

"val10to12" (multiplier values for 10-12 atoms) and "decmark" (leftmost fragment for multipliers from 13 to 19).

The number of terminal symbols that is allowed from a point of failure and, hence, the numbers of reliable interpretations and possible correct fragments are dependent on where in a name the failure occurred. For example, if failure occurred within a multiplying term clause, there would be few symbols allowed. If however the failure occurred at a point where a substituent clause could be present, then there would be many terminal symbols to choose from.

In the semantic-correction process, there are several more sophisticated investigations that could be added, at the expense of more complex code and increased processing time. For example, in the case of invalid locants, consider the name *12-dichloropentane*. Here, the following deductions could be made concerning the faulty halogen substituent:

- (1) The locant value of 12 is too large for the parent aliphatic chain length of five carbon atoms.
- (2) The explicit multiplier "di" implies that the user probably intended to give more than one locant. (From our experience, it is quite common for multiplier terms to be omitted, but the presence of unnecessary ones is rare.)
- (3) A valid name is created if the 2-digit number "12" is converted by insertion of a comma to create two locants, i.e., "1,2-...".

Thus, the user could be shown the valid name *1,2-dichloropentane* and asked if that is what was intended.

With this more computationally intensive type of correction, it is important for the system to give up if no solution has been found after some predetermined length of time, or when a certain level of detail has been reached. Nevertheless, as processing power of PCs increases, the number and complexity of attempts to correct erroneous names can expand.

It will be a definite advantage to automatic correction, if a semantic check is applied where two or more alternative syntactically correct names have been constructed by the syntax error correction system. For example, consider the name *pentane-1,3-dol*, in which the following two syntactically correct names are automatically produced by the system described:

pentane-1,3-diol (Replacement of "d" by "di")
pentane-1,3-ol (Deletion of "d")

By applying a semantic check on each of these names, it can be seen that while the first is acceptable, the second has a

locant/multiplier term conflict in the position where the syntax correction has just taken place. Thus, both names can be presented to the user, along with a suitable message explaining why the system believes the first to be the more likely candidate.

The principal conclusion of this work is that it is possible to correct semiautomatically, i.e., with some limited input from the user, many of the errors commonly made in the use of systematic chemical nomenclature. An automatic correction mode can provide one or more names that are syntactically correct, but some user judgment is necessary to determine whether these include the intended name.

Applications of the software we have developed could include industrial/commercial data entry and validation of names where input is by nonchemically trained personnel and for computer-based teaching of chemical nomenclature.

ACKNOWLEDGMENT

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DETERM: Thermophysical Property Data for the Optimization of Heat-Transfer Equipment

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A physical-property calculation system coupled with a very comprehensive and extensive literature database is described. Methods and methodologies for generating the thermophysical property data necessary for carrying out detailed and accurate design and check-rating calculations of heat-transfer equipment are discussed.

INTRODUCTION

With the ever-increasing sensitivity of economic and pollution issues, the requirements for the performance of heat-

generation and heat-transfer equipment are becoming continually more stringent. The "overall" methodologies and algorithms with LMTD values and correction factors traditionally used for the mathematical modeling of fired heaters,

```

*****
THREE PHASE LLE FLASH
*****
STREAM      4
TEMPERATURE: 25.00 CEL      298.15 K      77.00 DEG F
PRESSURE:    1.0000 BAR      1.0197 KP/CM2  14.504 PSIA
CODE         NAME           MOLE FRACT.  MOL AMOUNT  WEIGHT  WEIGHT AM.
                        KMOL      FRACTION      KG
    28  HEPTANE             0.271790    81.537    0.555539    8170.46
   120  BENZENE             0.042730    12.819    0.068086    1001.35
    10  WATER               0.420594   126.178    0.154559    2273.14
   300  ACETONITRILE        0.264887    79.466    0.221816    3262.31
    SUM              1.000000   300.000    1.000000    14707.25
AVERAGE MOLAR MASS: 49.024 G/MOL
MODEL USED FOR LIQUID PHASE NON-IDEALITY: UNIFAC

RESULT OF 3-PHASE CALCULATION:

PHASE 1:    31.324 MOLE %
PHASE 2:    32.618 MOLE %
PHASE 3:    36.057 MOLE %
* THE SYSTEM IS STABLE *

*****
THERMOPHYSICAL PROPERTIES OF LIQUID PHASE # 1 OF STREAM      4
*****
CODE         NAME           MOLE FRACT.  MOL AMOUNT  WEIGHT  WEIGHT AM.
                        KMOL      FRACTION      KG
    28  HEPTANE             0.000431     0.040    0.001842     4.06
   120  BENZENE             0.000937     0.088    0.003123     6.88
    10  WATER               0.767645    72.138    0.590282   1299.59
   300  ACETONITRILE        0.230988    21.707    0.404752     891.12
    SUM              1.000000    93.973    1.000000    2201.63
AVERAGE MOLAR MASS      23.43 G/MOL

*****
THERMOPHYSICAL PROPERTIES OF LIQUID PHASE # 2 OF STREAM      4
*****
CODE         NAME           MOLE FRACT.  MOL AMOUNT  WEIGHT  WEIGHT AM.
                        KMOL      FRACTION      KG
    28  HEPTANE             0.828120    81.036    0.878389    8120.23
   120  BENZENE             0.121340    11.874    0.100332     927.52
    10  WATER               0.002798     0.274    0.000534     4.93
   300  ACETONITRILE        0.047741     4.672    0.020746     191.79
    SUM              1.000000    97.855    1.000000    9244.46
AVERAGE MOLAR MASS      94.47 G/MOL

*****
THERMOPHYSICAL PROPERTIES OF LIQUID PHASE # 3 OF STREAM      4
*****
CODE         NAME           MOLE FRACT.  MOL AMOUNT  WEIGHT  WEIGHT AM.
                        KMOL      FRACTION      KG
    28  HEPTANE             0.004259     0.461    0.014156     46.17
   120  BENZENE             0.007924     0.857    0.020532     66.96
    10  WATER               0.497045    53.766    0.297018    968.62
   300  ACETONITRILE        0.490771    53.088    0.668293    2179.40
    SUM              1.000000   108.172    1.000000    3261.14
AVERAGE MOLAR MASS      30.15 G/MOL

