

**PACKAGE ID** - 000344IBMPC02 PMOD 1.6

**KWIC TITLE** - A Pyrolysis and Primary Migration Model

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

**LIMITATION CODE** -UNL                   **AUDIENCE CODE** - UNL

**COMPLETION DATE** - 01/06/1993   **PUBLICATION DATE** - 01/01/1992

**DESCRIPTION** - PMOD-Version 1.6 is a copyrighted computer program for simulating oil generation, cracking, and other chemical reactions occurring during the pyrolysis of petroleum source rocks over a specified history of temperature and either depth or hydrostatic pressure. The chemical reaction mechanism is defined by the user and, within limits, can be as simple or complex as desired. The model also simulates compaction of the source rock and expulsion of a liquid water phase and a liquid hydrocarbon phase. The expulsion is done by either a simple, constant-fluid-density model or by a more rigorous model using a modified Redlich-Kwong-Soave equation of state. The latter model also calculates overpressuring. An auxiliary program, PLOTPMOD, permits graphical display and hardcopy of the results, as well as preparation of ASCII-file subsets of the results for use with a spreadsheet or other graphics program.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; UCRL-MA-107789 Rev.1; Media Includes Source Code, Executable Module, Sample Problem Input Data;

**SOURCE CODE INCLUDED?** - No

**MEDIA QUANTITY** - 3 3.5 Diskettes

**METHOD OF SOLUTION** - The governing equations (a set of ordinary differential equations) are numerically integrated using LSODE.

**COMPUTER** - IBM PC

**OPERATING SYSTEMS** - MS-DOS

**PROGRAMMING LANGUAGES** - FORTRAN 77

**SOFTWARE LIMITATIONS** - Maximum of 12 oil species, 9 gases, 14 solid organic species, and 6 solid inorganic species are allowed. Maximum of 100 chemical reactions, including distributed activation energies.

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

**PACKAGE ID** - 000344IBMPC02 PMOD 1.6

**UNIQUE FEATURES** - User-definable chemical composition (carbon, hydrogen, oxygen, nitrogen, and sulfur) of all species.  
User-definable chemical reaction network.

**RELATED SOFTWARE** - Our earlier model, PYROL, used a fixed set of species and chemical reactions.

**OTHER PROG/OPER SYS INFO** - The graphics library PCDIGLIB (for IBM PC) is required to compile the program. PCDIGLIB library not included.

**HARDWARE REQS** - 550 K RAM.

**TIME REQUIREMENTS** - Execution time of seconds to tens of minutes, depending on the complexity of the problem.

**REFERENCES** - Robert L. Braun and Alan K. Burnham, PMOD: A flexible model of oil and gas generation, cracking, and expulsion, UCRL-JC-105371 Rev. 1, January 1992; R.L. Braun and A.K. Burnham, User's Manual for PMOD, A Pyrolysis and Primary Migration Model, UCRL-MA-107789, July 1991.

**ABSTRACT STATUS** - Submitted August 1993. Released screened August 31, 1993.

**SUBJECT CLASS CODE** - U

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
P CODES  
CRACKING  
PETROLEUM  
PYROLYSIS  
COMPUTERIZED SIMULATION  
EQUATIONS OF STATE  
MIGRATION

**EDB SUBJECT CATEGORIES** -  
990200 023000

**SPONSOR** - DOE/DP

**PACKAGE TYPE** - SCREENED