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Unified system for the prediction of retention data in gas–liquid chromatography

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Abstract

A unified system of calculating retention data in advance (data of more than 400 stationary phases between 60–130 [°C] column temperature) has been worked out based on research work of more than four decades and on the results of hundreds of researchers and research teams. The system is suitable for multiplication of horizontal (from a given stationary phase calculating from one column temperature [T1] to another [T2]) and vertical (on standard column temperature from one stationary phase to another) counting between isothermal circumstances without any limitation. The system can be used in programmed gas–liquid chromatography including double (carrier gas and column temperature and/or special vaporizater) programming. We present a system software with a protocol and some tables to help in its use. Zerolane (hypothetical stationary phase), squalane and OV-101 stationary phases are used as the fundamental stationary phases for precalculation. © 1998 Elsevier Science B.V.

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1. Introduction

The importance of calculation and counting of retention data in advance is well-known. Some aspects of the topic have already been mentioned by James and Martin who invented this method [1].

This method got widespread use and more and more researchers and teams worked on the calculation of retention data in advance [2]. Most of these works can be found in three reviews [3–5] and in a monograph [6]. Related to these observations we paid attention [7,8] to the importance of these methods (Rohrschneider conception [9], McReynolds system [10], etc.).

It should be noted that a specific utilization of

theoretical and practical results of solubility parameters according to Kersten and Poole [11], Pomaville and coworkers [12,13], Sanchez et al. [14], Abraham et al. [15,16], Li et al. [17,18] and Laffort et al. [19,20] are also important sources of the precalculation of retention data in gas–liquid chromatography (GLC) including the retention index system [21].

Thanks to these works and researches, specialists paid more attention to this field and a vivid debate resulted [22,23] leading to a lot of development in the increment method [24–26] and perfection of it by introduction of the double environmental factor [27].

Summing up the results and the experiences of the last 45 years in this field we decided to base our paper on the Rohrschneider conception and on the

McReynolds system, also agreeing the theoretical importance of the methods which used solubility parameters. Our decision is based on the knowledge of the dependence of retention index on column temperature, on the easy usage of relationships by computer [3] and the direct availability of the Tekler equation [28] and Tekler's modified equation by Santiuste [29].

Zerolane [36] (hypothetical stationary phase), squalane and OV-101 stationary phases are used as fundamental stationary phases for precalculation.

The retention index system gives some extras to the library resulting from the gas chromatography (GC)–mass spectrometry system perspective.

2. Theory

The first step in the elaboration of the system was based on the usage of the quotient equation with the Rohrschneider conception [9] which is based on the first five McReynolds [10] standards: benzene (1), *n*-butanol (2), 2-pentanone (3), 1-nitropropane (4) and pyridine (5):

$$I_{x,Tc}^{\text{st.ph.}}/I_{x,Tc}^{\text{OV-101}} = \sum_{i=1}^5 (I_i^{\text{st.ph.}}/I_i^{\text{OV-101}})_{Tc} \cdot s_i \quad (1)$$

where: I = isotherm retention index according to Kováts [30] [dimensionless]; x = symbol of substance examined; st.ph. = symbol of stationary phase used; T_c = column temperature [°C]; i = serial number of i^{th} McReynolds standard from the first five ones; $s_i = i^{\text{th}}$ substance specific factor of the compound examined [31] [dimensionless].

It is obvious from the first equation that we must get to know each data of the retention index of the first five McReynolds standard substances used at every column temperature in the interval of column temperature system (between 60–130 [°C]) when we want to count the retention data in advance.

Previously we declared that the substance specific factors (s_i values) do not depend on the stationary phase used and the column temperature [31]. Poole demonstrated [32] that the substance-specific factors (s_i values) depend theoretically on individual interactions of the substance examined and standard compound used on squalane stationary phase as follows:

$$f_i = I^{\text{SQ}}(i)/I^{\text{SQ}}(x) = [I_M(i)/I_M(x)][\pi(i)/\pi(x)] \quad (2)$$

where: f_i = quotient of interaction values of i^{th} standard compound and the substance examined; π = individual interaction value and I_M is molecular index contribution [33].

Since the two retention indices in Eq. (2) depend on column temperature and the quality of the substance studied, f_i depends theoretically on column temperature and the quality of the substance studied, so the substance specific factors depend theoretically on column temperature and the quality of the substance studied. Fortunately, in practice, we can omit the results of these effects but they cause the difference between the theoretical and the measured values in the sum of substance specific factors and so the 0.1–0.5% errors of the precalculation of retention data.

Data calculation of substance specific factors (s_i values) will be mentioned in Section 3.

Because the connection between retention index and the stationary phase used can be obvious from the definition equation of the retention polarity [33], we are able to make up the following:

$$I_{i,Tc}^{\text{st.ph.}} = \frac{a_{i,1} + a_{i,2} RP^{\text{st.ph.}}(120.0 [\text{°C}])}{1 + a_{i,3} RP^{\text{st.ph.}}(120.0 [\text{°C}])} \quad (3)$$

where: RP = retention polarity [33] [dimensionless] and $a_{i,1}$, $a_{i,2}$, $a_{i,3}$ are constants of Eq. (3). Retention polarity can be counted on the ΔI values of the first five McReynolds standards as follows:

$$RP^{\text{st.ph.}}(T_c) = 20 \sum_{i=1}^5 (\Delta I_i / I_i^{\text{Squalane}})_{T_c} \quad (4)$$

where: RP = retention polarity [dimensionless] at T_c isotherm column temperature

$$\Delta I_i = I_i^{\text{st.ph.}} - I_i^{\text{Squalane}} \quad (5)$$

Retention polarity depends on the column temperature since the retention indices depend on column temperature. If we are in need of other retention polarity data of other column temperatures, we can count them in the following way:

$$RP^{\text{st.ph.}}(T_c) = \frac{A_{RP} + B_{RP} T_c}{1 + C_{RP} T_c} \quad (6)$$

where: A_{RP} , B_{RP} and C_{RP} are constants of Eq. (6).

It should be noted that Santiuste [34] presented very good results for retention polarity at different column temperatures on various stationary phases.

In the following we recognised that the constants of McReynolds standard substances in Eq. (3) depend on the column temperature as follows:

$$a_{i,j} = A_{i,j} + \frac{B_{i,j}}{T_c + C_{i,j}} \quad (7)$$

where j is the serial number of constants ($j=1, 2$ and 3 , respectively) and $A_{i,j}$, $B_{i,j}$ and $C_{i,j}$ are constants of Eq. (7). Putting the data of Eq. (7) into Eq. (3), we can see the following:

$$I_{i,T_c}^{\text{st.ph.}} = \frac{A_{i,1} + \frac{B_{i,1}}{T_c + C_{i,1}} + \left(A_{i,2} + \frac{B_{i,2}}{T_c + C_{i,2}} \right) RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])}{1 + \left(A_{i,3} + \frac{B_{i,3}}{T_c + C_{i,3}} \right) RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])} \quad (8)$$

The system standardised onto the required column temperature is ready to count retention index and other GLC parameters in advance, but calculation of other data (specific retention volume, activity coefficient, etc.) can be done only by introducing extra equations. There are some of these in Eqs. (9)–(19) as follows:

$$\ln [Q]^{\text{st.ph.}}(T_c) = \frac{C_{Q,1} + C_{Q,2} RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])}{1 + C_{Q,3} RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])} \quad (9)$$

where: $\ln[Q]$ = the logarithm naturale of relative volatility of two consecutive n -alkanes [dimensionless] and $C_{Q,1}$, $C_{Q,2}$ and $C_{Q,3}$ are constants of Eq. (9). In the following we recognised that the constants of Eq. (9) depend on the column temperature as follows:

$$C_{Q,i} = A_j + \frac{B_j}{T_c + C_j} \quad (10)$$

where j is serial number of constants ($j=1, 2$ and 3 respectively) and A_j , B_j and C_j are constants of Eq. (10). Similarly:

$$K_c^{\text{st.ph.}}(T_c) = \frac{K_{1,j} + K_{2,j} RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])}{1 + K_{3,j} RP^{\text{st.ph.}}(120.0 [^\circ\text{C}])} \quad (11)$$

where: K_c = Kováts coefficient [$-\ln(\text{cm}^3/\text{g})$] [35] and $K_{1,j}$, $K_{2,j}$ and $K_{3,j}$ are constants of Eq. (11). Moreover we recognised the dependence of the constants in Eq. (11) on column temperature:

$$K_{i,j} = A_{i,j}^* + \frac{B_{i,j}^*}{T_c + C_{i,j}^*} \quad (12)$$

where: j = serial number of constants ($j=1, 2$ and 3 , respectively) and $A_{i,j}^*$, $B_{i,j}^*$ and $C_{i,j}^*$ are constants of Eq. (12). We must mention that the value of $K_c^{\text{Apolane-87}}(T_c)$, that is the retention polarity (at $120.0 [^\circ\text{C}]$) equals to 2.30 , was counted by substitution. We used these data in the McReynolds polarity calculation [35]:

$$MP(T_c)^{\text{st.ph.}} = 2[K_c^{\text{st.ph.}}(T_c)/K_c^{\text{Apolane-87}}(T_c)] - 1 \quad (13)$$

where: MP = the McReynolds polarity [dimensionless]. Calculations of the retention polarity data at $120.0 [^\circ\text{C}]$ of some stationary phases is given in Table 1. With the assistance of the $\ln(Q)$ value, the specific retention volume of n -octane can be counted with Kováts coefficient definition equation [35] as follows:

$$V_g\{[n\text{C}_8](T_c)\} = \exp\{[0.08 - 0.01K_c(T_c)] \ln [Q(T_c)]\} \quad (14)$$

where: V_g = the specific retention volume [cm^3/g] and $n\text{C}_8$ = symbol of n -octane. Thus we can calculate the data of all n -alkanes, since:

$$\ln [Q]^{\text{st.ph.}}(T_c) = \ln [V_g\{z+1\}(T_c)] - \ln [V_g\{z\}(T_c)] \quad (15)$$

where: z is the carbon(atom) number of the first eluted n -alkane used. On returning to the definition equation of retention index according to Kováts [30], we can write [35]:

$$\begin{aligned} S_c^{\text{st.ph.}}(T_c) &= I^{\text{st.ph.}}(T_c) - K_c^{\text{st.ph.}}(T_c) \\ &= 100\{\ln [V_g^{\text{st.ph.}}(T_c)] / \ln [Q]^{\text{st.ph.}}(T_c)\} \end{aligned} \quad (16)$$

where S_c is the molecular structural coefficient [35] [$\ln(\text{cm}^3/\text{g})$].

