  1.41630E+02
9.97000E+00  4.00853E+02  1.52020E+02
1.01300E+01  4.03163E+02  1.63740E+02
1.02900E+01  4.05253E+02  1.76350E+02
1.04500E+01  4.07433E+02  1.90000E+02
1.06100E+01  4.09623E+02  2.04620E+02
1.07700E+01  4.11863E+02  2.20790E+02
1.09300E+01  4.14103E+02  2.38150E+02
1.10900E+01  4.16283E+02  2.56540E+02
1.12500E+01  4.18483E+02  2.76430E+02
1.14100E+01  4.20683E+02  2.98610E+02
1.15700E+01  4.22943E+02  3.22350E+02
1.17300E+01  4.25123E+02  3.46750E+02
1.18900E+01  4.27313E+02  3.72570E+02
1.20500E+01  4.29503E+02  4.00390E+02
1.22100E+01  4.31713E+02  4.30580E+02
1.23700E+01  4.33913E+02  4.61510E+02
1.25300E+01  4.36083E+02  4.94010E+02
1.26900E+01  4.38283E+02  5.28210E+02
1.28500E+01  4.40493E+02  5.64560E+02
1.30100E+01  4.42693E+02  6.02020E+02
1.31700E+01  4.44863E+02  6.38960E+02
1.33300E+01  4.47043E+02  6.76430E+02
1.34900E+01  4.49263E+02  7.16190E+02
1.36500E+01  4.51503E+02  7.56250E+02
1.38100E+01  4.53703E+02  7.92820E+02
1.39700E+01  4.55883E+02  8.25830E+02
1.41300E+01  4.58053E+02  8.53350E+02
1.42900E+01  4.60253E+02  8.75020E+02
1.44500E+01  4.62453E+02  8.87920E+02
1.46100E+01  4.64673E+02  8.89930E+02
1.47700E+01  4.66933E+02  8.78950E+02
1.49300E+01  4.69113E+02  8.51870E+02
1.50900E+01  4.71303E+02  8.05130E+02
1.52500E+01  4.73433E+02  7.39040E+02
1.54100E+01  4.75603E+02  6.58320E+02
1.55700E+01  4.77933E+02  5.68040E+02
1.57300E+01  4.80013E+02  4.74940E+02
1.58900E+01  4.82173E+02  3.87330E+02
1.60500E+01  4.84333E+02  3.10920E+02
1.62100E+01  4.86483E+02  2.49050E+02
1.63700E+01  4.88673E+02  2.00610E+02
1.65300E+01  4.90883E+02  1.62630E+02
1.66900E+01  4.93133E+02  1.32950E+02
1.68500E+01  4.95323E+02  1.09360E+02
1.70100E+01  4.97533E+02  8.99300E+01
1.71700E+01  4.99773E+02  7.38300E+01
1.73300E+01  5.01923E+02  6.06200E+01
1.74900E+01  5.04123E+02  4.95000E+01
1.76500E+01  5.06313E+02  4.04500E+01

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1.78100E+01  5.08673E+02  3.31800E+01
1.79700E+01  5.10753E+02  2.72400E+01
1.81300E+01  5.12943E+02  2.19700E+01
1.82900E+01  5.15133E+02  1.76000E+01
1.84500E+01  5.17353E+02  1.42600E+01
1.86100E+01  5.19543E+02  1.18100E+01
1.87700E+01  5.21713E+02  9.81000E+00
1.89300E+01  5.23963E+02  8.55000E+00
1.90900E+01  5.26093E+02  7.36000E+00
1.92500E+01  5.28283E+02  6.32000E+00
1.94100E+01  5.30453E+02  5.36000E+00
1.95700E+01  5.32613E+02  4.69000E+00
1.97300E+01  5.34813E+02  4.24000E+00
1.98900E+01  5.37043E+02  3.87000E+00
2.00500E+01  5.39273E+02  3.73000E+00
2.02100E+01  5.41413E+02  3.21000E+00
2.03700E+01  5.43553E+02  2.84000E+00
2.05300E+01  5.45803E+02  2.46000E+00
2.06900E+01  5.48013E+02  2.24000E+00
2.08500E+01  5.50213E+02  1.72000E+00
2.10100E+01  5.52403E+02  2.09000E+00
2.11700E+01  5.54703E+02  1.95000E+00
2.13300E+01  5.56803E+02  1.50000E+00
2.14900E+01  5.58973E+02  1.43000E+00
2.16500E+01  5.61153E+02  1.28000E+00
2.18100E+01  5.63323E+02  1.13000E+00
2.19700E+01  5.65503E+02  1.20000E+00
2.21300E+01  5.67633E+02  1.13000E+00
2.22900E+01  5.69923E+02  1.13000E+00
END
```

In the standard format for a **Kinetics2015** data file, the first line is reserved for any user-specified title. The second line contains the time and temperature units, as described in detail in the next paragraph. Each line thereafter must contain three entries (space- or comma-delimited, with any mixture of F, E, or I format): time, temperature, and reaction data. The END line after the data is optional. However, if the user wishes to have additional information (e.g., sample description) at the end of the file, then the END line is required, followed by the additional line(s) of information.

