

As mentioned above, the system, mkdir, chdir, and perror functions are not in this release version 3.6c. Furthermore, the fgetc function is not compatible.

Some simple graphic functions have been added to the MS-DOS version, though the Macintosh version of the Aztec C does not contain them but gives an easy access to the Macintosh Toolbox functions. For every manager of the Macintosh Toolbox there is a header file, which defines the manager's functions and constants. Thus, the Macintosh Quickdraw graphic functions are easy to use, but are not present on other systems. It would be a nice feature to implement the graphic functions in each Aztec C product.

Source Level Debugger (SDB). With the Aztec C version 3.6 Manx Software Systems have provided a C interpreter with an interactive editor. It has three windows: one for the C source, a second one for output, and a third one for entering

commands. Using SDB, one can debug programs at C and assembly language levels, display all active function names and values of passed parameters, tracing function-by-function or line-by-line, set break points by line functions, or variables, do post mortem debugging, etc. SDB uses about 180K memory, and it runs under the Aztec Shell, the MPW Shell, or the Finder. It is able to handle very large programs as well. This product reduces the time normally spent in debugging fairly well.

Overall, the Aztec C compiler was able to handle a very large program system, HTSS. It performed well and was quite satisfactory. The code it generated is efficient, and the overall compilation time was reasonable. The newly released version 3.6 has a new source level debugger that cuts the development time greatly and is a major improvement in productivity. The Aztec C is a powerful tool for Macintosh program developers.

TDS DIPPR:[†] An Efficient, Helpful Tool!

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It's early Monday morning as John Newgrad enters the office of Dave Oltimer...

"Dave, I have an assignment I need some help on."

"Be glad to help, if I can; what's the problem?"

"Well," John said, "I have to do a process design for a speculative air oxidation process, and I need to find a good solvent, first of all."

"Do you have any specs on the solvent?" Dave asked.

"Not in detail," John replied. "But, something that's liquid at room temperature would be best. And, to simplify separation, the solvent should boil between maybe 100 and 150 °C. Of course, it would need to be miscible with the aromatic feed and the various oxidation products."

"What have you considered so far for a solvent?" Dave asked.

"Hey, Dave, I'm just getting started on this; I don't know...maybe an ester?"

"Well, maybe," said Dave. "But, even though an ester might complicate things through side reactions, let's leave that decision for later. At this point, have I got a deal for you!"

"What do you mean?" John asked.

"I just recently obtained a copy of TDS's Numerica DIPPR program for my PC."

"What's this DIPPR program?"

"It's a search program and database, developed by Technical Database Services, Inc., for the AIChE's Design Institute of Physical Property Data thermophysical properties database," said Dave. "It has really super capabilities and can do nested searches for entire homologous series, as well as searches on combinations of 13 temperature-dependent and 26 constant properties. We can quickly get a list of compounds that satisfy

your mp and n-bp requirements and then narrow the choices down."

"Sounds great," said John. "How does it work?"

"Well, we could take the 'Class Search' option and list the n-bp and mp for all compounds in the four classes of esters (see Figure 1). That would be a lot of data to go through, though. Let's do it the easy way. We'll just search the entire database of 766 compounds for those that satisfy your requirements."

"What do you mean?" asked John.

"We'll ask DIPPR to find all of the compounds that have melting points between 250 and 295 K and normal boiling points between 373 and 395 K."

"Hey, that was quick! How many compounds are on the printout?" asked John.

"There are 20 compounds, John, and one of them reminds me of something I forgot."

"What's that?" asked John.

"Notice that acetic acid is on the list. It satisfies your mp and n-bp restrictions; I recall that it is frequently used as a solvent for aromatic oxidations: terephthalic acid from either tolualdehyde or *p*-xylene are two examples that come to mind, now."

"Sounds good to me," asked John. "I'll use it for the first-pass process design. But, I'll need property data."

"No problem," said Dave. "I'll just search on the name 'acetic acid' and get a printout of all the properties for you. Are SI units O.K.?"

"I don't think very good in SI units, Dave. Actually, I prefer English units."

"No problem, again, John. With the DIPPR system, you can easily get any units you want. I'll also include the notes and references in the printouts, in case you need to refer to them later. Maybe it would also be a good idea to print out a graph for acetic acid's heat of vaporization vs temperature. Unlike most other common compounds, the lower carboxylic acids have a maximum in their latent heat curves; the graph

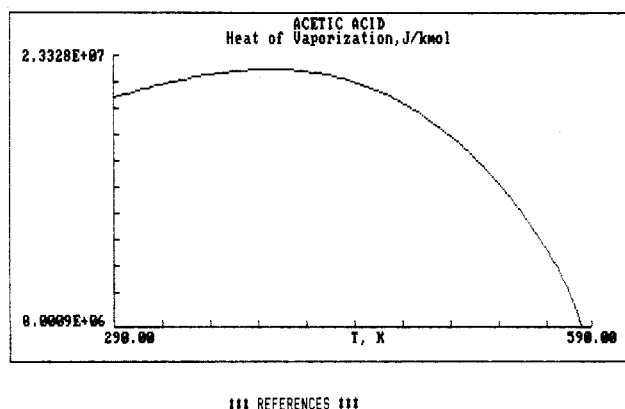
[†] Hardware requirements and pricing information: Version 1, 766 compounds, IBM PC (or compatible) with math coprocessor; 256-kB memory; 4-MB hard disk; unit price, \$850; site license, available on request; demo diskette, \$35; university discount, 20%. Version 2, 1023 compounds, math coprocessor not required; unit price, \$1250. Vendor: Technical Database Services, Inc. (TDS), 10 Columbus Circle, New York, NY 10019 [(212) 245-0044; telex 6714962].