Table 1
Retention polarity of some stationary phases at 120.0 (°C)

Stationary phase	RP^a
<i>n</i> -Hexadecane	0.35
Nujol	0.50
C78 [46]	1.10
Apiezon-L (2127)	4.83
Apiezon-L (TREATED)	4.49
Apiezon-L (2012)	5.11
DC-330	6.37
Apiezon-J	6.60
SF-96	6.44
Apiezon-N	6.73
SE-30	6.96
TFPS-00 [43,49]	7.00
OV-1	7.10
PCN-C78 [44]	7.17
OV-101	7.30
SE-52	10.94
SE-54	11.05
OV-3	13.80
Dinonyl sebacate	17.50
OV-7	18.00
TFPS-15 [43,49]	18.30
DC-550	19.10
DINA	19.20
DEG stearate	20.00
Diisodecyl phthalate	21.50
DC-703	22.23
Dinonyl phthalate	22.90
TFPS-26 [43,49]	29.10
UCON-LB-550-X	29.30
UCON-LB-1800	29.90
PPG-2000	32.10
Acetyl- <i>n</i> -tributylcitrate	34.25
TFPS-35 [43,49]	34.80
OV-25	37.60
QF-1	45.99
PPG sebacate	46.63
TFPS-50	49.80
OV-225	55.70
NPGS	69.80
PEG-20M	69.90
PEG-6000	70.45
PEG-4000	71.70
FFAP	75.86
PEG-600	80.40
Reoplex-400	81.70
PDEAS	89.20
DEGS	109.90
EG-bis-cyanoethyl ether	116.70
EGS	122.50
TCEP	132.35
BCEF	145.34

^a In calculating we did limit the number of decimal figures.

Using the molecular structural coefficient, the McReynolds standard specific factor can be counted as follows:

$$MF^{st.ph.}(Tc) = S_{c,i}^{st.ph.}(Tc) / S_{c,i}(Tc)^{Zerolane} \quad (17)$$

where: MF = the McReynolds standard specific polarity factor [dimensionless] and Zerolane = an absolute apolar hypothetical stationary phase [36,37].

The average standard specific polarity factor can be counted with the help of the following equation:

$$APF^{st.ph.}(Tc) = (1/5) \sum_{i=1}^5 MF_i^{st.ph.}(Tc) \quad (18)$$

where: APF = average standard specific polarity factor [dimensionless]

Finally, data describing the real polarity circumstances, the effective polarity, in the best way can be counted according to the following equation:

$$P_e^{st.ph.}(Tc) = 10MP^{st.ph.}(Tc)[MF^{st.ph.}(Tc) - 1] \quad (19)$$

where P_e is the effective polarity of the stationary phase used [dimensionless]. System data of the most important constants in Section 3 including other relationships are listed in Tables 2 and 8.

3. Practice

The practical part is based on the software of the system shown in Table 2. As you can see in Table 2, the system software wants the name of the compound examined as first input data asking the number of the stationary phases to be considered. It is followed by the name of the first stationary phase, its retention polarity at 120.0 [°C] (Table 1) and isotherm column temperature [°C]. After these the program calculates the constants of the equation, the values of the retention index of the first five McReynolds standards and the wanted parameters of them on three base stationary phases either (squalane, Zerolane and OV-101 with 7.17 retention polarity value). Then the program calculates retention index values of the first five McReynolds standards in the given GC circumstances including other important parameters. The calculation process ends with the calculation of differences of guessed value of the retention index and the measured and