```

Figure 1. Three-phase liquid-liquid-liquid equilibrium flash.

reformers, and heat exchangers are in many cases no longer adequate to meet these more rigorous specifications. Either overdesign will occur, which is wasteful of capital and materials, or underdesign will produce an exchanger which will operate at less than optimum conditions. This means loss of heat throughout the life of the unit. An approach which allows a much more satisfactory representation of the physical reality within these types of equipment and of their mode of functioning is the "stepwise" method.^{1,2} In these methodologies the heat-transfer or heat-generation units are divided mathematically into a finite number of subunits, each one of which is treated individually and locally as a separate entity. The equations describing each local unit are solved individually and collectively with appropriate boundary conditions. This procedure is iterated until the desired convergence of the entire

system is achieved. Certainly a more refined mathematical treatment of the simulation of these devices is of little value if the physical property data necessary for stepwise-type calculations do not also have the appropriate accuracy. Most important is that physical property data be available under the local conditions of composition, temperature, and pressure actually attendant in each of the individual local units of the model employed. In general, tables of values covering the complete range of temperature, pressure, and composition of the thermophysical and transport properties for the vapor and the condensed states of the pure components and complex mixtures utilized are necessary.

These requisite values of density, viscosity, enthalpy, thermal conductivity, heat capacity, surface tension, and critical pressure are generated by the systems DETHERM-SDR,³⁻⁶