The default unit for time is minutes and the default unit for temperature is degrees Celsius. The time unit may optionally be specified in line 2 of the data file as: Time(s), Time(m), Time(h), Time(d), Time(y), or Time(my), for seconds, minutes, hours, days, years, or millions of years, respectively. Likewise, the temperature unit may optionally be specified as Temp(K) for Kelvins. Note that the words Time and Temp must appear and the respective unit must follow in parentheses. The time and temperature units may be different for each data file.

The Wildcat Technologies' HAWK® and the Weatherford SR Analyzer® both have options for saving their data in the standard **Kinetics2015** format. Although the **Kinetics2015** Data Module was originally programmed to directly read and interpret the file formats generated by Rock-Eval® 6 and Pyromat®, it is recommended that the user manually convert that data to the standard format outside of **Kinetics2015**. The large Rock-Eval files must be thinned to an appropriate number of data points and re-saved to leave out extraneous information. Because of the variability of the formats for TGA, DTA, and DSC data from Thermal Analysis instruments,

the user must manually convert that data to the standard format prior to **Kinetics2015** analysis. In these cases, the third column of the data file can be the relative signal, which can be converted to rate or integral data using the graphical editing tools of the Data Module.

Four data types are permitted for the reaction data:

1. Relative reaction rate (arbitrary scale)
2. Relative cumulative reacted (arbitrary scale)
3. Fraction reacted per second (fraction ranging from 0 to 1)
4. Fraction reacted (fraction ranging from 0 to 1)

Obviously, the reaction can be measured by either reaction rate or extent of reaction (cumulative reacted or fraction reacted, hereafter referred to as integral data). In both cases, the data may be on a relative scale for each experiment or they may be on an absolute scale (i.e., fraction reacted per second for rate and fraction reacted for integral). Data types 1 and 4 are the most common. During the kinetic analysis, relative data are normalized by the final integral data point, so precautions should be taken to assure that the final point is a representative one and not unduly affected by scatter. A mixture of rate files and cumulative files can be analyzed simultaneously. If one or more files contain absolute data, any relative data files are converted to absolute by assuming that the data extend to complete reaction.

A total of 20000 data points are allowed for the combined data files being analyzed. Analysis time is proportional to the number of points, and we have found that approximately 150 points per experiment are usually adequate. The time entries in each data file must be in ascending order. If **Kinetics2015** finds a non-ascending time, it issues a warning message and discards that data point. This procedure does not always find the truly invalid data point; therefore, the user should further examine and correct the data file for use in future runs. The data file is read until a blank line or an end-of-file is encountered.

In some experiments, the reaction signal can undergo considerable dispersion before reaching the detector. This can cause serious errors in the data analysis. A tracer signal measured under the same conditions will help quantify the dispersion. To supply tracer data, enter the tracer signal as the fourth entry in each data line. The tracer data can be rate (pulse) or integral (step), but it cannot be a square wave. The tracer data can be on a relative scale and must be supplied for each experiment in the set being analyzed. Use of the tracer data requires that each data file have a constant time step. Blank entries for the tracer rate are permitted once it has decreased to zero. **Kinetics2015** permits the use of tracer data only in the nth-order, Gaussian, Weibull, and nucleation analysis methods.

The theoretical reaction rates and integrals are determined in **Kinetics2015** using the arbitrary thermal history specified by the experimental data. This ordinarily requires that the time and temperature data begin at a negligibly small reaction rate. This requirement is necessary (with one exception, noted later) to initialize the regression analysis for distribution models, because the program has to know how to partition the initial fraction reacted among the various parallel reactions. By beginning at a negligibly small reaction rate, the starting integral can be initialized to zero for each energy component in the activation energy distribution. This requirement is easily fulfilled by merely extending the thermal history that specifies the actual or estimated sample

heatup to an earlier time at which no reaction has taken place. Negative times are acceptable in the data file and are conveniently used in this extension. For a constant heating rate experiment, a single earlier point with a reaction rate or integral of zero will suffice. For a more complex early thermal history (and to supply enough data points to make smooth plots, even for the constant heating rate case) additional points are needed. For each of the extra points, including the very first one, the experimental rate or integral must be entered as -999 to avoid using it in the regression analysis, other than to enable accurate calculation of the rate and integral at the first real data point.

Using one contiguous block of -999 data, starting with the first data point, is the safest way of using this feature. Another contiguous block of -999 data, ending with the last data point, can also be safely used. A random mixture of -999 points with true data points is not yet permitted in the **Kinetics2015** graphical user interface (KineticsGUI.EXE). It is permitted by the Fortran executable code (KINETICS.EXE), but the results must be carefully examined for the following two cases: (1) if rate data are interspersed with -999's and then integrated by **Kinetics2015** for parameter refinement based on cumulative values and (2) if cumulative data are interspersed with -999's and then differentiated by **Kinetics2015** for parameter refinement based on rates. Peculiar results in these cases are sometimes obtained, especially for sparse data sets. Discrete model distribution parameters determined using KINETICS versions prior to Dec. 97 from cumulative reacted data files having –999 data suffer from truncation of the distribution at too high an initial energy and should be rerun for increased accuracy.

As mentioned above, we allow one exception to the complete thermal history requirement. If the data are on the absolute scale defined above, the first data point may begin at a positive fraction reacted if, and only if, a single Gaussian reaction is being used with the energy distribution parameter constrained to zero. For this case, -999 data must not be used and the calculated integral is initialized to the fraction reacted at the first data point.

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