Scaled Random Number Simulation of High Correlation Coefficients for Gasoline Range Compound Concentrations (unpublished preprint)

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Abstract

It has been common practice to plot gasoline range parameters as absolute concentrations within crude oils of either single compounds, sums of compound pairs, or the square root of the products of concentrations of compounds. If a sample of crude such as a condensate has a relatively high concentration of volatile components, then the concentration of all of the gasoline range components tends to be high. Conversely, heavy oil with very low concentrations of volatile compounds tends to have low concentrations of each of the compounds in the gasoline range (C_5 - C_8). By using absolute concentrations, much of the apparent correlation between and among various gasoline range compound parameters derives simply from the differential scaling through three or four orders of magnitude which results from the simple presence or absence of large amounts of the gasoline fraction within a given crude oil sample. This variance due to scaling overwhelms the variation in the concentration of these components that may be ascribed to different genetic signatures or different generation or alteration processes to which the samples may have been subjected. Statistically, this is referred to as a "spurious correlation" between parameters. It is caused by a third, possibly unknown, "lurking variable". To prevent "spurious correlation" parameters must only be considered within groups or categories of samples which are similar with respect to third or additional properties.

Introduction

In order to try to elucidate geochemical processes and relationships within, between and among crude oil and condensate samples, stochastic correlations between the absolute concentrations of individual and groups of gasoline range (C_5-C_8) compounds in crude oil samples have been used (Mango 1987, figure 1; 1990 figure 6; 1997 figures 2, 3, 4, and 10; 2000 figures 2, 3, 4, 5, 6, 10, 11, 13, 14, 15, 16, and 17; tenHaven, 1996 figures 5, 8, 10, 12, 14). These absolute concentrations range from a few parts per million to a few percent by weight of the whole oil sample, that is,

through about four orders of magnitude (equivalent to about e^{-8} to e^{2} on a natural log scale). Plots in the Mango (1987, 1997, 2000) papers were made using either natural or base 10 multi-cycle log-log plots, whereas the tenHaven (1996) figures were made on a linear scale ranging from zero to a few percent with a large proportion of the data points falling close to the origin. In contrast to the above noted publications, Mango (1994, figure 1) cross plotted sums of C_7 compounds from a more restricted data set on a linear scale (about 0.1 to about 0.9 weight percent) and demonstrated two linear correlations with very different slopes.

Another publication (Mango, 2000) shows "correlations [that] are the strongest yet disclosed for the [light hydrocarbons]" by using the square root of the product of the absolute concentration of a compound times the sum of the concentrations of two other compounds versus a similar mathematical construction for a set of homologous compounds with one additional carbon atom. It is the "strength" of the correlation that has been used, in part, to draw inferences regarding a causal relationship through chemical and geological processes inferred to have given rise to the observed compound distributions.

"Spurious correlations" (Perles and Sullivan, 1969, p317; Simon, 1954) are statistical phenomena in which two parameters have a high level of correlation that is primarily due to one or more "other" variables (also called "lurking variables"). These "other controlling variables" may be identifiable and thus easily compensated by restricting the correlation of interest to narrow categories of samples in which the "other" variable is held constant. It is also quite possible that the "other" variables cannot be easily identified. Examples of "spurious correlations" include (1) the high correlation between the total amount of fire damage incurred at a fire and the number of firemen called out to fight that fire; (2) the time series average salary of teachers in a selected, large North American city and the price of Jamaica rum in that same city; and (3) the correlation noted in the 1988 U.S. census between the number of churches and number of violent crimes in a geographic area. In the first example, the "lurking variable" is clearly the size or value of the facility or building that is on fire, and this variable dictates both the number of fire fighters and the probable magnitude of damage. There is no causal relationship between the measured parameters that would suggest that sending fewer fire fighters to a fire would result in a reduction in the amount of damage. In fact, quite the opposite is true. If there are "lurking variables" in the other two examples, they could include inflation and population density, respectively, or they could be something rather more subtle and difficult to identify.

