

ezGC and Pro ezGC

for Fast, Economical GC Method Development

The March 1993 issue of *The Restek Advantage* previewed ezGC, a new software program that uses computer modeling to accurately simulate changes to a GC analysis. The software calculates the peak widths and retention times for a given set of chromatographic conditions and then displays the resulting chromatogram. In addition, the software predicts the optimum temperature program for a given analysis that provides baseline resolution in the shortest time. A chromatographer can see, within seconds, the effect of changes in column dimensions, carrier gas, and operating conditions instead of spending hours or days in the laboratory. The ezGC software improves column selection, optimizes peak resolution, minimizes analysis times, and greatly increases laboratory productivity. Both method development labs and analytical labs performing routine analysis can benefit from ezGC. The following examples demonstrate the capabilities of ezGC using a typical set of columns and chromatographic conditions.

Let ezGC optimize your GC method for resolution in the shortest analysis time

To begin optimizing a GC method, first obtain two sets of retention times for the components of interest at two different temperature programs. In the following example, retention times were collected from two injections of a volatile fragrance mixture using temperature program rates of 3 and 8C/min. Next, the chromatographic conditions and retention times were entered using the menu driven screens of the ezGC program.

Figure 1 - Easily enter information into ezGC from menu driven screens.

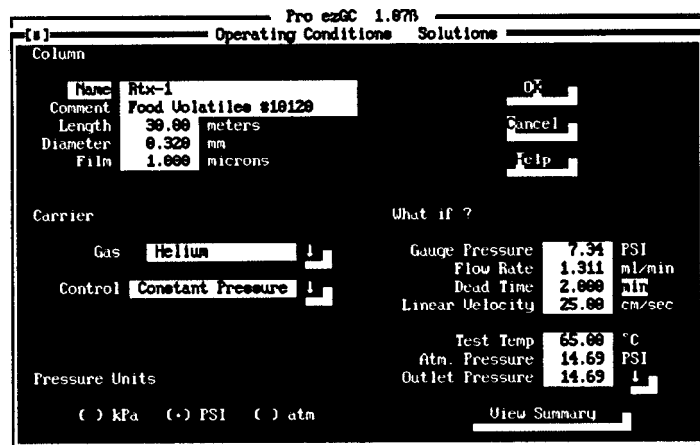
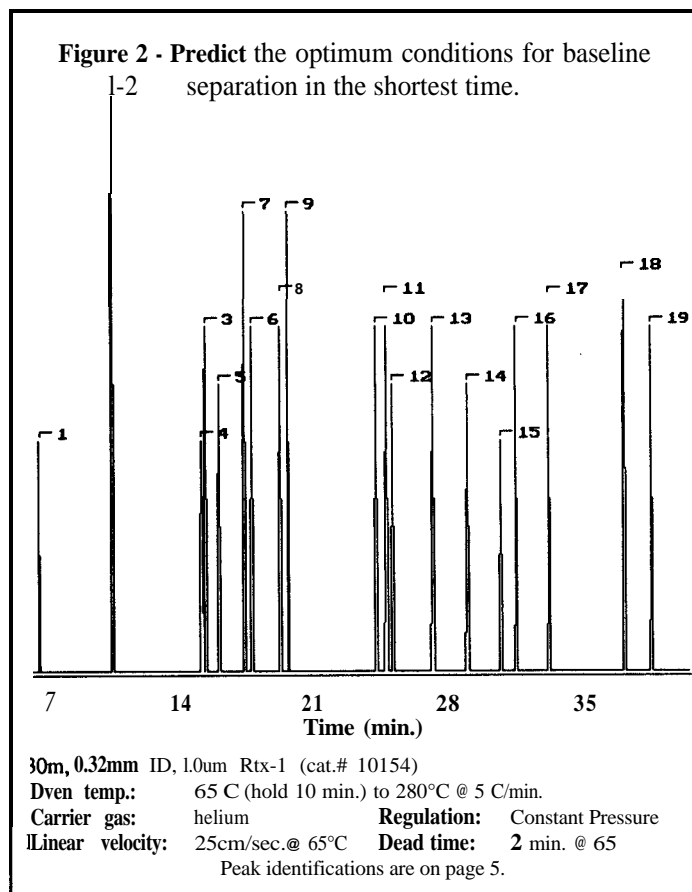


Figure 1 shows the screen used to input the retention time data. The first scenario we will investigate is where a particular column is already installed and the chromatographer wants to determine the conditions that will separate all components with the shortest analysis time. The ezGC software can be set to automatically evaluate different temperature programs and print a solution list. The solution list is prioritized according

to the temperature(s) that resolve the most components in the shortest time. A resolution factor can be specified, or defaulted to a value of 1.5, which approximates baseline separation. Figure 2 illustrates the predicted chromatogram obtained for 19 flavor and fragrance compounds using a 30 meter, Rtx-1 column with a 1.0um film thickness. The program predicted a 10 minute initial hold at 65C, providing baseline resolution in under 40 minutes.