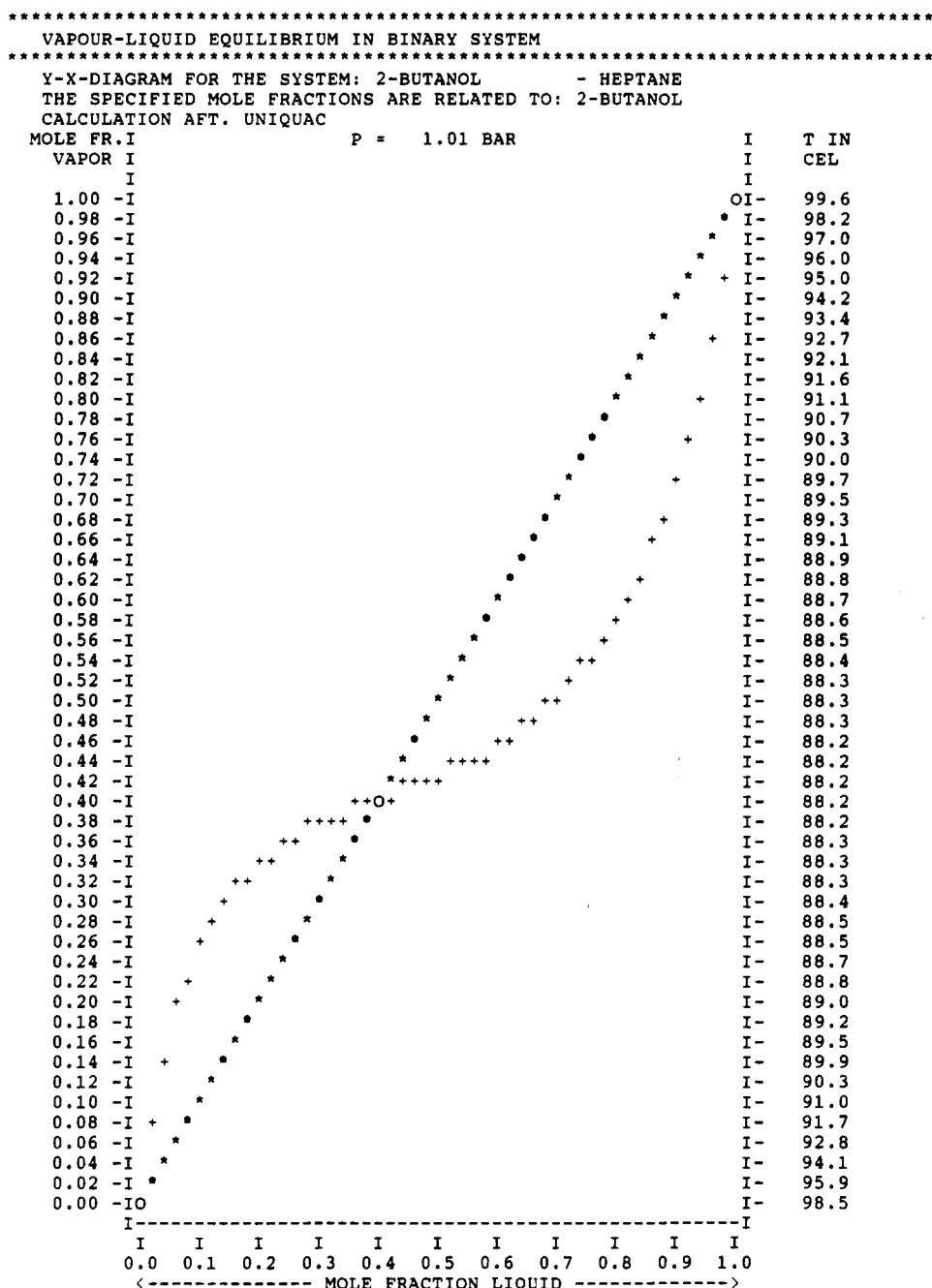


Figure 2. Isobaric binary vapor-liquid equilibrium diagram.

-SDC, and -SDS. DETHERM-SDR provides access to a literature database consisting at present of more than 16 600 documents, 85 500 tables, and 845 500 data records for 3700 compounds. Many of these data, i.e., for VLE, GLE, and transport properties, have been published in the DECHEMA Chemistry Data Series (CDS).¹¹

DETERM-SDC is a calculational program which allows the determination of properties for complex mixtures. Its internal database contains the pure component data for more than 550 chemical compounds. These data are stored in records of fixed length—the data vectors. Each data vector contains 240 basic data properties for each compound. Examples are density at various temperatures, critical constants, boiling temperature, viscosity, etc. These data are taken from the literature. If several literature values are available for a given property, a data analysis is carried out: The data are carefully evaluated and compared by statistical methods.

Data for all properties for a given pure component in the system are always entered into the data vectors. If a desired

property cannot be obtained from the literature, then it is estimated from the molecular structure or from other already-known properties such as the normal boiling point. DETHERM-SDS is very useful in this regard. DETHERM-SDS provides estimates of data based on the boiling point and whatever other empirical values are available. Of course, the more completely the data vectors are filled with measured values for the individual components, the more satisfactory the estimations are likely to be. For VLE and GLE calculations, appropriate binary interaction parameters are needed for the desired method for calculating phase equilibria, such as Wilson, NRTL, or UNIQUAC. These values are taken from such references as Gmehling et al.⁷ Recommended parameters, which are computed from several literature sources, are available for approximately 140 binary pairs. The interaction parameters for 410 other binaries are calculated from reliable single data sets. For the equation of state methods including Lee-Kesler-Ploecker, Redlich, Kwong-Soave, and Peng-Robinson, the binary interaction parameters