The purpose of this contribution is to demonstrate that the high degree of correlation between and among the concentrations of gasoline range parameters may

be largely due to a "lurking variable", namely the total amount of gasoline within the sample, and to make recommendations as to how to avoid this problem.

Method and Results

Synthetic Data: Scaled Random Numbers

Scaled random numbers are defined as sets of random numbers that have all been multiplied by a common random number or scaling factor. The distributions of these random numbers have been constrained to simulate absolute concentrations of individual gasoline range compounds within whole crude oil or condensate samples as shown by Mango (1987, 1997, 2000) and ten Haven (1996) . That is, six sets (A to F) of 1000 random numbers have been chosen with a uniform distribution (Figure 1a) within a numerical range of either three to six or three to 10. The various sets of random numbers are thus surrogates for relative concentrations of various compounds within the gasoline range of any given crude oil. These random numbers have then been compared and contrasted in various combinations similar to those published for absolute gasoline range concentrations (Mango 1987; 1997; 2000; ten Haven 1996).

For the random numbers sets selected over the range of three to six, the relative concentration of two compounds A and B (or any of the values A through F) will fall within the range of A/B = 2:1 and B/A = 2:1. That is, the amount of A varies relative to the amount of B by up to a factor of four. However, both A and B might be present in any given crude oil in concentrations ranging from a few parts per million to a few percent by weight. This range of observed concentration is accommodated by multiplying both A and B by 10^X where X is selected from a table of random numbers with normal or Gaussian distribution with a mean value of 2.3 and a standard deviation of 0.7 (Figure 1b shows two examples of two sets of random numbers with a Gaussian distribution cross plotted to allow visualization). The Gaussian scaling factors with a mean of 2.3 and standard deviation of 0.7 rarely are less than zero or greater than 4. They yield pseudo-concentrations of individual compounds that center around a few hundred parts per million with relatively fewer "data points" at the extremes. This construction provides for pairs of A and B that are similar in both magnitude and distribution to observed, absolute gasoline range compound distributions. The construction of these random number sets requires that pairs of results for any given sample do not range by more than a factor of four. Similarly, a second set of scaled random numbers has been generated with a range of three to 10 and in which the variability is allowed to be as high as a factor of 11 (A/B < 3.33 and B/A < 3.33).

All random numbers in this work have been generated in sets of 1000 numbers using the RAND() function in the spreadsheet software Microsoft Excel 97. All of the scaling factors have been extracted from a table of 100 sets of 1000 random numbers each generated using the Data Analysis function of the same software. All of the coefficients of determination (CoD = r^2) have been calculated using the Trendline function in Excel for a linear correlation with no constraint on the intercept. Figure 2 shows an example of a cross plot of 1000 values of B versus A with a variability of four and a Gaussian scaling factor. The CoD ranges from about 0.87 to 0.98 with a mean CoD of 0.93 (Table 1). The range in the coefficient of determination has been determined by tabulating the r^2 values for 120 sets of 1000 random numbers. That is, each set of 1000 random values of A and B will have a specific CoD because the numbers and scaling factors are, indeed, random. Repeating the calculation 120 times provides a statistical distribution of CoD values. If the variability between pairs of random number sets is as high as a factor of 11, then the r^2 values range from 0.70 to 0.96 with a mean CoD of 0.82 (Table 1).

Additional cross plots have been made using the sum of two scaled random numbers versus the sum of two scaled random numbers (A+B versus C+D) as well as the square root of the product of the sum of two scaled random numbers times a third scaled random number versus the same construction ($[(A+B)*C]^{1/2}$ versus $[(D+E)*F]^{1/2}$). This was done to simulate the method in which gasoline range data have been plotted (Mango, 2000) and to demonstrate the impact on the CoD when two or three random numbers are combined on each axis to construct a variable. Figures 3 and 4 are examples of cross plots of sums and square roots of products of scaled random numbers, respectively.

Table 1 shows the r^2 for sums and square roots of products of scaled random numbers for data sets in which the variability among the parameters has been limited to factors of four and 11. In each case, 160 sets of 1000 random numbers have been plotted and the observed r^2 values tabulated with the maximum, minimum and mean noted.