Class Selection

n-Alkanes	Polyols	Other amines, imines
Methylalkanes	n-Aliphatic acids	Nitriles
Cycloalkanes	Other aliphatic acids	C,H,N,O ₂ compounds
Other alkanes	Aromatic carbox. acids	Other monofunc. C,H,O,N
1-Alkenes	Anhydrides	C, H, S compounds
Other alkenes	Formates and acetates	Polyfunctional C,H,O
Dialkenes	Other sat. aliph. esters	Polyfunctional C,H,O,N
Alkynes	Unsat. aliphatic esters	Polyfunkt. C,H,O,S (hal)
n-Alkyl benzenes	Aromatic esters	Polyfunkt. C,H,O, halide
Other Alkylbenzenes	Ethers	Polyf. C,H,N,(O), halide
Other monoaromatics	Epoxides and Peroxides	Organic/Inorganic cmpds
Polyaromatics	Aliphatic chlorides	Inorganic acids
Other hydrocarbon rings	Aromatic chlorides	Inorganic bases
Inorganic gases	C, H, Br compounds	Sodium salts
Aldehydes	C, H, I compounds	Other salts
Ketones	C, H, F compounds	Elements
n-Alcohols	C, H, multihalogen cmpds	Inorganic halides
Other aliph. alcohols	Aliphatic amines	Other inorganics
Aromatic alcohols	Aromatic amines	

ARROW KEYS: move highlight. ENTER: make selection. F10: quit.

Figure 1.



- *** REFERENCES ***
1. International Critical Tables of Numerical Data, Physics, Chemistry, and Technology (7 Vols. + Index), edited by E.W. Washburn, McGraw-Hill, New York (1926-1933).
 2. Stull, D.R., Westrum, E.F., Jr., Sinke, G.C., "The Chemical Thermodynamics of Organic Compounds," John Wiley and Sons, New York (1969).
 3. Young, S., "The Vapour-Pressure, Specific Volumes, Heats of Vaporization, and Critical Constants of Thirty Pure Substances," Royal Dublin Society, Scientific Proceedings, Ser. A, Vol. 12, 374 (1910).
 4. Weltner, W., Jr., "The Vibrational Spectrum Associative and Thermodynamic Properties of Acetic Acid Vapor," J. Am. Chem. Soc. 77, 3941 (1955).
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Figure 2.

will help remind you that the tabulated data aren't peculiar, but correct."

"Dave, that's certainly a little unusual!"

"I know—just check the references, though. That behavior is well documented (see Figure 2)."

"O.K., I will. But say, Dave, that DIPPR system has really helped me here! I have another problem, too...maybe you might try DIPPR there, if it wouldn't be a big effort?"

"What's that, John?"

"Well, Dave, it seems like I'm involved with a lot of 'odd-

ball' compounds recently. I need property data for 4-hydroxyacetophenone (4-HAP) for another project and haven't found much, even in Beilstein."

"Let's look. Hmm...it's not in the DIPPR databank either. But, that doesn't mean that DIPPR can't help."

"Oh?"

"Sure. One of the better ways to predict property data for an oddball compound is to use Generalized Corresponding States Principle (GCSP) procedures with two reference compounds that are similar to the oddball; that ensures that the various properties are at least reasonable. DIPPR can help us to select the reference compounds; their acentric factors should bracket that for 4-HAP. First, we'll look at the acentric factors for a few compounds that are like 4-HAP and then do a 'property search' over the entire database for compounds with values below and above what we think its value may be. Later, after you've estimated the acentric factor and critical properties for 4-HAP, choose two reference compounds from the list, and I'll get you complete property data for each one from DIPPR."

"Dave, I'm really glad I talked to you! Thanks for showing me DIPPR; I'm farther along in half an hour than I expected to be by the end of the week!"

"John, from your standpoint, I know that property data are just a means to an end; there's no reason why you should spend an inordinate amount of time hunting for data when you don't need to! I'm glad, too, that you can see what a valuable tool DIPPR is!"

This 'true-to-life' story illustrates some practical applications of the TDS DIPPR software and database. If you have similar problems, you might want to check out previous reviews for details (references 1, 2, and particularly 3) and/or request further information from Technical Database Services, Inc. (see below).

REFERENCES

- (1) Ergol, Len. *Chem. Eng.* **1988**, 95(5), 114.
- (2) Hughson, Roy V. More Programs Reviewed for Ch.E.'s. *Chem. Eng.* **1988**, 95(16), 109-112.
- (3) Larsen, A. H. The TDS DIPPR PC Package. *Chem. Eng. Prog.* **1989**, 85(2), 78-79.