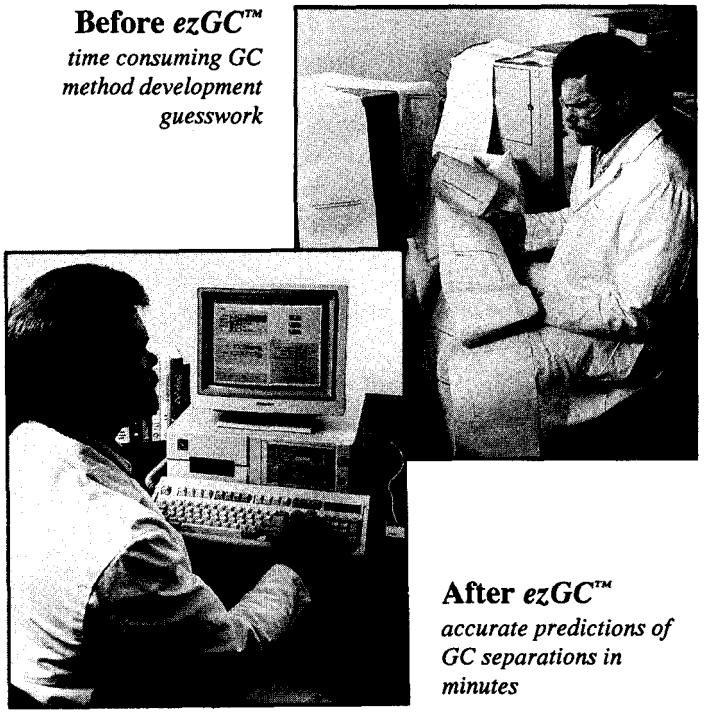
THE
# RESTEK
ADVANTAGE

## Sneak Preview! ezGC Software
### *Simplifies GC Method Development*

- Saves time and money by reducing analysis times and improving sample resolution.
- Automatically determines optimum temperature program rates and column flow rates.
- Works with constant flow, constant pressure, or electronic pressure/ flow programming.
- Visually demonstrates changes in resolution when the column parameters and operating conditions are changed.
- Easy to use, mouse driven software with built in help menus.
- Takes the guesswork out of capillary column selection.
- Easy to install and works on all DOS operating systems with 512K of free RAM.
- Costs about the same as a 30-meter column.

**Before *ezGC™***
*time consuming GC method development guesswork*



**After *ezGC™***
*accurate predictions of GC separations in minutes*

Did you ever work with a chromatographer who seems to know how to pick the best temperature program and flow conditions? After years and years of experience they seem to inherently know which GC parameters work best. They have learned how parameters such as temperature, flow, and distribution coefficients affect a separation. Why wait years? Use ezGC and quickly become a master at capillary column selection and optimization.

*In this issue...*



Even experienced chromatographers will benefit by using ezGC. Restek's applications department was hard at work trying to optimize the temperature program rate for the 60 compounds in EPA Method 502.2. They tried 4, 10, 12, and 16C/min., but there were so many compounds that new coelutions occurred at each temperature program ramp. The separations were so complex that they couldn't figure out whether faster or slower program rates were better. After several frustrating days of working on the project, they tried ezGC. They entered the retention times into the ezGC program and let the software do the optimization. ezGC predicted 7.5C/min. as the optimum temperature program rate and printed a simulated chromatogram illustrating the expected separations. They were impressed but still not convinced. Actual chromatograms were then generated at 7 and 8C/min., but only 7.5C gave the best separation, just as the program predicted. Now our applications department is so convinced of the power of ezGC that they use it for all optimization work.

You can save time and money in your laboratory by using ezGC to optimize all your analyses. If you have a simple analysis with no coelutions, you can use the software to predict the fastest temperature program and flow conditions while

maintaining baseline resolution (R2 1.5). And, if your sample contains compounds which may switch elution orders at the new optimized conditions, ezGC will list the new elution order.

Did you ever wonder how your sample would look on a different film thickness? If you are using a 0.25um film and you suspect that a 0.5um film would improve resolution, use ezGC to print a simulated chromatogram with the 0.5um film. In fact, you can try any other film thickness and ezGC will provide simulated chromatograms at optimized run conditions. How about a longer length or different inside diameter? Enter the desired column dimensions into the ezGC program and it will provide a simulated chromatogram for visual examination. Now you don't have to waste your time or money buying experimental columns to optimize your analysis, ezGC can do it for you.

How does ezGC work?