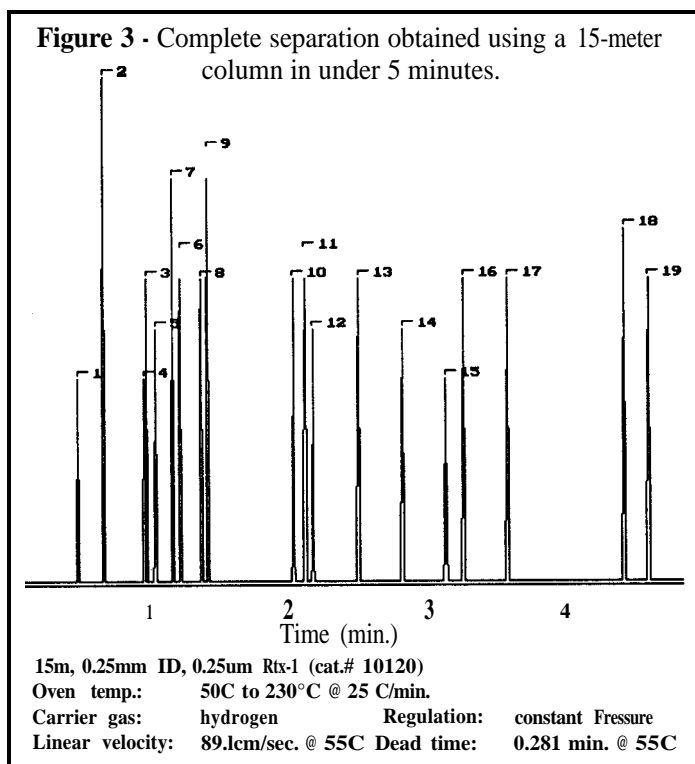
Determine how changes in column and carrier gas will improve separations

GC method development can be very costly when considering the expense of evaluating different stationary phases, column dimensions, and oven temperatures. Many chromatographers empirically optimize their chromatographic conditions for a particular column and then accept these as the "best separation" achievable. This is understandable considering the cost of buying and installing new columns. With ezGC you can determine within minutes how changes in the column and operating conditions will effect separations.(Table I). All that is needed are the retention times for your components from two temperature programs using any column which has the same stationary phase. Previously calculated indices can be retrieved either from disk or loaded from a commercial data base or library.

Table I - Parameters that can be optimized using ezGC

oven temperature and program rate (multi-ramp)
 minimum analysis time
 maximum resolution
 column length
 film thickness
 internal diameter
 carrier gas type (He, H₂, N₂, Ar)
 carrier gas flow or velocity
 constant pressure or pressure program

To illustrate how ezGC can be used to quickly determine the optimum analysis time for a particular sample, Restek's applications group optimized each of the parameters listed in Table I for the flavor and fragrance compounds shown in Figure 1. ezGC predicted that a 15meter column, 0.25mm ID, a 0.25um film thickness, in conjunction with a 25C/min. temperature program would greatly decrease the analysis time without sacrificing resolution. The new optimum analysis was obtained using a lower-cost 15-meter column with an analysis time under 5 minutes with 1/10 the analysis time and 1/2 the column length originally used (Figure 3). ezGC more than pays for itself.



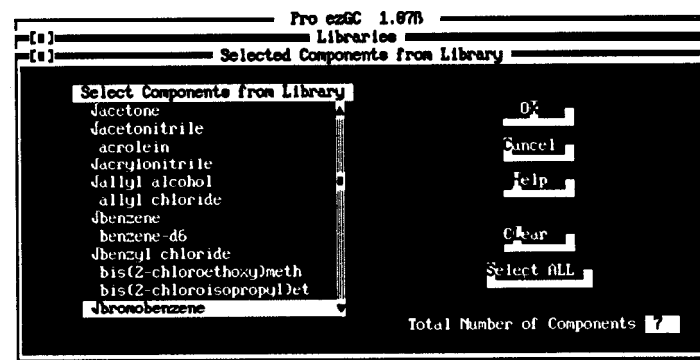
Peak Identification for Figures 2 & 3

1 ethylbutyrate	8 ~rymene	15 eugenol
2 trans-2-hexenol	9 D-limonene	16 vanillin
4 benzaldehyde	10 methone	17 ethyl vanillin
3 a-pinene	11 menthofuran	18 ethyl laurate
5 camphene.	12 menthol	19 amyl cinnamic aldehyde
7 b-pinene	13 carvone	
6 octanal	14 cinnamic alcohol	

Do method development without installing a column
 Method optimization is much faster using ezGC but is it possible to make column selection easier? Restek now offers data bases of thermodynamic retention indices called libraries, making it possible to select a column and predict chromatographic separations without even installing a column. These libraries contain hundreds of commonly analyzed components. These libraries have been generated in Restek's Applications Laboratory using the most appropriate stationary phases. Entries are added to the library after certifying each identification using GC/MS. Once the libraries are complete, it is possible to select components by simply choosing the entry from the library section of either ezGC or **Pro ezGC** Figure 4 is an example of the select menu, showing a portion of the Environmental Volatiles library. This library currently contains 138 organic components (along with surrogates and internal standards) commonly analyzed in water and solid wastes, analyzed on three different stationary phases (Rtx-502.2, Rtx-1 and Rtx-624). Furthermore, using **Pro ezGC** makes it possible for each laboratory to create their own "User" libraries, adding compounds which can be modeled along with library data supplied by Restek. Restek now offers five libraries and plans to introduce several more libraries in the upcoming months. We also have plans to continue expanding the number of compounds offered and the number of stationary phases in each library.

Almost every chromatographic method currently in use could be made more efficient by separating the components of interest in less time. The thought of spending days of additional method time and/or purchasing columns which may not give better results often keeps analysts from investigating these options. With ezGC it is possible to quickly and easily determine: "What is the best column?" and "What is the optimum temperature program and carrier flow?". The advanced features of **Pro ezGC** make GC computer modeling

Figure 4 - Select the specific components for a stationary phase to separate and then optimize your method for any column, oven temperature and carrier gas parameters.



(ezGC article is continued on page 6.)