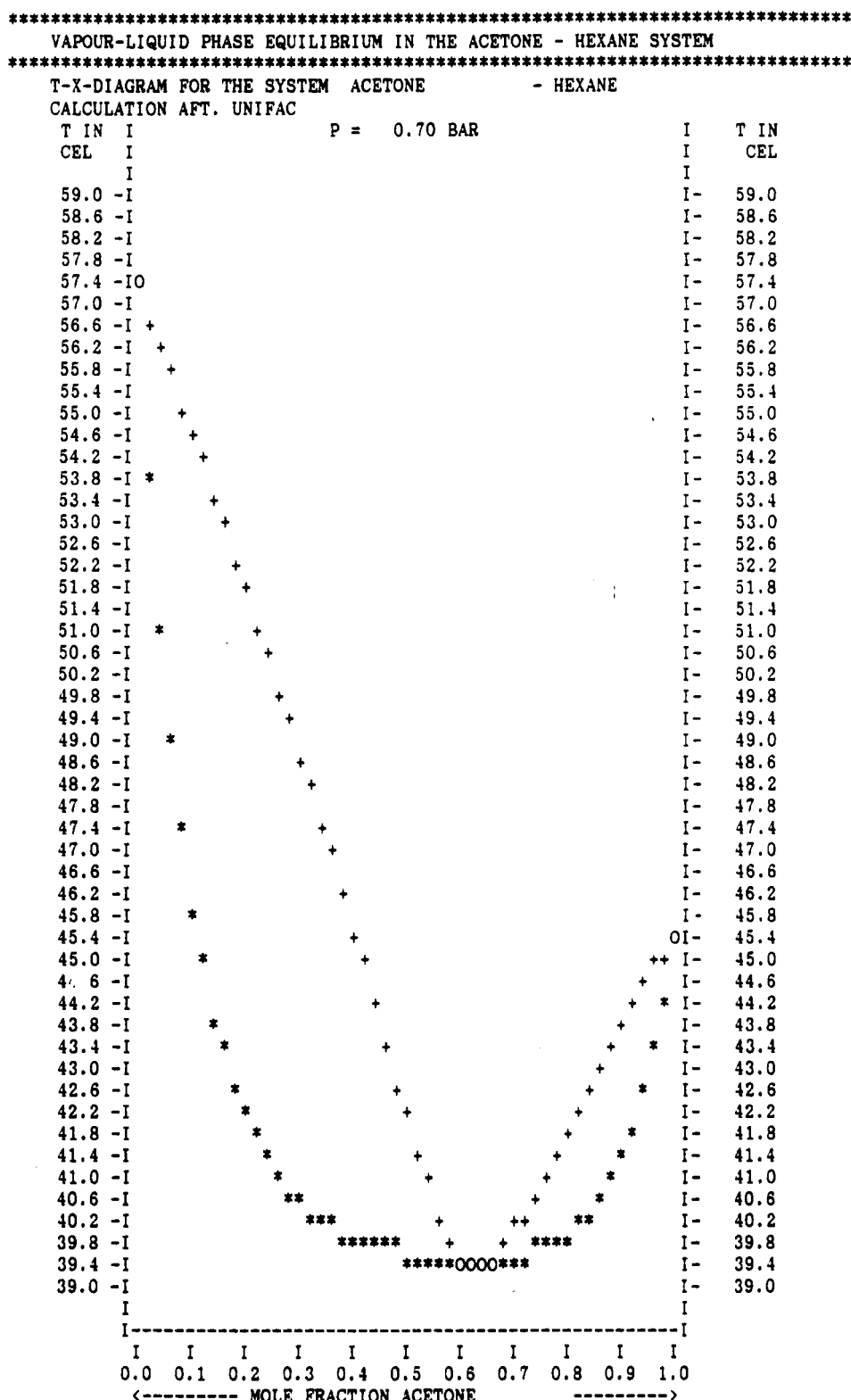


Figure 3. Isobaric binary boiling temperature diagram.

are taken from Knapp et al.⁸ The recommended parameters for 130 binaries consisting of low-boiling substances are available.

These data, so generated and appropriately formatted, can then be used as input parameters for such simulation packages as SST (Heat Exchangers), FRNC-5 (Fired Heaters), or REFORMER for performing stepwise simulation calculations of high accuracy. These types of calculations are especially important if studies of fouling are undertaken.¹²⁻¹⁸ Direct links have been written for such general chemical plant simulation

packages as ASPEN-PLUS.

Several examples of data retrieval and calculational capabilities of DETHERM are given in Figures 1-7.

RESULTS

The comparison of heat-exchanger calculations carried out according to the averaging method with those calculated according to the stepwise method show that there are decided advantages to the stepwise method, assuming that adequate

```

* D E T H E R M - S D C
* DATA CALCULATION SYSTEM VERSION 2.6
* 04/21/88
*****
TABLE AND DIAGRAM OUTPUT
*****
STREAM 5
CODE NAME MOLE FRAC. MOLE AMOUNT WEIGHT WEIGHT AM.
      KMOL FRACTION KG
22 METHANE 0.300000 0.300 0.180613 4.81
23 ETHANE 0.300000 0.300 0.338530 9.02
24 PROPANE 0.100000 0.100 0.165482 4.41
116 NITROGEN 0.300000 0.300 0.315376 8.40
SUM 1.000000 1.000 1.000000 26.65
* D E T H E R M - S D C
* DATA CALCULATION SYSTEM VERSION 2.6
* 04/21/88
*****
TABLE AND DIAGRAM OUTPUT
*****
TABLE OF THE VISCOSITIES OF STREAM 5
*****
TEMP. PRES. STATE VISCOSITY ( IN MPA.S )
CEL BAR AGGR. MOLAR AFTER LEE AFTER WILKE AFTER STIEL
      I I I AVERAGE AND DEAN
*****
0.0 1.50 I G 0.01124 0.01064 0.01067
10.0 1.50 I G 0.01160 0.01100 0.01103
20.0 1.50 I G 0.01196 0.01136 0.01139
30.0 1.50 I G 0.01231 0.01171 0.01174
40.0 1.50 I G 0.01266 0.01206 0.01209
50.0 1.50 I G 0.01301 0.01241 0.01244
60.0 1.50 I G 0.01335 0.01275 0.01278
70.0 1.50 I G 0.01369 0.01309 0.01312
80.0 1.50 I G 0.01403 0.01343 0.01345
90.0 1.50 I G 0.01436 0.01376 0.01378
100.0 1.50 I G 0.01468 0.01409 0.01411
110.0 1.50 I G 0.01501 0.01441 0.01444
120.0 1.50 I G 0.01533 0.01473 0.01476
130.0 1.50 I G 0.01565 0.01505 0.01507
140.0 1.50 I G 0.01596 0.01537 0.01539
150.0 1.50 I G 0.01627 0.01568 0.01570
160.0 1.50 I G 0.01658 0.01599 0.01601
170.0 1.50 I G 0.01688 0.01629 0.01631
180.0 1.50 I G 0.01718 0.01659 0.01661
190.0 1.50 I G 0.01748 0.01689 0.01691
200.0 1.50 I G 0.01777 0.01719 0.01721
210.0 1.50 I G 0.01807 0.01749 0.01750
220.0 1.50 I G 0.01836 0.01778 0.01779
230.0 1.50 I G 0.01864 0.01807 0.01808
240.0 1.50 I G 0.01893 0.01835 0.01837
250.0 1.50 I G 0.01921 0.01864 0.01865

```

Figure 4. DETHERM-SDC viscosity table.

Property	DETHERM-SDS	Literature Value	Deviation %
normal boiling point (K)	352	347	1.2
critical temperature (K)	555	545	1.8
critical pressure (bar)	41.2	44.8	-8.7
standard heat of formation, gas, at 25°C (kJ/Mol)	-141.3	-142.4	0.8
density, liquid, at 20°C (g/cc)	1.342	1.338	0.3
viscosity, liquid, 20°C (cP)	0.769	0.824	-7.2
thermal conductivity, liquid, at 20°C (W/mK)	0.118	0.102	13.1

Figure 5. Synthesized data compared with literature data for 1,1,1-trichloroethane.

physical-property data are available for all relevant values of temperature and pressure occurring in the system. Also, a complete, detailed description of the various regions within the heat exchanger or the furnace or the tubes of the reformer can be achieved. This is important for determining eddy currents and studying the special effects which might occur within the piece of equipment.