Real Williston Basin Data: Raw and Normalized

In addition to the scaled random number sets, real analytical data for a suite of about 175 crude oils from the Canadian Williston Basin (Obermajer et al. 1998; 1999) have also been examined in two ways (Figures 5a and 5b). Absolute quantitation of the gasoline range compounds was not available for these samples because the sample size was only semi-quantitatively controlled. Thus the best approximation of absolute compound concentrations is the raw peak areas determined by the software integrator coupled to the gas chromatograph. Figure 5a is a plot of integrator counts

(micro-volt seconds) of 2-methylhexane plus 2,3-dimethylpentane versus 3-methylhexane plus 2,4-dimethylpentane showing a CoD of 0.96 and a distribution through about 4 orders of magnitude. All of the available data have been included in Figure 5 even though some of the samples may have experienced some post generation and accumulation alteration due to water washing and/or biodegradation. Figure 5b shows the same results but with the individual peak areas normalized to the total area of the peaks eluting between iC_5 and nC_8. The overall CoD for the normalized Williston Basin data is about 0.73, but this is almost certainly not meaningful because there are at least two separate populations of data readily apparent in Figure 5b.

Discussion

The cross plots and correlations of individual and combinations of two or three scaled random numbers show high degrees of correlation (Figures 2 to 4, Table 1). Because the source of the "data" is from a random number generator, it is clear that the observed correlation is entirely a "spurious correlation" caused by a "lurking variable", namely the scaling factor. This was tested by calculating CoD for the unscaled sets of random numbers. In each case, r^2 was nearly zero. As expected, an increase in the underlying or true variability results in a decrease in the CoD of the scaled parameters (Table 1).

By plotting sums of two random numbers (A+B) versus sums of two other random numbers (C+D), the coefficient of determination shifts to higher values than those noted for correlations between two random variables (A versus B). This simply results from the fact that there is a low probability of a co-occurrence of two scaled random numbers that are close to the extreme of the allowed range of values. Thus there is a tendency to reduce the number of end member values. The result is that the average CoD for a variability of four shifts from about 0.93 for a single compound on each axis (Figure 2) to about 0.96 for the two compound case (Figure 3) and to about 0.97 for the three compound case (Figure 4, Table 1).

The results for the Williston Basin oils (Figures 5a and 5b) demonstrate that while multi-cycle log-log plots of absolute integrator counts yield very high CoD values, they tend to mask the real information content within a data set. Figure 5b clearly shows two separate groups of samples with different slopes indicating that the concentrations of the four compounds are controlled by one or more processes that are fundamentally different for those two groups. Thus the apparent relationship shown in Figure 5a might be taken to suggest that there is a single, universal process linking the various compounds used in the cross plot, whereas, Figure 5b indicates that the situation is more complex and the two trends could be taken to indicate that there are at least two processes active. It must be noted that both the relative quantities and the

slope or rate of change of one variable with respect to the other are different. For this particular data set, the two groups of data points in Figure 5b correspond with oils interpreted as belonging to different genetic families on the basis of other geochemical parameters (Obermajer et al. 1998; 1999). That is, the two processes might be considered as the biosynthesis of two different types of organic matter followed by catagenetic breakdown via different routes. Figure 5b indicates that differences occur among the oils in the basin and those differences may be related to source rock characteristics which, in turn, control the processes by which the gasoline range products are ultimately derived.

As with all statistical correlations, it is very important to be aware that a co-variance between any pairs of measured parameters does not imply that there is any causal relationship between the parameters (Perles and Sullivan, 1969, p316). Much, if not all, of the strong correlation between and among gasoline range compound concentrations is apparently due to a "lurking variable" and thus it is doubly important to avoid inferring any causal relationships. Even when measures are taken to compensate for one or more known "lurking variables", the residual correlation or correlations still do not necessarily imply any causal relationship.