Table 2
System software

```

10 REM "THE GREATEST SYSTEM OF PRECALCULATION IN GLC BETWEEN 60–130 [C]"
20 DIM I(3,5),SC(3,5),VG(3,5),LG(3,5),PS(3,5),DI(3,5),S(3,5),DZ(3,5)
30 CLS
40 PRINT SPC(10) "THE GREATEST SYSTEM OF PRECALCULATION IN GLC BETWEEN 60–130 [C]"
50 INPUT "TYPE OF COLUMN APPLIED (COATED=1;DIFFERENT=0)";CT
60 INPUT "DATE(in quotation marks MONTH—DAY—YEAR)=";DAS
70 LPRINT SPC(5) "THE GREATEST SYSTEM OF PRECALCULATION IN GLC BETWEEN 60–130 [C] ";DAS
80 FOR W=1 TO 80:LPRINT"*";NEXT W
90 PRINT SPC(5) "PARAMETERS of COLUMN USED"
100 INPUT "No. and/or sign of COLUMN (in quotation marks)";NUS
110 INPUT "COLUMN LENGHT,[cm]=";L
120 INPUT "COLUMN I.D.[cm]=";D
130 INPUT "BETA of COLUMN=";BE
140 INPUT "df of COLUMN[cm]=";DF
150 INPUT "QUANTITY of STATIONARY PHASE USED in the COLUMN APPLIED[g]=";MS
160 INPUT "NAME of COMPOUND EXAMINED (in quotation marks)";NS
170 INPUT "NUMBER OF STATIONARY PHASES EXAMINED";N
180 INPUT "COLUMN TEMPERATURE,[C.]=";TC
190 T=273.16+TC
200 RT=T*62362.7
210 LPRINT SPC(20) " TC,[C.]=";TC;"T=";T;"[K.]"
220 LPRINT SPC(15) "PARAMETERS of COLUMN USED"
230 LPRINT SPC(5) NUS;"L=";L;"[cm],I.D.=";D;"[cm],ms=";MS;"[g]"
240 LPRINT SPC(5) "df=";DF;"[cm],BETA=";BE
250 FOR W=1 TO 80:LPRINT"*";NEXT W
260 PRINT SPC(2) "CALCULATIONS OF CONSTANTS"
270 GOSUB 1250
280 KA=AK+(BK/(2.3+CC))
290 ST$(1)="ZEROLANE":PR(1)=-20.83
300 ST$(2)="SQUALANE":PR(2)=0
310 ST$(3)="OV-101":PR(3)=7.17
320 GOSUB 1850
330 FOR E=1 TO N
340 PRINT SPC(5)E
350 INPUT "ST.PH.=";ST$
360 INPUT "RP OF ST..PH. at 120.0[C]=";PR
370 INPUT "RETENTION INDEX MEASURED;IF YOU HAVEN'T THEN INPUT:0)=";MI
380 INPUT "RETENTION INDEX DIFFERENCE MEASURED (IF YOU HAVEN'T THEN INPUT:0)=";XX
390 PRINT SPC(2) "CALCULATIONS"
400 GOSUB 470
410 REM "PRINTING"
420 GOSUB 1550
430 GOSUB 2550
440 FOR W=1 TO 80:LPRINT"#";NEXT W
450 NEXT E
460 END
470 I1=(A11+A12*PR)/(1+A13*PR)
480 I2=(A21+A22*PR)/(1+A23*PR)
490 I3=(A31+A32*PR)/(1+A33*PR)
500 I4=(A41+A42*PR)/(1+A43*PR)

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(Cont.)

Table 2. Continued

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510 I5=(A51+A52*PR)/(1+A53*PR)
520 DD(1)=I1-IS(1)
530 DD(2)=I2-IS(2)
540 DD(3)=I3-IS(3)
550 DD(4)=I4-IS(4)
560 DD(5)=I5-IS(5)
570 KA=AK+(BK/(2.3+CC))
580 CK=AK+(BK/(PR+CC))
590 PM=(2*(CK/KA))-1
600 LQ=AQ+(BQ/(PR+CQ))
610 Q=EXP(LQ)
620 B=LQ/LOG(10)
630 R=8.31434
640 REM[R]=[J/K*MOL]
650 DG=R*T*LQ
660 L8=(8-(CK/100))*LQ
670 V8=EXP(L8)
680 S1=I1-CK
690 S2=I2-CK
700 S3=I3-CK
710 S4=I4-CK
720 S5=I5-CK
730 L1=(LQ/100)*S1
740 L2=(LQ/100)*S2
750 L3=(LQ/100)*S3
760 L4=(LQ/100)*S4
770 L5=(LQ/100)*S5
780 V1=EXP(L1)
790 V2=EXP(L2)
800 V3=EXP(L3)
810 V4=EXP(L4)
820 V5=EXP(L5)
830 RP=20*((DD(1)/IS(1))+(DD(2)/IS(2))+(DD(3)/IS(3))+(DD(4)/IS(4))+(DD(5)/IS(5)))
840 P1=S1/SC(1,1)
850 P2=S2/SC(1,2)
860 P3=S3/SC(1,3)
870 P4=S4/SC(1,4)
880 P5=S5/SC(1,5)
890 AP=(P1+P2+P3+P4+P5)/5
900 P=ABS(10*PM*(AP-1))
910 LPRINT SPC(5) ST$
920 DR=PR-RP
930 FOR W=1 TO 80:LPRINT"*";NEXT W
940 LPRINT SPC(5)"DATA OF POLARITY"
950 FOR W=1 TO 80:LPRINT"-";NEXT W
960 LPRINT SPC(5)"RP(MEAS.) at 120.0[C]=";PR;" RP(CALC.)=";RP;"DELTA RP=";DR
970 LPRINT SPC(5)"APF=";AP;"MP(C)=";PM
980 LPRINT SPC(5)"SPF1=";P1;"SPF2=";P2;"SPF3=";P3;"SPF4=";P4;"SPF5=";P5
990 LPRINT SPC(5)"EFFECTIVE POLARITY=";P
1000 FOR W=1 TO 80:LPRINT"*";NEXT W
1010 LPRINT SPC(5)"DATA OF n-ALKANES"

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Table 2. Continued

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1020 FOR W=1 TO 80:LPRINT“-”;NEXT W
1030 LPRINT SPC(5)“KC(C)=”;CK;“KC(APOLANE-87)=”;KA
1040 LPRINT SPC(5)“Vg(n-C8)=”;V8;“ln[Vg(nC8)]=”;L8;“Q=”;Q;“LQ(C)=”;LQ;“b=”;B;“DG(CH2)=”;DG;“[J/MOLE]”
1050 FOR W=1 TO 80:LPRINT“*”;NEXT W
1060 LPRINT SPC(5)“RETENTION INDICES”
1070 FOR W=1 TO 80:LPRINT“-”;NEXT W
1080 LPRINT SPC(5)“I(BENZENE)=”;I1;“I(n-BUTANOL)=”;I2;“I(2-PENTANONE)=”;I3
1090 LPRINT SPC(5)“I(1-NITROPROPANE)=”;I4;“I(PYRIDINE)=”;I5
1100 LPRINT SPC(5)“DI(BENZENE)=”;DD(1);“DI(n-BUTANOL)=”;DD(2);“DI(2-PENTANONE)=”;DD(3)
1110 LPRINT SPC(5)“DI(1-NITROPROPANE)=”;DD(4);“DI(PYRIDINE)=”;DD(5)
1120 FOR W=1 TO 80:LPRINT“*”;NEXT W
1130 LPRINT SPC(5)“RETENTION DATA”
1140 FOR W=1 TO 80:LPRINT“-”;NEXT W
1150 LPRINT SPC(5)“SC(BENZENE)=”;S1;“SC(n-BUTANOL)=”;S2;“SC(2-PENTANONE)=”;S3
1160 LPRINT SPC(5)“SC(1-NITROPROPANE)=”;S4;“SC(PYRIDINE)=”;S5
1170 FOR W=1 TO 80:LPRINT“-”;NEXT W
1180 LPRINT SPC(5)“VG(BENZENE)=”;V1;“VG(n-BUTANOL)=”;V2;“VG(2-PENTANONE)=”;V3
1190 LPRINT SPC(5)“VG(1-NITROPROPANE)=”;V4;“VG(PYRIDINE)=”;V5
1200 LPRINT SPC(5)“LG(BENZENE)=”;L1;“LG(n-BUTANOL)=”;L2;“LG(2-PENTANONE)=”;L3
1210 LPRINT SPC(5)“LG(1-NITROPROPANE)=”;L4;“LG(PYRIDINE)=”;L5
1220 FOR W=1 TO 80:LPRINT“*”;NEXT W
1230 FOR W=1 TO 80:LPRINT“*”;NEXT W
1240 RETURN
1250 REM“CALCULATIONS OF CONSTANTS”
1260 A11=1390.06313#-(1368658.6#/(TC+1735.95194#))
1270 A12=1.47345878#+(161.447847#/(TC+18.1898927#))
1280 A13=-.00413282551#+(.321027518#/(TC+24.2498456#))
1290 A21=275.437726#+(177645.18#/(TC+444.913517#))
1300 A22=-18.7228445#-(19462.3258#/(TC-861.031445#))
1310 A23=-.018387103#-(10.8224202#/(TC-692.815625#))
1320 A31=561.421254#-(13504.3319#/(TC-316.647771#))
1330 A32=22.9791448#+(16272.9574#/(TC-959.97109#))
1340 A33=-.00529014563#+(.904001794#/(TC+122.818624#))
1350 A41=813.008951#-(148747.176#/(TC+823.997937#))
1360 A42=-164.296161#-(431030.292#/(TC-2597.55827#))
1370 A43=-16.1613972#-(6470778.29#/(TC-400472.085#))
1380 A51=1195.29103#-(279997.158#/(TC+443.580041#))
1390 A52=65.1506145#-(97733.4632#/(TC+1591.28027#))
1400 A53=.0202064645#-(20.1826992#/(TC+897.312106#))
1410 AQ=2.83618+(98.623/(TC-218.674))
1420 BQ=1010.115-(5711.395/(TC-30.478))
1430 CQ=-858.442+(4245.836/(TC-31.2))
1440 AK=-7682.288+(36283853.7#/(TC+4806))
1450 BK=300481.718#+(200594658#/(TC-612.573))
1460 CC=-859.492+(959818.103#/(TC+1386.56))
1470 REM“CALCULATIONS OF RETENTION INDICES OF 1,4-DIOXANE AND FIRST 5 McREYNOLDS’ CONSTANTS ON SQUALANE”
1480 IS(0)=634.5118-(974.19302#/(TC-169.305966#))
1490 IS(1)=1385.76244#-(1352925.75#/(TC+1725.35765#))
1500 IS(2)=278.519494#+(174278.749#/(TC+439.734271#))
1510 IS(3)=562.086191#-(13220.7335#/(TC-314.318583#))
1520 IS(4)=807.608523#-(138154.861#/(TC+788.273358#))

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(Cont.)

Table 2. Continued

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1530 IS(5)=1193.83974#-(278541.673#/(TC+442.264007#))
1540 RETURN
1550 N$="1,4-DIOXANE"
1560 REM"QUOTIENT-EQUATION"
1570 X1#=.4729641304#
1580 X2#=1.125373686#
1590 X3#=-.1137505687#
1600 X4#=-.7097169762#
1610 X5#=.2250829962#
1620 X6#=679.3-(839.135/(TC-161.6))
1630 Z1=I(1,1)/I(3,1)
1640 Z2=I(1,2)/I(3,2)
1650 Z3=I(1,3)/I(3,3)
1660 Z4=I(1,4)/I(3,4)
1670 Z5=I(1,5)/I(3,5)
1680 Y1=I1/I(3,1)
1690 Y2=I2/I(3,2)
1700 Y3=I3/I(3,3)
1710 Y4=I4/I(3,4)
1720 Y5=I5/I(3,5)
1730 II=(Y1*X1#+Y2*X2#+Y3*X3#+Y4*X4#+Y5*X5#)*X6#
1740 DD(0)=II-IS(0)
1750 IM=XX+IS(0)
1760 KD=XX-DD(0)
1770 IZ=(Z1*X1#+Z2*X2#+Z3*X3#+Z4*X4#+Z5*X5#)*X6#
1780 LPRINT SPC(5)N$
1790 LPRINT SPC(5)"I(SQ)=",IS(0);"I(ZEROLANE)=",IZ;"I(M)=",IM
1800 PRINT SPC(5)"I(SQ)=",IS(0);"I(ZEROLANE)=",IZ;"I(M)=",IM
1810 LPRINT SPC(5)"I(C)=",II;"DI(M)=",XX;"DI(C)=",DD(0);"DELTA DI=";KD
1820 PRINT SPC(5)"I(C)=",II;"DI(M)=",XX;"DI(C)=",DD(0);"DELTA DI=";KD
1830 FOR W=1 TO 80:LPRINT"*";:NEXT W
1840 RETURN
1850 REM"CALCULATIONS OF FUNDAMENTAL STATIONARY PHASES"
1860 FOR J=1 TO 3
1870 FOR K=1 TO 5
1880 LQ(J)=AQ+(BQ/(PR(J)+CQ))
1890 CK(J)=AK+(BK/(PR(J)+CC))
1900 CK(1)=KA/2
1910 PM(J)=(2*(CK(J)/KA))-1
1920 Q(J)=EXP(LQ(J))
1930 B(J)=LQ(J)/LOG(10)
1940 R=8.31434
1950 REM"[R]=[J/K*MOL]"
1960 DG(J)=R*T*LQ(J)
1970 L8(J)=(8-(CK(J)/100))*LQ(J)
1980 V8(J)=EXP(L8(J))
1990 I(J,1)=(A11+A12*PR(J))/(1+A13*PR(J))
2000 I(J,2)=(A21+A22*PR(J))/(1+A23*PR(J))
2010 I(J,3)=(A31+A32*PR(J))/(1+A33*PR(J))
2020 I(J,4)=(A41+A42*PR(J))/(1+A43*PR(J))
2030 I(J,5)=(A51+A52*PR(J))/(1+A53*PR(J))