Stepwise Shell and Tube Exchanger Simulation (SST) can improve the efficiency of heat transfer and monitor fouling in a plant and consequently reduce fuel consumption and flue gas emission from furnaces and boilers. Since FRNC-5 can improve the efficiency of fired heaters and boilers, the resulting optimized designs will release fewer flue gas tons with pollutants to the atmosphere. This is especially true for pollutants such as hydrocarbons, CO, and sulfur compounds. This may not apply to NO_x because some waste heat recovery with FRNC-5 lowers flue gas temperature and thus increases NO_x. However, if NH₃ injection is used to lower NO_x, the FRNC-5 program can be used to optimize the points of NH₃ injection and thereby help to reduce NO_x.

Those properties which are needed for the calculation are the following: density, viscosity, thermal conductivity, heat capacity, enthalpy, surface tension, and liquid critical pressure.

ND: 0.0-PRP-2.49 COPYRIGHT 06/03/86 DECHEMA E.V., FRANKFURT/MAIN
 LA: ENGL
 DT: 02
 ID: CDB
 AU: FREISER, H.; GLOWACKI, W. L.
 TI: SOME PHYSICAL PROPERTIES OF ISOQUINOLINE.
 JA: J. AM. CHEM. SOC.
 CO: JACSAT
 VO: 71
 PA: 514
 PY: 1949

(1) C9H7N
 ISOQUINOLINE
 NUMBER: 119-65-3

COLUMN 1: TEMPERATURE			
TAG:	TSY#ULUUDSTU	UNIT:	K
PURE COMPOUND	LIQUID		VALUE
COLUMN 2: VISCOSITY			
TAG:	VIS#ULUUDSTU	UNIT:	PA.S
PURE COMPOUND	LIQUID		VALUE
COLUMN 3: DENSITY			
TAG:	DNS#ULUUDSTU	UNIT:	KG/M3
PURE COMPOUND	LIQUID		VALUE
1:	TSY	2:	VIS
3:	DNS		
303.15	0.0032528	1091.0	
313.15	0.0026034	1083.1	
323.15	0.0021323	1075.2	
333.15	0.0017872	1067.3	
343.15	0.0015269	1059.4	
353.15	0.0013223	1051.4	
373.15	0.0010230	1035.4	
398.15	0.00077870	1015.5	
423.15	0.00062170	994.98	
448.15	0.00050670	974.21	
473.15	0.00042230	953.00	

*** END OF TABLE ***

Figure 6. Typical document with data on a coal chemical (extract).

Viscosity and thermal conductivity have recently been treated in detail by Stephan and Heckenberger.¹¹ Especially correlations giving a functional representation of the variation of these transport properties with temperature, pressure, and composition as well as diagrams of the results are presented. Only three methods can effectively describe viscosity over the entire fluid range: 1, the method of Chung; 2, the method of Ely and Hanley; 3, the residual viscosity method. Some illustrative examples of the results of Stephan and Heckenberger demonstrating the dependencies of these properties on the variables temperature, pressure, and composition are given.

The data for the liquid viscosity of water-ethanol mixtures demonstrate how greatly the viscosity can vary with temperature and composition. If the 80% composition line for water is considered, the viscosity varies from roughly 6500 to 632 μ Pa-s as the temperature is increased from 275 to 350 K. Thus, errors in the position of measuring the temperature can result in large errors in determination of the apparent local temperature. This in turn would lead to very great errors in the viscosity, which brings with it extreme errors in the heat-transfer coefficient of the apparatus. Obviously this will influence the design of the heat exchanger. Assuming an error of 5 K is made in determining the temperature at 275 K (280 instead of 275 K is measured), then the viscosity of 5039.1 instead of 6487.0 μ Pa-s, an error of 1447.9 or 22%. For 90% water the percentage error is just as great: 3971.5 instead of 5115.5 μ Pa-s, and an error of 1144 μ Pa-s or 22% as well (cf. p 318 in ref 4 and Figure 8). The thermal conductivity also varies greatly. At 275 K it assumes a value of 392.4 mW/m-K for a concentration of 0.8 and 460.0 mW/m-K for a mole fraction of 0.9 in water at a pressure of 0.1 MPa (cf. p 199 in ref 4 and Figure 9).

This illustrates how essential accurate temperature and pressure values are to the stepwise method. In their treatment of the viscosity of liquids and gases Reid et al.¹² recommend methods for correlating viscosities with temperature, estimating viscosities when no experimental data are available, estimating the effects of pressure on viscosity, and estimating the viscosity of mixtures.⁵ These have partially been incorporated into

DATA BANK: CHEMSAFE
 ND: 8.1-FXL-1001.89
 AU: Nabert, K.; Schoen, G.
 JA: Deutscher Eichverlag; Braunschweig (Pub.)
 JS: 2. ED.
 PY: 1963-1989