In the case of gasoline range compounds, it would seem to be essential to avoid "spurious correlations" by either (1) using normalized rather than absolute compound concentrations or (2) by considering groups of crude oil samples in categories that have similar amounts of gasoline range compounds. Taking this first step still does not preclude the existence of influence or control by additional "lurking variables" that have not yet been identified, but should at the very least provide an opportunity to extract information from the data that would otherwise be lost. The example shown in Figure 5a and 5b suggests that normalizing the data to the total gasoline range content provides at least two groups of oils in which there *may* be two separate links among the compounds that are cross plotted. The multi-cycle log-log plot compresses what are apparently real differences to the point that the chemical distinction between the groups would be missed.

Conclusions

A series of scaled random numbers along with real gasoline range data from the Williston Basin (Obermajer et al., 1998; 1999) provide examples of the statistical impact of using absolute concentrations ranging over four orders of magnitude as opposed to normalized amounts of the gasoline range (C_5 - C_8) compounds. Highly variable concentrations of gasoline within a whole crude oil comprise a "lurking variable" giving rise to "spurious correlations" when gasoline range compounds are investigated using multi-cycle log-log plots of absolute concentrations. The results suggest that most of the potentially revealing genetic information contained in the data are lost by using absolute rather than normalized data.

Coefficients of determination (r^2) for correlations of scaled random numbers increase as the number of compounds used to construct the parameters used on each axis is increased. This result derives from the low probability of the coincidence of extreme values for any given set of numbers. It is not immediately clear to what extent the increase in r^2 as a function of the number of compounds used in real data sets can be attributed to a similar phenomenon in which at least some of the variability may be due to simple sampling or analytical errors.

Acknowledgments

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Tables

Table 1. Table of Coefficients of Determination (r^2) for scaled random numbers versus scaled random numbers: A versus B; A+B versus C+D; and $\sqrt{(A*(B+C))}$ versus $\sqrt{(D*(E+F))}$ with variability factors of four and 11.

	variability factor	**4**	**11**
Single variable	r^2 maximum	.98	.96
	r^2 mean	**.93**	**.82**
	r^2 minimum	.87	.70
Sum of variables			
	r^2 maximum	0.98	0.97
	r^2 mean	**0.96**	**0.90**
	r^2 minimum	0.92	0.77
Square root (product)			
	r^2 maximum	0.98	0.97
	r^2 mean	**0.97**	**0.92**
	r^2 minimum	0.94	0.79

Figure Captions

Figure 1.   Cross plots of examples of two sets of 1000 random numbers with (a) uniform distributions ranging between 3 and 10, and (b) Gaussian distributions with a mean of 2.3 and a standard deviation of 0.7.

Figure 2.   Cross plot of A versus B where A and B are sets of 1000 Scaled Random Numbers in which the variability of A relative to B is a factor of 4 and a Gaussian Scaling factor (mean = 2.3, standard deviation = 0.7) has been applied.

Figure 3.   Cross plot of (A+B) versus (C+D) where A, B, C, and C are sets of 1000 Scaled Random Numbers. See Figure 2 and text for construction.

Figure 4. Cross plot of square roots of products of Scaled Random Numbers.   See Figure 2 and text for construction.

Figure 5. Cross plots of gasoline range data for 2,3-dimethylpentane plus 2-methylhexane versus 2,4-dimethylpentane plus 3-methylhexane for about 175 Canadian Williston Basin oils: (a) raw integrator counts and (b) area percent normalized to the gasoline range (C_5-C_8).