```

Table 2. Continued

```

2040 DI(J,K)=I(J,K)-IS(K)
2050 DZ(J,K)=I(J,K)-I(1,K)
2060 SC(J,K)=I(J,K)-CK(J)
2070 LG(J,K)=(LQ(J)/100)*SC(J,K)
2080 VG(J,K)=EXP(LG(J,K))
2090 PS(J,K)=SC(J,K)/SC(1,K)
2100 NEXT K
2110 AP(J)=(PS(J,1)+PS(J,2)+PS(J,3)+PS(J,4)+PS(J,5))/5
2120 P(J)=ABS(10*PM(J)*(AP(J)-1))
2130 RP(J)=20*((DI(J,1)/IS(1))+(DI(J,2)/IS(2))+(DI(J,3)/IS(3))+(DI(J,4)/IS(4))+(DI(J,5)/IS(5)))
2140 NEXT J
2150 FOR J=1 TO 3
2160 LPRINT SPC(5) ST$(J)
2170 PRINT SPC(5) ST$(J)
2180 FOR W=1 TO 80:LPRINT"*";NEXT W
2190 LPRINT SPC(5)"DATA OF POLARITY"
2200 PRINT SPC(5)"DATA OF POLARITY"
2210 FOR W=1 TO 80:LPRINT"-";NEXT W
2220 LPRINT SPC(5)"RP(120.0[C.]="";PR(J)
2230 PRINT SPC(5)"RP(120.0[C.]="";PR(J)
2240 LPRINT SPC(5)"APF="";AP(J);"MP(C)="";PM(J)
2250 LPRINT SPC(5)"PS(BENZENE)="";PS(J,1);"PS(n-BUTANOL)="";PS(J,2);"PS(2-PENTANONE)="";PS(J,3)
2260 LPRINT SPC(5)"PS(1-NITROPROPANE)="";PS(J,4);"PS(PYRIDINE)="";PS(J,5)
2270 LPRINT SPC(5)"EFFECTIVE POLARITY ="";P(J)
2280 FOR W=1 TO 80:LPRINT"*";NEXT W
2290 LPRINT SPC(5) "DATA OF n-ALKANES"
2300 FOR W=1 TO 80:LPRINT"-";NEXT W
2310 LPRINT SPC(5)"KC(C)="";CK(J);"KC(APOLANE-87)="";KA
2320 LPRINT SPC(5)"Vg(n-C8)="";V8(J);"ln[Vg(nC8)]="";L8(J);"Q="";Q(J);"
LQ(C)="";LQ(J);"b="";B(J);"DG(CH2)="";DG(J);"[J/MOLE]"
2330 FOR W=1 TO 80:LPRINT"*";NEXT W
2340 LPRINT SPC(5)"RETENTION INDICES"
2350 FOR W=1 TO 80:LPRINT"-";NEXT W
2360 LPRINT SPC(5)"I(BENZENE)="";I(J,1);"I(n-BUTANOL)="";I(J,2);"I(2-
PENTANONE)="";I(J,3)
2370 LPRINT SPC(5)"I(1-NITROPROPANE)="";I(J,4);"I(PYRIDINE)="";I(J,5)
2380 LPRINT SPC(5)"BASE SQ:DI(BENZENE)="";DI(J,1);"DI(n-BUTANOL)="";DI(J,2);"
DI(2-PENTANONE)="";DI(J,3)
2390 LPRINT SPC(5)"DI(1-NITROPROPANE)="";DI(J,4);"DI(PYRIDINE)="";DI(J,5)
2400 LPRINT SPC(5)"BASE ZEROLANE:DI(BENZENE)="";DZ(J,1);"DI(n-
BUTANOL)="";DZ(J,2);"DI(2-PENTANONE)="";DZ(J,3)
2410 LPRINT SPC(5)"DI(1-NITROPROPANE)="";DI(J,4);"DI(PYRIDINE)="";DZ(J,5)
2420 FOR W=1 TO 80:LPRINT"*";NEXT W
2430 LPRINT SPC(5)"RETENTION DATA"
2440 FOR W=1 TO 80:LPRINT"-";NEXT W
2450 LPRINT SPC(5)"SC(BENZENE)="";SC(J,1);"SC(n-BUTANOL)="";SC(J,2);"SC(2-
PENTANONE)="";SC(J,3)
2460 LPRINT SPC(5)"SC(1-NITROPROPANE)="";SC(J,4);"SC(PYRIDINE)="";SC(J,5)
2470 LPRINT SPC(5)"VG(BENZENE)="";VG(J,1);"VG(n-BUTANOL)="";VG(J,2);"VG(2-
PENTANONE)="";VG(J,3)
2480 LPRINT SPC(5)"VG(1-NITROPROPANE)="";VG(J,4);"VG(PYRIDINE)="";VG(J,5)

```

(Cont.)

Table 2. Continued

```

2490 LPRINT SPC(5)“LG(BENZENE)=”;LG(J,1);“VG(n-BUTANOL)=”;LG(J,2);“ LG(2-
PENTANONE)=”;LG(J,3)
2500 LPRINT SPC(5)“LG(1-NITROPROPANE)=”;LG(J,4);“LG(PYRIDINE)=”;LG(J,5)
2510 FOR W=1 TO 80:LPRINT“*”;NEXT W
2520 NEXT J
2530 FOR W=1 TO 80:LPRINT“*”;NEXT W
2540 RETURN
2550 REM“tR CALCULATIONS”
2560 LV=(LQ/100)*(II-KC)
2570 VV=EXP(LV)
2580 NV=VV*MS
2590 INPUT“INLET PRESSURE of CARRIER GAS APPLIED,[kp/cm2]=”;IP
2600 INPUT“OUTLET PRESSURE of CARRIER GAS APPLIED,[kp/cm2]=”;OP
2610 INPUT“FLOW-RATE of CARRIER GAS USED at the COLUMN
TEMPERATURE,[cm3/min]”;FC
2620 LPRINT SPC(5)“FC=”;FC;“[CM3/MIN]”
2630 PRINT SPC(5)“FC=”;FC;“[CM3/MIN]”
2640 PP=IP/OP
2650 J=1.5*((PP×2-1)/(PP×3-1))
2660 FR=J*FC
2670 IF CT=0 THEN 2700
2680 IF CT=1 THEN INPUT“TM[MIN]=”;TM
2690 GOTO 2710
2700 TM=((D/2)×2*3.14*L)/FR
2710 TR=(NV/FR)+TM
2720 LPRINT SPC(5)“INLET PRESSURE=”;IP;“[kp/cm2]”
2730 LPRINT SPC(5)“OUTLET PRESSURE=”;OP;“[kp/cm2]”
2740 LPRINT SPC(5)“J-FACTOR[1]=”;J;“J*FC=”;FR;“[cm3/min]”
2750 LPRINT SPC(5)“VG(CALC.)=”;VV;“[cm3/g], VN(CALC.)=”;NV;“[cm3]”
2760 PRINT SPC(5)“VG(CALC.)=”;VV;“[cm3/g], VN(CALC.)=”;NV;“[cm3]”
2770 LPRINT SPC(5)“tR(CALC.)=”;TR;“[min] to =”;TM;“[MIN]”
2780 PRINT SPC(5)“tR(CALC.)=”;TR;“[min] to =”;TM;“[MIN]”
2790 REM“STATIONARY PHASE ACTIVITY CALCULATION”
2800 INPUT“IS THERE P0-VALUE OF COMPOUND EXAMINED (YES=1;NO=0)”;QW
2810 IF QW=0 THEN 2880
2820 INPUT“VAPOR PRESSURE of COMPOUND EXAMINED AT COLUMN
TEMPERATURE,[TORR]=”;P0
2830 LPRINT SPC(5)“P0=”;P0;“[torr]”
2840 PRINT SPC(5)“P0=”;P0;“[torr]”
2850 AS=RT/(P0*VV)
2860 PRINT SPC(5)“AS(CALC.)[g/mol]=”;AS
2870 LPRINT SPC(5)“AS(CALC.)[g/mol]=”;AS
2880 FOR W=1 TO 80:LPRINT“*”;NEXT W
2890 FOR W=1 TO 80:LPRINT“#”;NEXT W
2900 RETURN

```

calculated values (Appendix A, Table 7). After printing, the program is ready to take the data of another stationary phase in the same GLC conditions. If we want to change the GLC circumstances of the calculation, we must start the program again.

In Appendix A we sum up the signs used in the system software (Table 2).