In the past 20 years, several attempts have been made to predict retention and elution in gas chromatography. Initially, elution order was predicted by Kovats indices (1). However, Kovats indices are restricted to isothermal conditions. With the increasing use of temperature programming, Kovats indices were not applicable in many situations. A modified retention index equation was developed by Van den Doo1 and Kratz2 that incorporated Kovats indices into temperature programming. This modified retention index works relatively well, as was demonstrated in *The Restek Advantage* (January 1992). However, neither the Kovats or Van den Doo1 and Kratz methods account for changes in carrier gas viscosity, linear velocity, film thickness, etc. Recently, advances have been made in developing a more sophisticated method to predict GC behavior. Several researchers, Dose3; Curvers and Rijks4; and Snow and McNairJ have contributed to a method for calculating temperature programmed or isothermal retention from thermodynamic parameters. The distribution coefficient K, is related to the Gibbs free energy of gases in solution by the following equation:

$$AG = RT \ln K_D \text{ and since } AG = AH - TAS$$

substituting $K_D = k * \beta$, the following equation can be derived:

$$\ln k = \left(\frac{\Delta H}{R}\right) * \left(\frac{1}{T}\right) + \ln\left(\frac{a}{\beta}\right)$$

where

$$a = \left(\frac{\Delta S}{R}\right)$$

This new equation is in the form of $y = mx + b$ where $\frac{\Delta H}{R}$ is the slope of the line and the quantity $\ln(a/\beta)$ is the y intercept. The ezGC software incorporates these fundamental concepts into a computer algorithm that makes it possible to accurately predict GC retention times routinely to within 2 %.

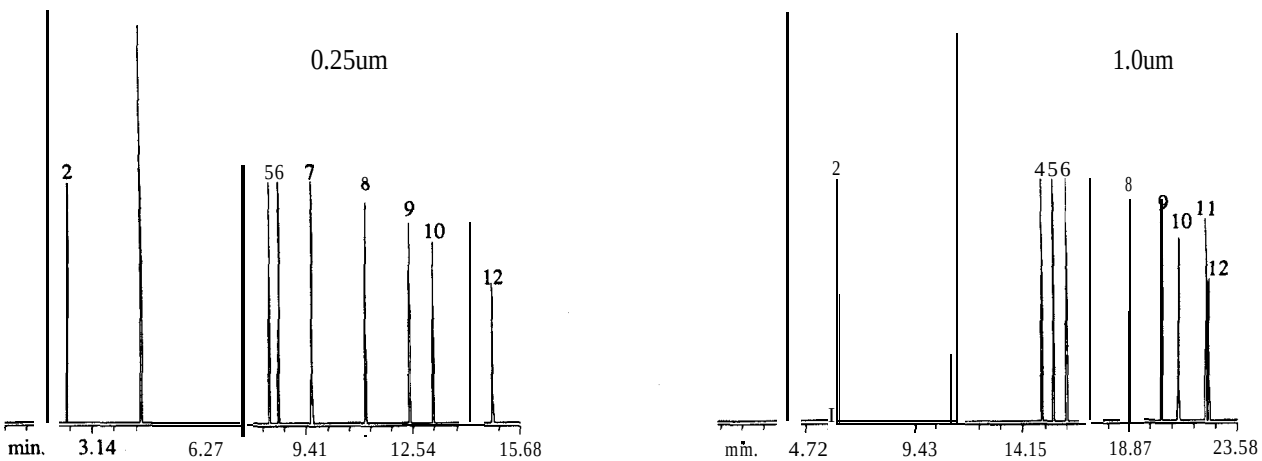
**How hard is it to use ezGC?**

By following a few simple steps, optimum operating conditions can easily be predicted for any analysis. To utilize ezGC simply obtain an accurate dead time and run your sample at fast and slow temperature program ramps. Enter the retention times for both runs in the program and you are ready to try new temperature program rates, flow rates, column IDs, film thicknesses, or column lengths. An on-line help manual is available at any time to answer questions, and in those rare cases when you need extra help, experienced Restek technical service chemists will be available to assist you with your more detailed questions.

**Ways to generate optimum conditions**

Optimum temperature programmed run conditions can be generated two ways. In one case, a specific set of GC conditions is entered and under those conditions, the ezGC program will predict the retention times of the components.

Figure **1 - ezGC** quickly predicts actual peak resolution when increasing the film thickness from 0.25 to 1.0um when using the same temperature program.




30m, 0.25mm ID Rtx-5

**Oven temp.: 35°C (hold 5 min.) @4C/min. to 280C** **Linear velocity: 43.0cm/sec @ 35C**

**Table I -** Comparison of Experimental vs. Calculated Retention Times

| # | Component Name | Exp. tR (min.) | Calc. tR (min.) | Exp. Calc. Error (min.) | /Exp. % Error (min.) |
|---|---|---|---|---|---|
| 1 | hexane | 3.891 | 3.900 | -0.009 | -0.2 |
| 2 | benzene | 6.032 | 6.117 | -0.085 | -1.4 |
| 3 | toluene | 11.001 | 11.076 | -0.075 | -0.7 |
| 4 | cblorobenzene | 15.002 | 14.991 | 0.011 | 0.1 |
| 5 | etbylbenzene | 15.500 | 15.495 | 0.005 | 0.0 |
| 6 | m-xylene | 16.184 | 16.059 | 0.125 | 0.8 |
| 7 | styrene | 17.395 | 17.129 | 0.266 | 1.5 |
| 8 | isopropylbenzene | 19.082 | 18.861 | 0.221 | 1.2 |
| 9 | n-propylbenzene | 20.5 17 | 20.345 | 0.172 | 0.8 |
| 10 | 1,3,5_trimetbylbenzene | 21.202 | 21.07 | 10.131 | 0.6 |
| 11 | tert-butylbenzene | 22.385 | 22.259 | 0.126 | 0.6 |
| 12 | decane | 22.501 | 22.364 | 0.137 | 0.6 |
| | | | | **Average error** | **0.7** |