Figure 1. Cross plots of examples of two sets of 1000 random numbers with (a) uniform distributions ranging between 3 and 10, and (b) Gaussian distributions with a mean of 2.3 and a standard deviation of 0.7.
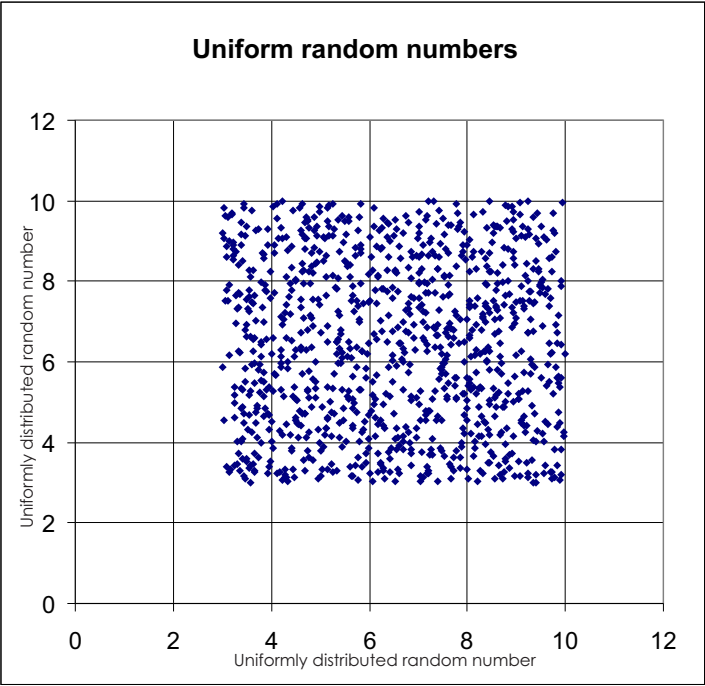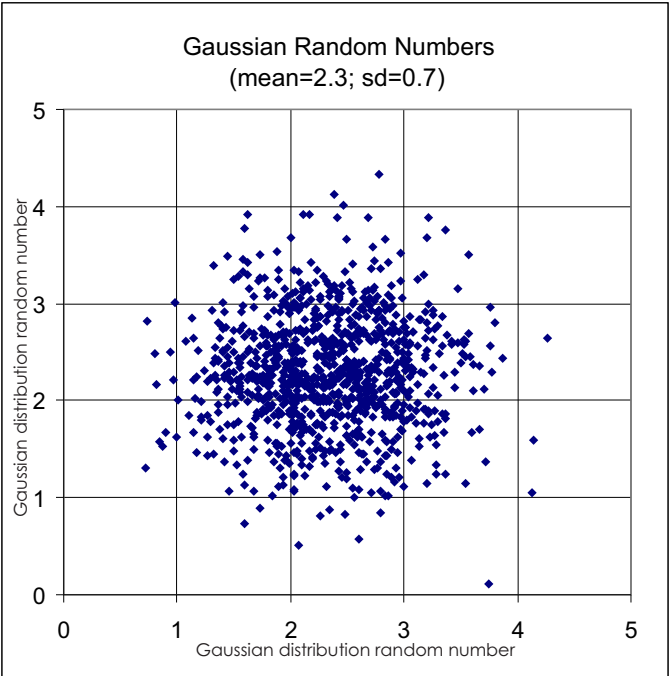

Figure 1a

Figure 1b

Figure 2. Cross plot of A versus B where A and B are sets of 1000 Scaled Random Numbers in which the variability of A relative to B is a factor of 4 and a Gaussian Scaling factor (mean = 2.3, standard deviation = 0.7) has been applied.