We present some retention index values at different column temperatures on three base stationary phases (squalane, Zerolane and OV-101 with 7.17

retention polarity value) in Appendix A. Our first model substance was 1,4-dioxane. Its substance specific factors were determined at 120.0 [°C] with a first order five unknown equation system by determinants and computer. It should be noted that in calculating we did not limit the number of decimal figures:

$$\begin{aligned} &(\text{SE-52/OV-101}): (693.9/680.9)s_1 \\ &+ (665.0/641.6)s_2 - (678.8/663.4)s_3 + \\ &(746.0/718.0)s_4 + (779.3/754.1)s_5 \\ &= (720.5/701.4) \end{aligned} \quad (20)$$

$$\begin{aligned} &(\text{DC-703/OV-101}): (734.8/680.9)s_1 + (735.6/ \\ &641.6)s_2 - (726.5/663.4)s_3 + (829.8/718.0)s_4 + \\ &(855.5/754.1)s_5 = (779.4/701.4) \end{aligned} \quad (21)$$

$$\begin{aligned} &(\text{NPGS/OV-101}): (942.2/680.9)s_1 \\ &+ (1047.2/641.6)s_2 + (963.8/663.4)s_3 \\ &+ (1184.6/718.0)s_4 + (1194.3/754.1)s_5 \\ &= (1060.2/701.4) \end{aligned} \quad (22)$$

$$\begin{aligned} &(\text{PEG-20M/OV-101}): (976.5/680.9)s_1 \\ &+ (1092.4/641.6)s_2 + (1002.4/663.4)s_3 \\ &+ (1234.1/718.0)s_4 + (1243.7/754.1)s_5 \\ &= (1103.9/701.4) \end{aligned} \quad (23)$$

Table 4

Substance specific factors of 1,4-dioxane in GLC

Substance specific factor	
Symbol	Value ^a
s_1	0.47296
s_2	1.12537
s_3	-0.11375
s_4	-0.70972
s_5	0.22508

^a We did limit the number of decimal figures in the calculation.

$$\begin{aligned} &(\text{BCEF/OV-101}): (1428.6/680.9)s_1 \\ &+ (1565.7/641.6)s_2 + (1488.9/663.4)s_3 \\ &+ (1725.1/718.0)s_4 + (1767.1/754.1)s_5 \\ &= (1617.1/701.4) \end{aligned} \quad (24)$$

Data calculated with this equation system are shown in Table 3. In our case the sum of substance specific factors was 0.99994 that can be the basis of a calculation. We presented according to Poole [32] in Section 2 that the cause of this deviation is the individual interactions of the substance studied and the McReynolds standards on the squalane stationary phase. In Table 4 some results of a comparing calculation can be found. We must keep in mind that use of the same names for the stationary phases (e.g., in Table 5) does not mean identical GLC conditions [38], because the complete and exact identification of stationary phases applied is very important in these cases (Table 6).

Table 3

Retention data of the first five McReynolds standards on Zerolane at different column temperatures (°C)

Standard	Column temperatures (°C)							
	60.0	70.0	80.0	90.0	100.0	110.0	120.0	130.0
Benzene	550.6	555.0	559.2	563.2	567.1	571.0	574.8	578.5
<i>n</i> -Butanol	497.8	487.7	477.6	467.5	457.5	447.5	437.4	427.4
2-Pentanone	508.4	512.0	516.1	520.7	525.8	531.3	537.4	544.1
1-Nitropropane	517.0	509.3	501.4	493.2	484.7	475.8	466.7	457.3
Pyridine	505.8	511.4	516.7	521.7	526.5	530.9	535.1	539.1
1,4-Dioxane	532.8	534.0	535.0	536.0	537.1	538.5	540.5	544.2

It should be noted that we can precalculate retention data of the first five McReynolds standards and any kind of substance examined on Zerolane at different column temperatures (°C) by the software presented in Table 2.

Table 5
Comparison of measured and calculated retention indices on some stationary phases at different column temperatures

Stationary phase	Column temp. (°C)	Retention index		
		Measured	Calculated	ΔI
DC-710	60	820.7 ^a	819.2	1.5
DC-710	70	822.6 ^a	823.6	−1.0
TFPS-00 ^{b,c}	80	688.8	684.5	4.3
TFPS-09 ^{b,c}	80	725.3	723.5	1.8
TFPS-15 ^{b,c}	80	753.4	751.2	2.2
TFPS-26 ^{b,c}	80	818.1	818.6	−0.5
Apiezon-L	100	687.0 ^d	687.3	−0.3
DC-200	100	697.0 ^d	696.1	0.9
Diethylhexyl sebacate	100	759.0 ^d	759.4	−0.4
Celanese ester No.9	100	778.0 ^d	777.6	0.4
Diisodecyl phthalate	100	779.0 ^d	779.2	0.2
DC-710	100	823.0 ^d	822.0	1.0
PPG	100	826.0 ^d	825.7	0.3
Acetyltributyl citrate	100	860.0 ^d	859.8	0.2
QF-1	100	876.0 ^d	877.4	−1.4
Tricresyl-phosphate	100	902.0 ^d	903.6	−1.6
Polyphenyl-ether	100	919.0 ^d	918.2	0.8
Marlophen-87	100	925.0 ^d	924.5	0.5
Polypropylene sebacate	100	931.0 ^d	931.5	−0.5
Marlophen-814	100	971.0 ^d	971.5	−0.5
NPGS	100	1080.0 ^d	1080.3	−0.3
PEG-20M	100	1081.0 ^d	1081.7	−0.7
XF-1150	100	1091.0 ^d	1091.5	0.5
PEG-4000	100	1091.0 ^d	1091.1	−0.1
Reoplex-400	100	1159.0 ^d	1158.6	0.4
DEGS	100	1363.0 ^d	1362.7	0.3
Ethyleneglycol-cyanoethyl ether	100	1402.0 ^d	1402.6	−0.6
TCEP	100	1517.0	1517.7	−0.7
<i>n</i> -C36	120	659.0 ^e	659.6	−0.6
Nujol	120	660.0 ^e	660.8	−0.8
Apiezon-M	120	682.0 ^e	682.5	−0.5
Apiezon-L(2127)	120	685.0 ^e	685.5	−0.5
Apiezon-L(2012)	120	687.0 ^e	687.2	−0.2
SF-96	120	695.0 ^e	694.7	0.3
Apiezon-J	120	696.0 ^e	696.1	−0.1
Apiezon-N	120	697.0 ^e	696.6	0.4
SE-30	120	698.0 ^e	697.9	0.1
OV-1	120	699.0 ^e	698.8	0.2
DC-200(2087)	120	700.0 ^e	699.9	0.1
OV-101	120	700.0 ^e	699.2	0.8
SE-52	120	721.0 ^e	721.6	−0.6
SE-54	120	722.0 ^e	721.9	0.1
APH	120	735.0 ^e	735.2	−0.2
OV-3	120	738.0 ^e	738.1	−0.1
APW	120	763.0 ^e	763.6	−0.6
DINA	120	770.0 ^e	770.9	−0.9
OV-7	120	774.0 ^e	774.6	−0.6
DC-550(2120)	120	782.0 ^e	781.6	0.4
DC-703	120	788.0 ^e	788.3	−0.3
Dinonyl phthalate	120	792.0 ^e	793.0	−1.0
OV-11	120	818.0 ^e	818.3	−0.3

Table 5. Continued

Stationary phase	Column temp. (°C)	Retention index		
		Measured	Calculated	ΔI
OV-22	120	882.0 ^e	881.9	0.1
OV-225	120	996.0 ^e	995.6	0.4
PEG-6000	120	1091.0 ^e	1091.1	-0.1
FFAP	120	1098.0 ^e	1097.6	0.4
PEG-600	120	1157.0 ^e	1157.8	-0.8
PDEAS	120	1216.0 ^e	1216.4	-0.4
BCEF	120	1518.0 ^e	1518.1	-0.1
C78 ⁱ	130	669.7 ^f	670.1	-0.4
MTF-C78	130	683.8 ^g	684.1	-0.3
PCI-C78 ⁱ	130	684.6 ^h	684.7	-0.1
PBr-C78	130	685.5 ^h	685.7	-0.2
PCN-C78	130	706.3 ^h	705.8	0.5
TMO-C78	130	716.3 ^h	716.1	0.2
POH-C78	130	716.9 ^f	717.3	-0.4
TTF-C78	130	718.2 ^g	717.9	0.3

^a Ref. [48]; ^b Ref. [43]; ^c Ref. [49]; ^d Ref. [5]; ^e Ref. [6]; ^f Ref. [46]; ^g Ref. [45]; ^h Ref. [44]; ⁱ Ref. [47].

4. Experimental

In most of the cases the experimental work meant controlling of the data and values read in literature (the GLC parameters of the essential experiment series are listed in Appendix A, Table 9).

The purpose was to define the equations of temperature dependence. With the help of computers, for this work we used data on 27 stationary phases and mathematical methods (regression relations, multivariable equations, etc.) based on hundreds of data in the literature [2–6,9,10].

Unfortunately, this heterogeneous database increased the number of faults in calculation as you can see below mostly because we found totally different data in different GLC circumstances; in the

case of data measured on filled columns. Differentiation on column temperature of data on literature was also a disadvantage because most of the measures have been done at 120.0 [°C]. Because of this, it is not obvious that the reliability of values is best at 120.0 [°C] and then decreases step by step towards 60.0 [°C] as the distribution of false measures was accidental.

With the contribution and assistance of other researchers and research teams the database can be recontrolled and the number of data could be recalculated and increased to make the basis more trustworthy and perfect because its trust-level is 92% at the moment.

5. Conclusions

Simulation of GLC processes with computer and precalculation of retention data in advance are three dimension processes.