PURE COMPONENT
 EG: 603-022-00-4
 UN: 1155

: LW: Regulations and laws concerning transportation and treatment
 : These classifications were made by the producer of the data base.
 : !class!subs.risks!pack.group!number/pack.instr.
 : -----!-----!-----!-----!-----!-----
 : UNO-recommendations ! 3 ! ! !
 : GGVSee (D) ! 3,1 ! ! !
 : IMDG-Code ! 3,1 ! ! !
 : GGVE-GGVS (D) ! 3 ! ! !2a
 : RDI-ADR ! 3 ! ! !2a
 : ICAO/IATA-regulat. ! 3 ! ! !pass. plane: FORBIDDEN
 : ! ! ! !cargo plane: 303
 : ChemG-Gefstoffv. (D) R-phrases: R12,19
 : S-phrases: S9,16,29,33
 : V.brennb.Fluess. (D) class: AI
 : electr. equipment temperature class (DIN): 4 ignition group (VDE): 4
 : electr. equipment explosion class: 1 explos. group (VDE/DIN): IIB
 : NM: 1,1'-OXYBISETHANE
 : FM: C4H10O
 : SD: FORMATION OF PEROXIDE
 : CR: 60-29-7

PROPERTIES	VALUES	UNITS
MEP#UUUUUD@TR: MAXIMUM EXPLOSION PRESSURE, RECOMMENDED	10.0	BAR
AIT#UUUUUF@TR: AUTOIGNITION TEMPERATURE, GERMAN STANDARD, RECOMMENDED	170.	CEL
UEL#UUUUUF@TR: UPPER EXPLOSION LIMIT, GERMAN STANDARD, RECOMMENDED	1100.	G/M3
LEL#UUUUUF@TR: LOWER EXPLOSION LIMIT, GERMAN STANDARD, RECOMMENDED	50.	G/M3
UEL#UUUUUF@TR: UPPER EXPLOSION LIMIT, GERMAN STANDARD, RECOMMENDED	36.0	VOLUME %
LEL#UUUUUF@TR: LOWER EXPLOSION LIMIT, GERMAN STANDARD, RECOMMENDED	1.7	VOLUME %
FLP#UUUG#D@TR: FLASH POINT, CLOSED CUP, RECOMMENDED	<	-20. CEL

Figure 7. Typical document with safety characteristics.

DETERM. Especially DETHERM-SDS, where thermo-physical properties are estimated for systems where no or only inadequate measured values exist, will employ more accurate methods and more efficient algorithms. Future versions of the DETHERM program will be oriented more toward modern interfaces and expert systems to aid the user in selecting the methods appropriate to the case at hand, depending upon the temperature, pressure, and composition of the mixture being studied. This is an undertaking which should rightly be shared among the various institutions engaged worldwide in thermochemical research.

The following mixing rules were used in making the calculations presented here:

thermal conductivity

$$y = (x_1 y_1^A + (1 - x_1) y_2^A)^{1/A} + x_1 (1 - x_1) B \quad (\text{C21})$$

viscosity

$$\ln y =$$

$$x_1 \ln y_1 + (1 - x_1) \ln y_2 + \ln \left[1 + \frac{(1 - x_1) x_1}{A + B(1 - x_1)^2} \right] \quad (\text{C22})$$

with x_1 = mole fraction of water, y_1 = viscosity of pure water, and y_2 = viscosity of pure alcohol.

In a database such as DETHERM it can be assumed that there will be an improvement of data quality as a function of time. That is, the reliability of the data increases—let us assume exponentially—as a function of the time that has elapsed since they were entered into the database. A time constant can be defined, γ , analogous to a relaxation time which depends (roughly) upon the number of users and the intensity of the use of the data.

The more intensively the data are used, the sooner and the more readily inaccuracies and inconsistencies can be discovered and corrected, whether these stem from the original literature or result from transfer of the data from one storage medium