Scaled Random Numbers
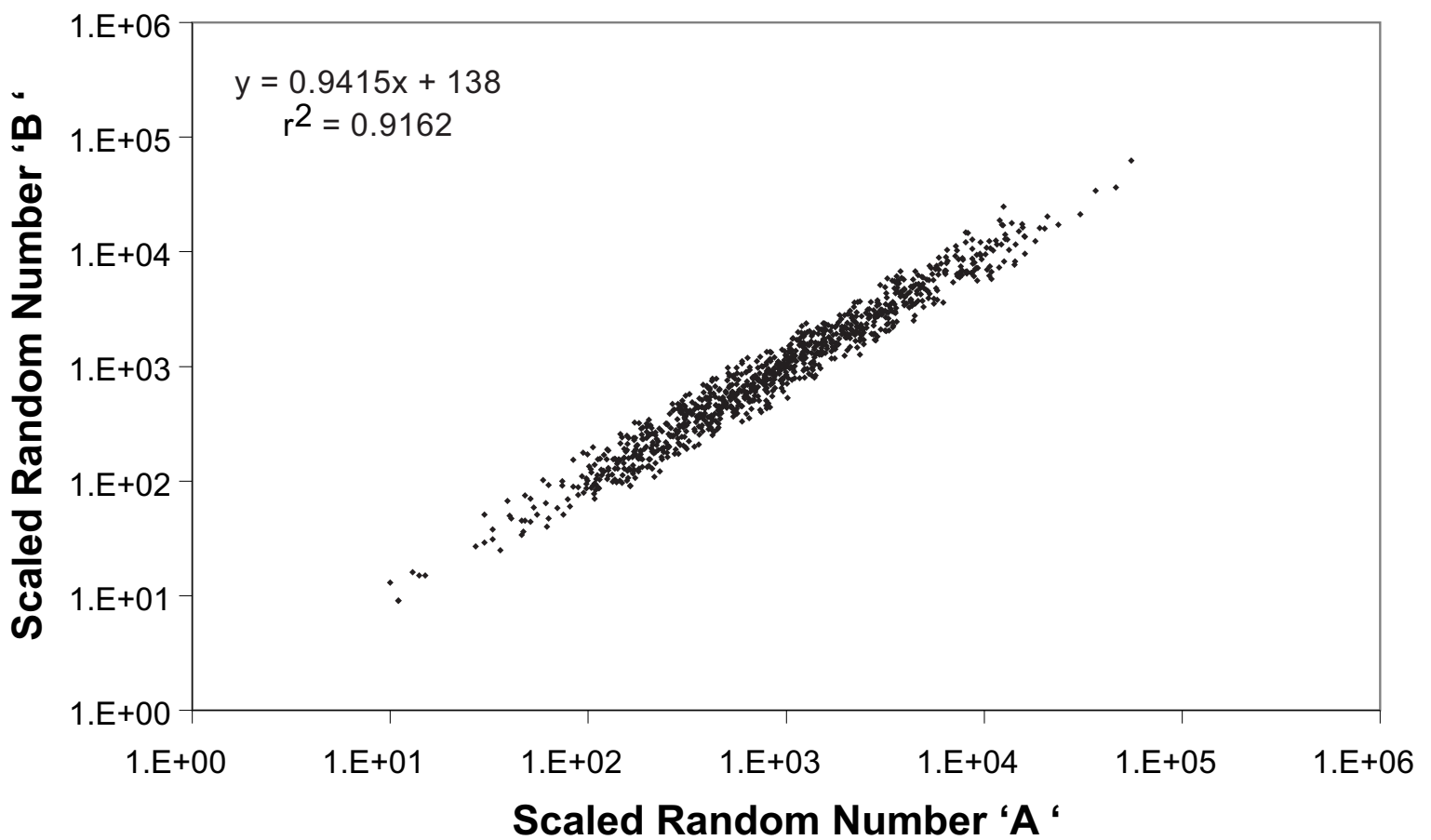
$y = 0.9415x + 138$