The first dimension is presented by the stationary phase used, the second by the used isothermal and/or programmed column temperature (including programmed temperature evaporator also if it is), the third by retention data given by the first two ones.

Table 6
Influence of the origin of the stationary phase on the retention polarity determined on DEGS at 120.0 (°C)

Supplier	Retention polarity
Supelco No. 1045	102.55
Chemical Research Services	106.63
Supelco No. 1303	108.87
PolyScience Corp.	110.03

Table 7

A protocol list of the system software

The greatest system of precalculation in GLC between 60–130 (°C); 09.02.1997

TC [°C]=120 T=393.16 [°K]

PARAMETERS OF COLUMN USED

HP-ULTRA 1, No.1909/1A-112, wall-coated open tubular column; L=2500 [cm], I.D.=0.032 [cm], $m_s=0.0171$ [g] $d_f=0.52$ [μm], $\beta=150$

ZEROLANE

DATA OF POLARITY

RP(120.0 [°C])=−20.83

APF=1 MP(C)=0

PS(BENZENE)=1 PS(*n*-BUTANOL)=1 PS(2-PENTANONE)=1

PS(1-NITROPROPANE)=1 PS(PYRIDINE)=1

EFFECTIVE POLARITY=0

DATA OF *n*-ALKANES $K_c(C)=84.26736$ KC(APOLANE-87)=168.5347 $V_g(nC8)=148.3833$ ln $[V_g(nC8)]=4.999799$ Q=2.010849 LQ(C)=0.6985568b=0.3033794 DG(CH₂)=2283.488 [J/mol]

RETENTION INDICES

I(BENZENE)=574.7573 I(*n*-BUTANOL)=437.4364 I(2-PENTANONE)=537.4384

I(1-NITROPROPANE)=466.7024 I(PYRIDINE)=535.1068

BASE SQ:DI(BENZENE)=±77.85413° DI(*n*-BUTANOL)=−152.4429 DI(2-PENTANONE)=−92.68421

DI(1-NITROPROPANE)=−188.799 DI(PYRIDINE)=−163.34

BASE ZEROLANE:DI(BENZENE)=0 DI(*n*-BUTANOL)=0 DI(2-PENTANONE)=0

DI(1-NITROPROPANE)=0 DI(PYRIDINE)=0

RETENTION DATA

SC(BENZENE)=490.49 SC(*n*-BUTANOL)=353.169 SC(2-PENTANONE)=453.171

SC(1-NITROPROPANE)=382.435 SC(PYRIDINE)=450.8394

VG(BENZENE)=30.76418 VG(*n*-BUTANOL)=11.78804 VG(2-PENTANONE)=23.7043

VG(1-NITROPROPANE)=14.46202 VG(PYRIDINE)=23.32135

LG(BENZENE)=3.426351 LG(*n*-BUTANOL)=2.467086 LG(2-PENTANONE)=3.165657

LG(1-NITROPROPANE)=2.671526 LG(PYRIDINE)=3.149369

SQUALANE

DATA OF POLARITY

RP(120.0 [°C])=0

APF=1.141382 MP(C)=0.9404731

PS(BENZENE)=0.9971696 PS(*n*-BUTANOL)=1.207308 PS(2-PENTANONE)=1.029579

PS(1-NITROPROPANE)=1.286281 PS(PYRIDINE)=1.186573

EFFECTIVE POLARITY=1.32966

DATA OF *n*-ALKANES $K_c(C)=163.5186$ KC(APOLANE-87)=168.5347 $V_g(nC8)=70.81283$ ln $[V_g(nC8)]=4.260041$ Q=1.952891 LQ(C)=0.6693111b=0.2906781 DG(CH₂)=2187.888 [J/mol]

RETENTION INDICES

I(BENZENE)=652.6203 I(*n*-BUTANOL)=589.9021 I(2-PENTANONE)=630.094

I(1-NITROPROPANE)=655.4375 I(PYRIDINE)=698.4723

BASE SQ:DI(BENZENE)=0 DI(*n*-BUTANOL)=0 DI(2-PENTANONE)=0

DI(1-NITROPROPANE)=0 DI(PYRIDINE)=0

BASE ZEROLANE:DI(BENZENE)=77.86291 DI(*n*-BUTANOL)=152.4658

DI(2-PENTANONE)=92.65558 DI(1-NITROPROPANE)=188.74 DI(PYRIDINE)=163.3655

RETENTION DATA

SC(BENZENE)=489.1017 SC(*n*-BUTANOL)=426.3836 SC(2-PENTANONE)=466.5754

SC(1-NITROPROPANE)=491.9189 SC(PYRIDINE)=534.9537

Table 7. Continued

VG(BENZENE)=26.40654 VG(*n*-BUTANOL)=17.35416 VG(2-PENTANONE)=22.7108
 VG(1-NITROPROPANE)=26.90918 VG(PYRIDINE)=35.89162
 LG(BENZENE)=3.273612 LG(*n*-BUTANOL)=2.853832 LG(2-PENTANONE)=3.122841
 LG(1-NITROPROPANE)=3.292467 LG(PYRIDINE)=3.580504
 OV-101
 DATA OF POLARITY
 RP(120.0 [°C])=7.17
 APF=1.216232 MP(C)=1.13024
 PS(BENZENE)=1.022169 PS(*n*-BUTANOL)=1.30853 PS(2-PENTANONE)=1.1.067794
 PS(1-NITROPROPANE)=1.408112 PS(PYRIDINE)=1.274553
 EFFECTIVE POLARITY=2.443934
 DATA OF *n*-ALKANES
 $K_c(C)=179.5097$ KC(APOLANE-87)=168.5347
 $Vg(nC8)=59.64256$ $\ln [Vg(nC8)]=4.088369$ $Q=1.932652$ $LQ(C)=0.6588934$
 $b=0.2861537$ $DG(CH_2)=2153.834$ [J/mol]
 RETENTION INDICES
 $I(BENZENE)=680.8731$ $I(n-BUTANOL)=641.642$ $I(2-PENTANONE)=663.4028$
 $I(1-NITROPROPANE)=718.021$ $I(PYRIDINE)=754.1285$
 BASE SQ:DI(BENZENE)=28.2616 DI(*n*-BUTANOL)=51.76264 DI(2-PENTANONE)=33.28027
 DI(1-NITROPROPANE)=62.51953 DI(PYRIDINE)=55.6817
 BASE ZEROLANE:DI(BENZENE)=106.1157 DI(*n*-BUTANOL)=204.2056
 DI(2-PENTANONE)=125.9645 DI(1-NITROPROPANE)=251.3186 DI(PYRIDINE)=219.0217
 RETENTION DATA
 $SC(BENZENE)=501.3634$ $SC(n-BUTANOL)=462.1323$ $SC(2-PENTANONE)=483.8932$
 $SC(1-NITROPROPANE)=538.5113$ $SC(PYRIDINE)=574.6188$
 $VG(BENZENE)=27.20633$ $VG(n-BUTANOL)=21.00916$ $VG(2-PENTANONE)=24.24814$
 $VG(1-NITROPROPANE)=27.20633$ $VG(PYRIDINE)=44.08523$
 $LG(BENZENE)=3.30345$ $LG(n-BUTANOL)=3.044959$ $LG(2-PENTANONE)=3.18834$
 $LG(1-NITROPROPANE)=3.548215$ $LG(PYRIDINE)=3.786125$
 DIMETHYLPOLYSILOXANE
 DATA OF POLARITY
 RP(MEAS.) at 120.0 [°C]=10.94 RP(CALC.)=10.95159 DELTA RP=−0.01159
 APF=1.254433 MP(C)=1.235181
 PS(BENZENE)=1.035071 PS(*n*-BUTANOL)=1.360097 PS(2-PENTANONE)=1.087602
 PS(1-NITROPROPANE)=1.469806 PS(PYRIDINE)=1.319589
 EFFECTIVE POLARITY=3.142709
 DATA OF *n*-ALKANES
 $K_c(C)=188.3529$ KC(APOLANE-87)=168.5347
 $Vg(nC8)=54.38782$ $\ln [Vg(nC8)]=3.99614$ $Q=1.921951$ $LQ(C)=0.6533408$
 $b=0.2837423$ $DG(CH_2)=2135.683$ [J/mol]
 RETENTION INDICES
 $I(BENZENE)=696.045$ $I(n-BUTANOL)=668.6969$ $I(2-PENTANONE)=681.2223$
 $I(1-NITROPROPANE)=750.4583$ $I(PYRIDINE)=783.2754$
 BASE SQ:DI(BENZENE)=43.43347 DI(*n*-BUTANOL)=78.81763 DI(2-PENTANONE)=51.09973
 DI(1-NITROPROPANE)=94.95691 DI(PYRIDINE)=84.82868
 BASE ZEROLANE:DI(BENZENE)=121.2877 DI(*n*-BUTANOL)=231.2605
 DI(2-PENTANONE)=143.7839 DI(1-NITROPROPANE)=283.7559 DI(PYRIDINE)=248.1686
 RETENTION DATA
 $SC(BENZENE)=507.6921$ $SC(n-BUTANOL)=480.3441$ $SC(2-PENTANONE)=492.8695$
 $SC(1-NITROPROPANE)=562.1055$ $SC(PYRIDINE)=594.9226$
 $VG(BENZENE)=27.57638$ $VG(n-BUTANOL)=23.06425$ $VG(2-PENTANONE)=25.03105$
 $VG(1-NITROPROPANE)=39.34875$ $VG(PYRIDINE)=48.75812$
 $LG(BENZENE)=3.31696$ $LG(n-BUTANOL)=3.138284$ $LG(2-PENTANONE)=3.220117$
 $LG(1-NITROPROPANE)=3.672464$ $LG(PYRIDINE)=3.886872$
 $1,4-DIOXANE I(SQ)=654.2699$ $I(ZEROLANE)=540.499$ $I(M)=721.2699$

(Cont.)