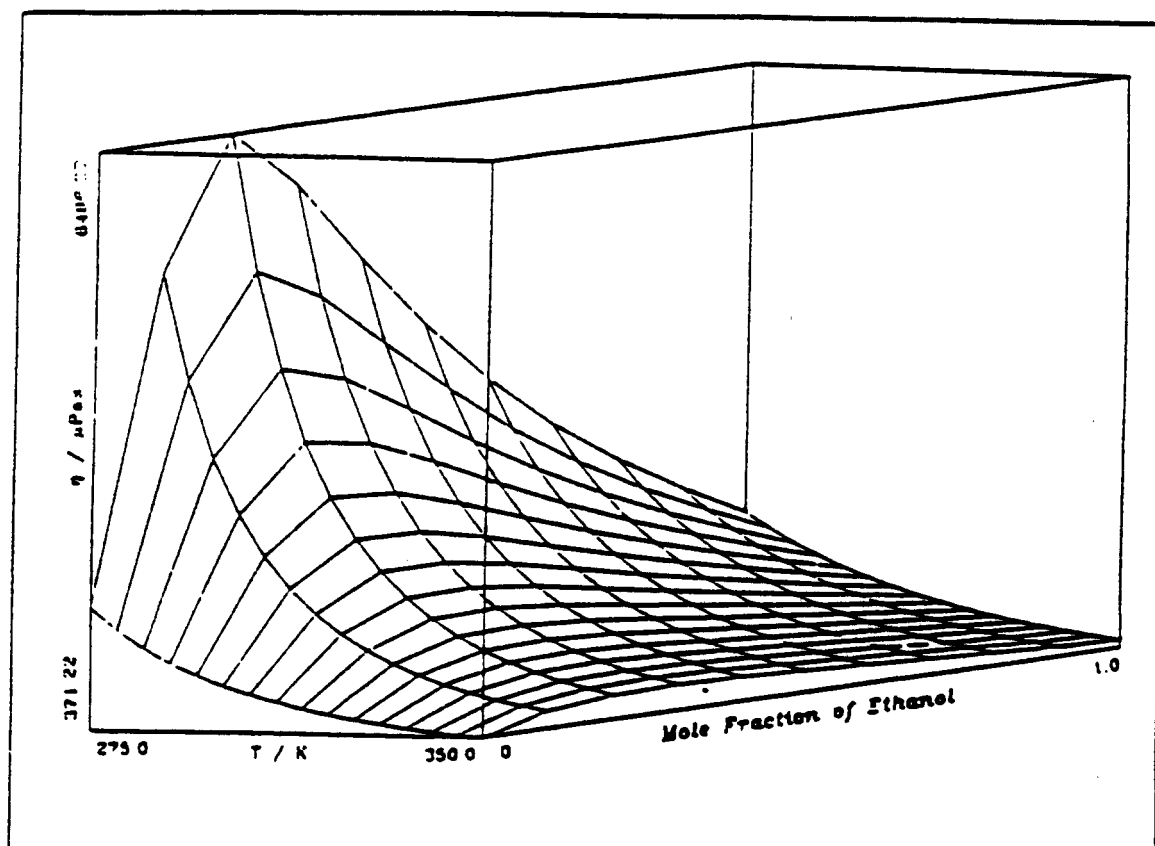


Figure 8. Liquid viscosity of water-ethanol mixtures at 0.1 μPa (linear axes) (cf. Stephan and Heckenberger¹¹).

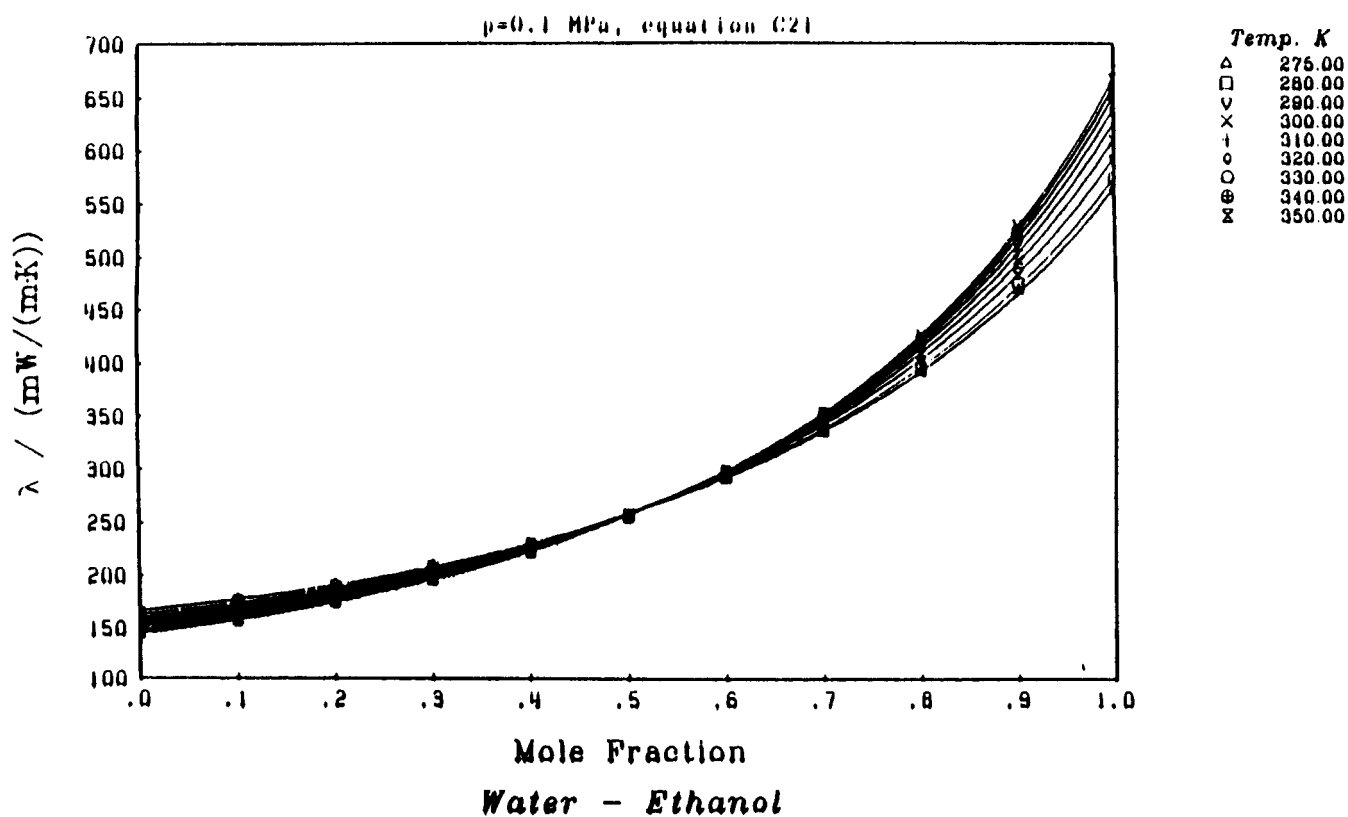


Figure 9. Thermal conductivity of water-ethanol mixtures.