Predicted results can be viewed in either a table format or a computer simulated chromatogram. Figure 1 shows simulated chromatograms demonstrating how the analysis would look if the stationary phase film thickness was increased from 0.25 to 1.0um with the same program conditions. The 30m, 1.0um film thickness increases the analysis times from approximately 14 to 22 minutes. Figure 2 shows the predicted optimum temperature program ramp for the 5m, 11.0um column to maximize resolution and minimize analysis times. Baseline resolution is obtained in under 6 minutes with the 5m column.

Another way to generate the optimum conditions is by entering a range of desirable temperature program conditions into the program. The optimum conditions, yielding the shortest analysis time with the best resolution, will be listed first with other possibilities listed sequentially. Computing time varies with the number of permutations requested.*

**Quickly compare differences in analysis and resolution changes when varying linear velocity, ID, film thickness, length, or theoretical plates**

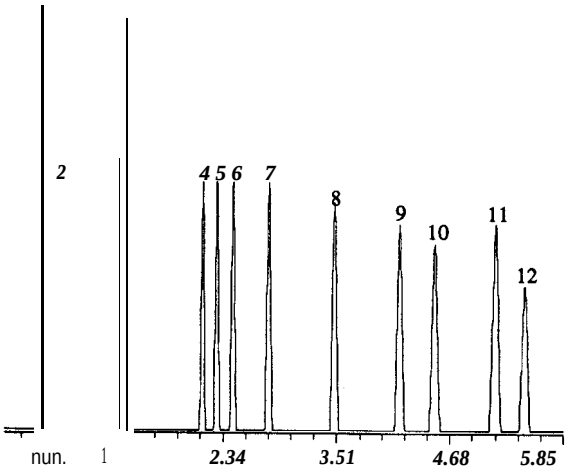
**etGC** permits a visual comparison of analysis times and resolution when column parameters such as linear velocity (including electronic pressure or flow programming), column diameter, theoretical plates, film thickness, and/or the column length are varied. Table I shows the predicted vs. actual retention times for a 1.0um Rtx-5 using data generated on a 0.25um capillary column. The absolute error is approximately 2%.

ezGC **simplifies method development**

**ezGc** greatly reduces the workload of GC method development. It also insures the best resolution and analysis time conditions for existing methods. This versatile program allows any parameter or combination of parameters to be changed and

*A 386SX-25 ***without a coprocessor was able to evaluate 350 temperature programs for I2 components in under I minute.***

**Figure 2 - ezGC** predicts the optimum resolution and fastest analysis times with a 5.0m, 1.0um column.




***5.0m, 0.25mm*** ID, 1.0um Rtx'd
**Oven temp.:** **50°C** @4C/min. to ***80C***
**Linear velocity:** **40.9cm/sec. @ 60C**

quickly viewed in either a table format or simulated chromatogram. ezGC can be installed on any IBM PC or compatible system with a hard drive and 512K of free memory.

After reading about ezGC, you may ask, "How could method development be easier?" The answer is, by having Restek generate thousands of thermodynamic retention index libraries on volatile organics, industrial solvents, pharmaceutical compounds, and flavors/fragrances using a wide variety of bonded phases. Restek has dedicated a large portion of our application chemists' time towards generating extensive libraries that interface to ezGC. See the July 1993 issue of The Restek Advantage for information on Restek's thermodynamic retention indice libraries. ■


**References**

(1) Kovats, E., Giddings, J.C., and Keller, R.A., ***Advances in Chromatography,*** Volume 1, Chapter 7. New York: Marcel Dekker (1965).
(2) Van den Dool, H. and Kratz, P.D., ***Journal of Chromatography,*** Volume 11, pp.463-471, (1963).
(3) Dose, E.V.,Anal. ***Chem.,*** 1987,59,2414-2419.
(4) Curvers, J., Rijks, J., Cramers, C., Knauss, K., Larson, P., ***HRC & CC,*** Vol. 8, Sept. 1985.
(5) Snow, N.H. and McNair, H.M., .I. ***of Chrom. Sci.,*** Vol. 30, July 1992.


# ezGC Software

(includes 5 1/4" and 3 1/2" disks)

**cat.# 21480, 21495**

**ezGC will be available for shipment in May 1993.**

ezGC" was developed jointly by Analytical Innovation, Inc. in cooperation with Restek Corporation.