Table 7. Continued

I(C)=721.5228 DI(M)=67 DI(C)=67.25293 DELTA DI= -0.2529297^b
 FC=1.51 [cm³/min]; J-FACTOR [1]=0.790858; J*FC=1.194196 [cm³/min]
 INLET PRESSURE=1.51 [kp/cm²]; OUTLET PRESSURE=1.01 [kp/cm²]
 VG(CALC.)=111.4976 [cm³/g], VN(CALC.)=1.906609 [cm³]
 tR(CALC.)=3.27937 [min], to=1.682807 [min]
 P0=2203.59 [Torr]; AS(CALC.)=99.79251 [g/mole]

^a It should be noted that retention indices are bigger on squalane than on zerolane stationary phase so their difference has a negative value. In calculating we did not limit the number of decimal figures.

^b In calculating we did not limit the number of decimal figures.

There has been a demand for a third dimension for a long time because the Rohrschneider concept and calculating method and the similar McReynolds system had only two dimensions (choice of stationary phase and 100.0, and column temperature at 120.0 [°C]). Up to this time this demand has not been satisfied because of the lack of the background relations.

Equations presented in this paper can solve this problem theoretically. But as was mentioned above, because of some databases at given column temperatures and of the heterogeneous databases, the certainty of calculations are not satisfying. Hopefully other researchers will help us and after a period of time, having more retention data, the constants of the equations are going to be more reliable.

This paper presents a new computer software to precalculate the retention data between 60–130 [°C] on different stationary phases.

This method can be used in GLC conditions of programmed temperature using data from literature [29].

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Appendix A

We can write according to Littlewood et al. [39]:

$$V_g^{\text{st.ph.}}(Tc) = \frac{V_N^{\text{st.ph.}}(Tc)}{m_s} = \frac{RT}{p^\circ(Tc)\gamma^{\text{st.ph.}}(Tc)M_s} \quad (25)$$

where: V_N =net retention volume [cm³]; m_s =mass of the stationary phase used in the column applied [g]; T =the column temperature [°K]; R =universal gas constant [cm³ Torr/mol °K], its value=62362.7 (1 Torr=133.322 Pa); p° =the vapor pressure of the pure substance studied [Torr] (hereby we notice that this dimension should be used in the SI system [Pa] but because of the ten times magnitude order (in Torr) and the difficulties in converting given data published before, the usage of the Torr dimension is allowed); γ =classical activity coefficient [41] [dimensionless]; M_s =mass of the used stationary phase [g/mol]. The polymer stationary phases made it necessary to have a new definition for activity. It is possible as reported by Schay [42]:

$$A_s(T)^{\text{st.ph.}} = \gamma^{\text{st.ph.}}(T)M_s^{\text{st.ph.}} \quad (26)$$

where: A_s =stationary phase activity [g/mol]. From Eq. (25):

$$A_s(T)^{\text{st.ph.}} = m_s RT/p^\circ(T)V_N(T)^{\text{st.ph.}} \quad (27)$$

Last but not least, we summarized a protocol list (Table 7) and the symbols of the system software (Table 8). The GLC parameters of the essential experiment series are given in Table 9.

Table 8

Symbols of system software

A11,A12,A13,A21,A22,A23,A31,A32,A33,A41,A42,A43,A51,A52 and A53 = a constants of Eqs. (3)–(5).
 AK = a constant of Eq. (11)
 AP = average standard specific polarity factor calculated of first 5 McReynolds standards on stationary phase used at TC column temperature [°C] [dimensionless]
 AP(1),AP(2) and AP(3) = average standard specific polarity factor calculated of first 5 McReynolds standards on basic stationary phases used at TC column temperature [°C] [dimensionless]
 AP = average standard specific polarity factor calculated of first 5 McReynolds standards on stationary phase used at TC column temperature [°C] [dimensionless]
 AP(1),AP(2) and AP(3) = average standard specific polarity factor calculated of first 5 McReynolds standards on basic stationary phases used at TC column temperature [°C] [dimensionless]
 AQ = a constant of Eq. (7)
 B = logarithm (on base: 10) of relative volatility of two consecutive *n*-alkanes used on stationary phase used at TC column temperature [°C] (the “b-value”), [dimensionless]
 B(1),B(2) and B(3) = logarithm (on base: 10) of relative volatility of two consecutive *n*-alkanes used on basic stationary phases used at TC column temperature [°C] [dimensionless]
 BK = a constant of Eq. (11)
 BQ = a constant of Eq. (7)
 CC = a constant of Eq. (11)
 CK = the Kováts coefficient calculated, [$-\ln(\text{cm}^3/\text{g})$], on a stationary phase used at TC column temperature [°C]
 CK(1),CK(2) and CK(3) = the Kováts coefficient calculated, [$-\ln(\text{cm}^3/\text{g})$], on basic stationary phases used at TC column temperature [°C]
 CQ = a constant of Eq. (7)
 DD(0) = difference of retention indices calculated between stationary phases used and squalane of the substance examined at TC column temperature [°C] [dimensionless]
 DD(1),DD(2),DD(3),DD(4) and DD(5) = difference of retention indices calculated between stationary phases used and squalane of first 5 McReynolds standards used at TC column temperature [°C] [dimensionless]
 DG = symbol of ΔG° , [J/mol]
 ΔG° = free energy of substance examined on a stationary phase used at TC column temperature [°C] [J/mol]
 $\Delta G^\circ(1)$, $\Delta G^\circ(2)$ and $\Delta G^\circ(3)$ = free energy of substance examined on basic stationary phases used at TC column temperature [°C] [J/mol]
 DI(1,1),DI(1,2),DI(1,3),DI(1,4) and DI(1,5) = difference of retention indices calculated between the Zerolane stationary phases and squalane of first 5 McReynolds standards at TC column temperature [°C] [dimensionless]
 DI(3,1),DI(3,2),DI(3,3),DI(3,4) and DI(3,5) = difference of retention indices calculated between an OV-101 stationary phases with retention polarity 7.17 at 120.0 [°C].and squalane of first 5 McReynolds standards at TC column temperature [°C] [dimensionless]
 DZ(2,1),DZ(2,2),DZ(2,3),DZ(2,4) and DZ(2,5) = difference of retention indices calculated between a squalane stationary phases and the Zerolane of first 5 McReynolds standards at TC column temperature [°C] [dimensionless]
 DZ(3,1),DZ(3,2),DZ(3,3),DZ(3,4) and DZ(3,5) = difference of retention indices calculated between an OV-101 stationary phases with retention polarity 7.17 at 120.0 [°C] and the Zerolane of first 5 McReynolds standards at TC column temperature [°C] [dimensionless]
 I(1,1),I(1,2),I(1,3),I(1,4) and I(1,5) = retention indices calculated of first 5 McReynolds standards on the Zerolane stationary phase at TC column temperature [°C] [dimensionless]
 I(2,1),I(2,2),I(2,3),I(2,4) and I(2,5) = retention indices calculated of first 5 McReynolds standards on a squalane stationary phase at TC column temperature [°C] [dimensionless]
 I(3,1),I(3,2),I(3,3),I(3,4) and I(3,5) = retention indices calculated of first 5 McReynolds standards at TC column temperature [°C] [dimensionless] on an OV-101 stationary phase with retention polarity

(Cont.)

Table 8. Continued

7.17 at 120.0 [°C]

DI(MEAS.)=difference of retention indices measured between stationary phases used and squalane of the substance examined at TC column temperature [°C] [dimensionless]

E=serial number of stationary phases examined

f=serial number

FC=flow-rate of the carrier gas used [cm³/min]

FR=adjusted flow-rate by j-factor [cm³/min]

I(1,1),I(1,2),I(1,3),I(1,4) and I(1,5)=retention indices calculated of first 5 McReynolds standards on the Zerolane stationary phase at TC column temperature [°C] [dimensionless]

I(2,1),I(2,2),I(2,3),I(2,4) and I(2,5)=retention indices calculated of first 5 McReynolds standards on a squalane stationary phase at TC column temperature [°C] [dimensionless]

I(3,1),I(3,2),I(3,3),I(3,4) and I(3,5)=retention indices calculated of first 5 McReynolds standards at TC column temperature [°C] [dimensionless] on an OV-101 stationary phase with retention polarity 7.17 at 120.0 [°C].