$r^2 = 0.9162$

Figure 2

Figure 3. Cross plot of (A+B) versus (C+D) where A, B, C, and C are sets of 1000 Scaled Random Numbers. See Figure 2 and text for construction.
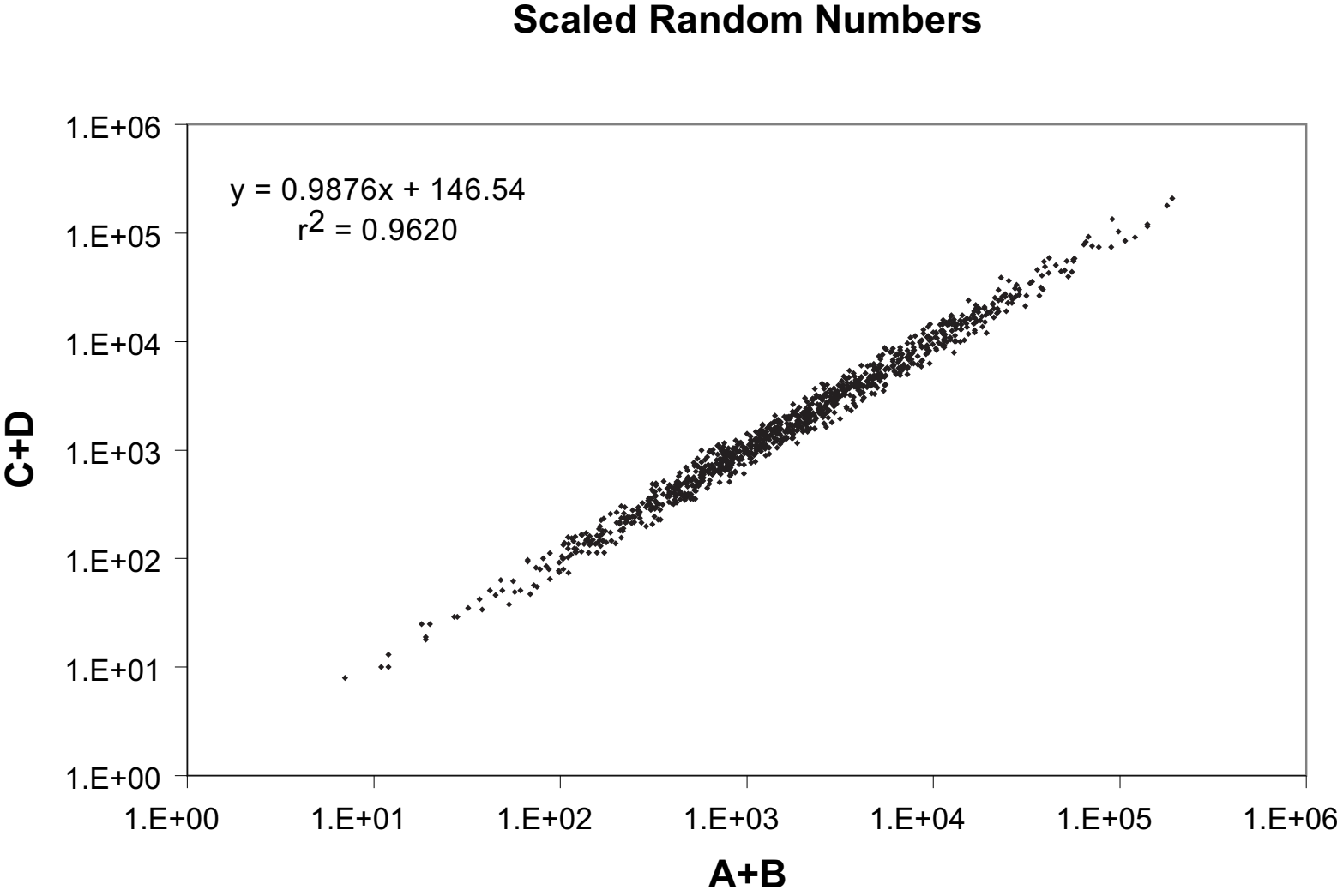
Scaled Random Numbers

$y = 0.9876x + 146.54$

$r^2 = 0.9620$

Figure 3

Figure 4. Cross plot of square roots of products of Scaled Random Numbers. See Figure 2 and text for construction.

