

**PACKAGE ID** - 000749IBMPC03 KINETICS98

**KWIC TITLE** - Pyrolysis Kinetic Analysis Program

**AUTHORS** - Braun, R.L.  
Lawrence Livermore National Lab., CA (United States)  
  
Burnham, A.K.  
Lawrence Livermore National Lab., CA (United States)

**LIMITATION CODE** -COPY           **AUDIENCE CODE** - LIM

**COMPLETION DATE** - 05/06/1998   **PUBLICATION DATE** - 05/06/1998

**DESCRIPTION** - KINETICS for Windows 95,98,NT (KINETICS98) is a kinetic analysis program designed for reactions such as kerogen, mineral, or polymer decomposition. It can fit rate parameters to chemical reaction data (rate or cumulative reacted) measured at a series of constant heating rate, isothermal, or arbitrary thermal histories. It uses 1st and nth order reaction models, a variety of activation energy distribution models, and an acceleratory nucleation model. Tracer data can be used to deconvolute instrumental dispersion. The program consists of a Fortran analysis module that does the analysis and a graphic user interface that edits data, sets up analysis problems, and views and prints results. New models are Miura methods, nth-order nucleation model, and a discrete model in which  $\ln(A)$  is a linear function of  $E$ . (This version supercedes version KINETICS97 (Fortran v4.05/GUI v 1.0) and DOS/UNIX version3.2)

**PACKAGE CONTENTS** - Media Directory; Software Abstract; Lawrence Livermore Copyright Notice; Media Includes Executable Modules, User's Guide;

**SOURCE CODE INCLUDED?** - No

**MEDIA QUANTITY** - 4 3.5 Diskettes

**METHOD OF SOLUTION** - The program uses a variety of approximate kinetic analysis methods to determine initial guesses for models fitted by nonlinear regression. The discrete activation energy distribution model uses a nested linear-nonlinear regression method.

**COMPUTER** - IBM PC

**OPERATING SYSTEMS** - Windows 95,98 or NT

**PROGRAMMING LANGUAGES** - Fortran and Visual Basic

**SOFTWARE LIMITATIONS** - 2000 data points.

**SOURCE CODE AVAILABLE (Y/N)** - N

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**UNIQUE FEATURES** - The only kinetics analysis software featuring discrete, Gaussian, and Weibull activation energy distribution models for broad reaction profiles and a 4-parameter nth order nucleation model for narrow reaction profiles.

**RELATED SOFTWARE** - None

**HARDWARE REQS** - 486 or greater microprocessor with 8 mbytes of memory.

**TIME REQUIREMENTS** - Kinetic analyses range from a few seconds to several minutes, depending on the speed of the computer and the number of data points.

**REFERENCES** - User's guide on media.

**ABSTRACT STATUS** - Released AS-IS 9/15/1998.

**SUBJECT CLASS CODE** - U

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
K CODES  
CHEMICAL REACTION KINETICS  
PYROLYSIS  
LEAST SQUARE FIT

**EDB SUBJECT CATEGORIES** -  
990200

**SPONSOR** - DOE/ER;DOE/FE

**PACKAGE TYPE** - AS - IS