I1,I2,I3,I4 and I5=retention indices calculated of first 5 McReynolds standards on a stationary phase used at TC column temperature [°C] [dimensionless]

II=retention index calculated of the compound examined on stationary phase used at TC column temperature [°C] [dimensionless]

IP=inlet pressure of the carrier gas used [kp/cm²]

IS(1),IS(2),IS(3),IS(4) and IS(5)=retention indices calculated of first 5 McReynolds standards on a squalane stationary phase at TC column temperature [°C]

IZ=retention index calculated of the substance studied on the Zerolane stationary phase at TC column temperature [°C] [dimensionless]

j=the compressibility factor according to James and Martin [1]

KA=the Kováts coefficient calculated, [$-\ln(\text{cm}^3/\text{g})$], on Apolane-87 stationary phase used at TC column temperature [°C]

KD=retention index difference of measured and calculated retention indices or retention index differences [dimensionless]

L1,L2,L3,L4 and L5=logarithm naturale (on base: $e=2.7182\dots$) of specific retention volume calculated of first 5 McReynolds standards on stationary phase used at TC column temperature [°C]

LG(1,1),LG(1,2),LG(1,3),LG(1,4) and LG(1,5)=symbol of the natural logarithm of specific retention volume of first 5 McReynolds standards, [$\ln(\text{cm}^3/\text{g})$], on the Zerolane phase used at TC column temperature [°C]

L8=symbol of the natural logarithm of *n*-octane's specific retention volume, [$\ln(\text{cm}^3/\text{g})$], on a stationary phase used at TC column temperature [°C]

L8(1)=symbol of the natural logarithm of *n*-octane's specific retention volume, [$\ln(\text{cm}^3/\text{g})$], on the Zerolane stationary phase used at TC column temperature [°C]

L8(2)=symbol of the natural logarithm of *n*-octane's specific retention volume, [$\ln(\text{cm}^3/\text{g})$], on a squalane stationary phase used at TC column temperature, [°C]

L8(3)=symbol of the natural logarithm of *n*-octane's specific retention volume, [$\ln(\text{cm}^3/\text{g})$], at TC column temperature, [°C] on an OV-101 stationary phase with retention polarity 7.17 at 120.0 [°C]

LQ=naturale logarithm (on base: $e=2.7182\dots$) of relative volatility of two consecutive *n*-alkanes used on stationary phase used at TC column temperature [°C] [dimensionless]

LV=symbol of the natural logarithm of 1,4-dioxane's specific retention volume, [$\ln(\text{cm}^3/\text{g})$], at TC column temperature [°C] on stationary phase used

MF=the McReynolds standard specific polarity factor

MS=mass of the stationary phase used in the column applied [g]

N=number of stationary phases examined

Table 8. Continued

N\$=name of the compound examined
 NV=net retention volume of 1,4-dioxane [cm³] at TC column temperature [°C] on stationary phase used
 OP=outlet pressure of the carrier gas used [kp/cm²]
 P_e=the effective polarity of stationary phase used at TC column temperature [°C] [dimensionless]
 P(1)=the effective polarity of Zerolane stationary phase used at TC column temperature [°C] [dimensionless]
 P(2)=the effective polarity of a squalane stationary phase used at TC column temperature [°C] [dimensionless]
 P(3)=the effective polarity of an OV-101 stationary phase used at TC column temperature [°C] [dimensionless] with retention polarity 7.17 at 120.0 [°C]
 P1,P2,P3,P4 and P5=substance specific polarity factor calculated of first 5 McReynolds standards on stationary phase used at TC column temperature [°C] [dimensionless]
 PM=the McReynolds polarity calculated on stationary phase used at TC column temperature [°C] [dimensionless]
 PP=relative pressure drop
 PR=retention polarity measured at 120.0 [°C] [dimensionless]
 PS(1,1),PS(1,2),PS(1,3),PS(1,4) and PS(1,5)=substance specific polarity factor calculated of first 5 McReynolds standards on Zerolane stationary phase at TC column temperature [°C] [dimensionless]
 PS(2,1),PS(2,2),PS(2,3),PS(2,4) and PS(2,5)=substance specific polarity factor calculated of first 5 McReynolds standards on a squalane stationary phase at TC column temperature [°C] [dimensionless]
 PS(3,1),PS(3,2),PS(3,3),PS(3,4) and PS(3,5)=substance specific polarity factor calculated of first 5 McReynolds standards on an OV-101 stationary phase with retention polarity 7.17 at 120.0 [°C] at TC column temperature [°C] [dimensionless]
 Q=relative volatility of two consecutive *n*-alkanes used on stationary phase used at TC column temperature [°C] [dimensionless]
 R=universal gas constant [J/°K·mol]
 RP=retention polarity calculated of stationary phase at TC column temperature [°C] [dimensionless]
 RP(1)=retention polarity calculated of Zerolane at TC column temperature [°C] [dimensionless]
 RP(2)=retention polarity calculated of a squalane stationary phase at TC column temperature [°C] [dimensionless]
 RP(3)=retention polarity calculated of an OV-101 stationary phase with retention polarity 7.17 at 120.0 [°C] at TC column temperature [°C] [dimensionless]
 ST\$=symbol of stationary phase examined
 ST.PH.=abbreviation of stationary phase
 ST\$(j)=name of the *j*th basic stationary phase used. It should be noted that the basic stationary phases are as follow: Zerolane, squalane and OV-101 with retention polarity 7.17 at 120.0 [°C]
 SC(1,1),SC(1,2),SC(1,3),SC(1,4) and SC(1,5)=molecular structural coefficient calculated of first 5 McReynolds standards on the Zerolane at TC column temperature [°C] [ln (cm³/g)]
 SC(2,1),SC(2,2),SC(2,3),SC(2,4) and SC(2,5)=molecular structural coefficient calculated of first 5 McReynolds standards on a squalane stationary phase at TC column temperature [°C] [ln (cm³/g)]
 SC(3,1),SC(3,2),SC(3,3),SC(3,4) and SC(3,5)=molecular structural coefficient calculated of first 5 McReynolds standards on an OV-101 stationary phase with 7.17 retention polarity at TC column temperature [°C] [ln (cm³/g)]
 S1,S2,S3,S4 and S5=molecular structural coefficient calculated of first 5 McReynolds standards on stationary phase used at TC column temperature [°C] [ln (cm³/g)]
 T=column temperature [°K]

(Cont.)

Table 8. Continued

TC = column temperature [°C]
 t_r = retention time [min]
 t_o = dead (hold-up) time [min]
V1,V2,V3,V4 and V5 = specific retention volume calculated of first 5 McReynolds standards [cm³/g] on stationary phase used at TC column temperature [°C]
VG(1,1),VG(1,2),VG(1,3),VG(1,4) and VG(1,5) = symbol of specific retention volume of first 5 McReynolds standards [cm³/g] on the Zerolane phase used at TC column temperature [°C]
V8 = specific retention volume of *n*-octane [cm³/g] on stationary phase used at TC column temperature [°C]
V8(1) = symbol of *n*-octane's specific retention volume [cm³/g] on the Zerolane at TC column temperature [°C]
V8(2) = symbol of *n*-octane's specific retention volume, [ln (cm³/g)], on a squalane at TC column temperature [°C]
V8(3) = symbol of *n*-octane's specific retention volume [cm³/g] at TC column temperature [°C] on an OV-101 stationary phase with retention polarity 7.17 at 120.0 [°C]
VV = symbol of 1,4-dioxane's specific retention volume [cm³/g] on the Zerolane at TC column temperature [°C]
W = serial number
X1,X2,X3,X4 and X5 = substance specific factor of first 5 McReynolds standards [dimensionless]
X6 = retention index at TC [°C] column temperature of the substance studied on an OV-101 stationary phase with 7.17 retention polarity at 120.0 [°C]
XX = difference of retention indices measured between stationary phases used and squalane of the substance examined at TC column temperature [°C] [dimensionless]
Y1,Y2,Y3,Y4 and Y5 = relative retention index of first 5 McReynolds standards measured on a stationary phase used at TC column temperature [°C] to an OV-101 stationary phase with 7.17 retention polarity at 120.0 [°C] [dimensionless]
Z1,Z2,Z3,Z4 and Z5 = relative retention index of first 5 McReynolds standards predicted on the Zerolane stationary phase at TC column temperature [°C] to an OV-101 stationary phase with 7.17 retention polarity at 120.0 [°C] [dimensionless]
ZZ = difference of measured and calculated retention indices of compound examined

Table 9

The gas–liquid chromatographic parameters of the essential experiment series

Gas chromatographs: different types of Carlo Erba and Hewlett–Packard
Detectors: flame ionization detectors
Attenuation: 10⁻⁹–10⁻¹⁰ [A]
Introduction of samples: 1.0 [mm³] from mixture by Hamilton or SGE syringes
Columns: different coated and wall-coated open tubular (WCOT)
Stationary phases: cited in this paper
Ratio of phases according to WCOT: 1:75–1:100
Carrier gas: nitrogen, argon and helium, respectively. It should be noted that the values of Kováts coefficient, molecular structural coefficient, specific retention volume, net retention volume, retention index, as well as, polarities are independent of the quality of the carrier gas used [39,40].
Inlet pressure: 2.14–2.95 [kp/cm²]
Flow-rate: 0.36–1.3 [cm³/min] on WCOT columns and 19–25 [cm³/min] on coated columns
Dead (hold-up) time: 3.567–4.386 [min] on WCOT columns and 0.3–0.5 [min] on coated columns
Column temperature: 60.0–150.0±0.1 [°C]
Temperature of evaporator: 200.0–250±1 [°C]
Temperature of detector: 230.0–250±1 [°C]

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