to another. This is, then, one of the specific advantages of a database that is used worldwide—the greater the number of users and the greater the variety of problems that are treated,

the sooner inaccuracies will be discovered and the more reliable the database will become. This is also one of the great advantages of the worldwide cooperation among those producing

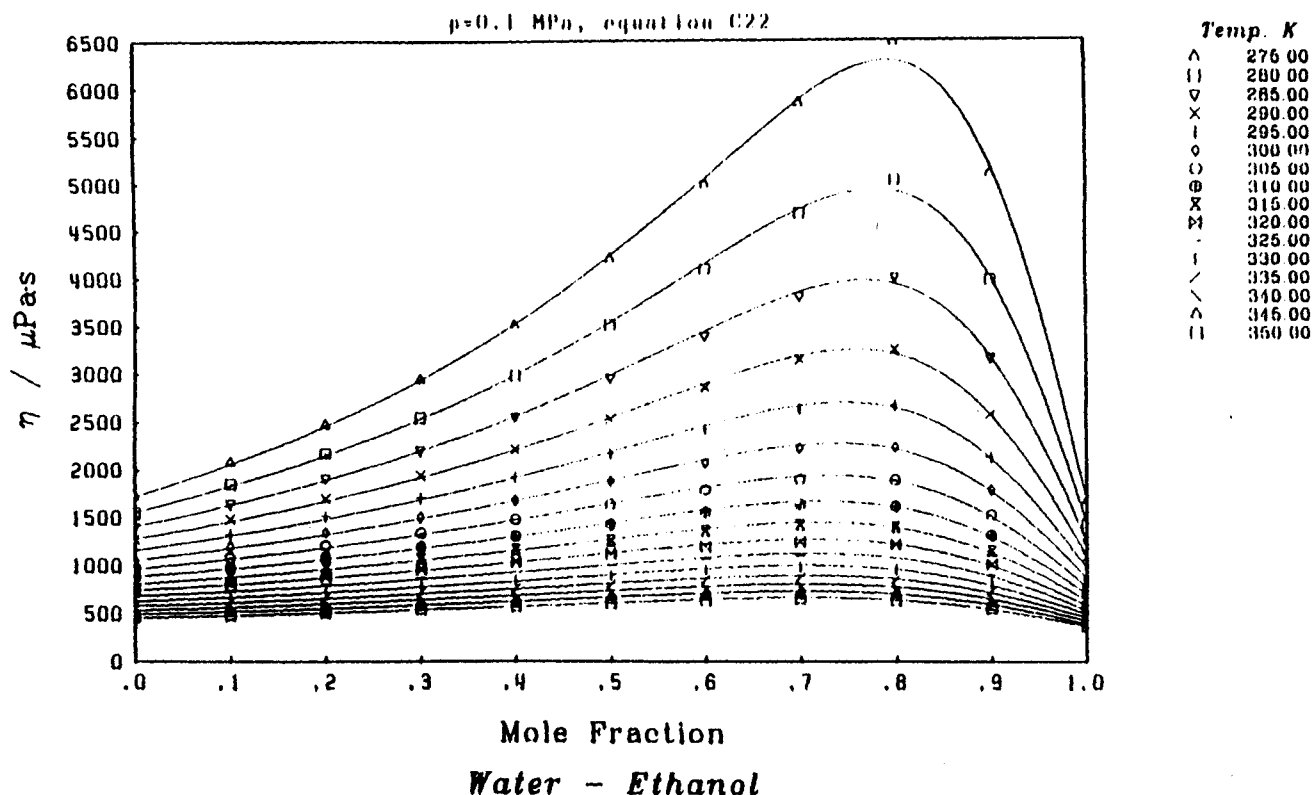


Figure 10. Viscosity of water-ethanol mixtures.

and distributing databases. The greater the use and the critical analysis of the database, certainly the more confidence one can have in using the values contained therein.

SUMMARY AND CONCLUSIONS

The more sensitive the mathematical simulation methods, the greater is the required accuracy of the physical-property data. Because the stepwise method yields results for the various regions of the furnaces and heat exchangers where temperature, pressure, and consequently the quality (percent of fluid in the vapor state) vary, it is necessary to reliably know the physical property and especially the transport property and phase equilibrium (VLE) data to high accuracy as a function of temperature and pressure and composition. This applies to the vapor and liquid states as well. The density certainly varies as a function of the temperature and the pressure. As indicated in the figures shown, the viscosity and the thermal conductivities are strong functions of the density. Consequently these properties are also strongly dependent upon temperature and pressure. The stepwise method is inherently more accurate and capable of yielding a more detailed description of the geometry of the heat-transfer equipment and of the internal flow conditions and regimes well.⁶⁻¹¹

It is of little avail, however, if adequate physical-property data are not available. It is the purpose of DETHERM to provide these thermophysical property data under the conditions required—whether from the literature, through correlations, or through estimation techniques such as incremental methods. Then, with the dual factors of increased mathematical simulation capability and adequate knowledge of the requisite thermophysical properties, the total simulation of the heat-transfer system can be carried out to greater accuracy. This allows a significantly more reliable optimization of the equipment so that the desired improvements in economy and environmental protection can be achieved. Thus, the more accurate stepwise simulation method brings advantages for

the plant operator and for the environment and is a logical starting point for the design of new equipment and the improvement of existing installations.

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