Scaled Random Numbers

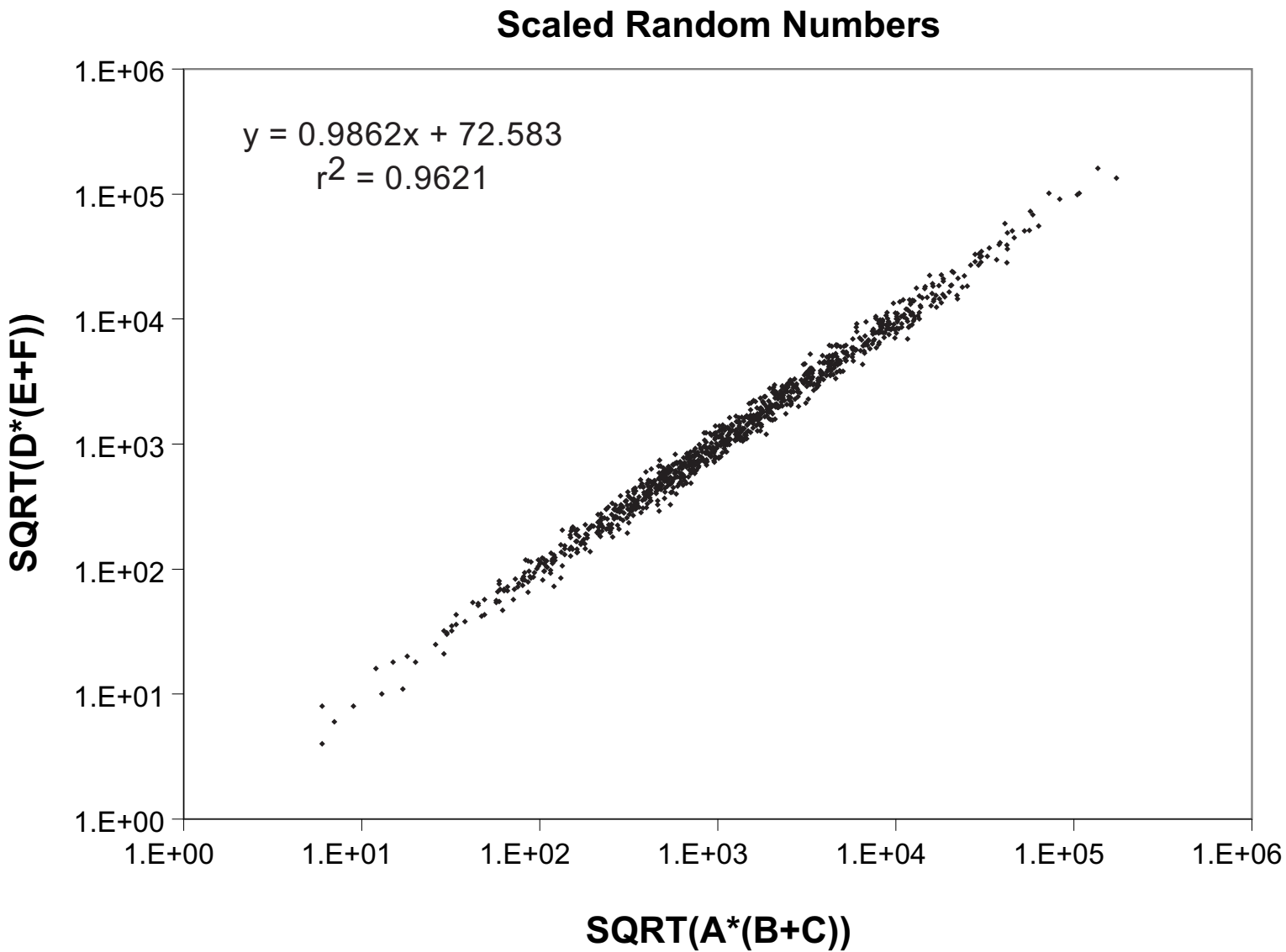$y = 0.9862x + 72.583$

$r^2 = 0.9621$

Figure 4

Figure 5. Cross plots of gasoline range data for 2,3-dimethylpentane plus 2-methylhexane versus 2,4-dimethylpentane plus 3-methylhexane for about 175 Canadian Williston Basin oils: (a) raw integrator counts and (b) area percent normalized to the gasoline range (C_5-C_8).

Williston Basin Oils
(absolute FID response)

Figure 5a

$y = 0.9208x + 11976$
$r^2 = 0.9597$

Williston Basin Oils
(normalized FID response)

Figure 5b

$y = 0.8034x + 0.7575$
$r^2 = 0.7308$