Easy-to-use Mathcad Computer Methods for Interconversion of Petroleum Distillation Curves. Part 4: ASTM - EFV (Equilibrium Flash Vaporization) Conversion Using Composite Functions

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Abstract

The procedure developed by Riazi and Daubert [1] [2] for EFV (Equilibrium Flash Vaporization) curve prediction starting from ASTM distillation data is transposed into Mathcad. A legible and easy-to-use worksheet for direct and reversed (EFV to ASTM) conversions is thus provided. Both input and predicted distillation curves are represented as 7 rows × 2 columns matrices, where first column contains the %vol. and the second column the corresponding temperatures. Correlations of Riazi & Daubert needed in the procedure are written as functions and composite functions which allow the conversion from one type of distillation into the other by a mere call of single-argument function and with the initial distillation data as input. Examples with distillation data taken from [1] allowed the verification of the Mathcad-written version and illustrate its convenient utilization.

Key words: *ASTM D 86, EFV, distillation, interconversion, Mathcad, petroleum*

Introduction

The main goal of this part of the work is to provide the Mathcad implementation of the Riazi and Daubert [1] procedure for estimation of EFV (Equilibrium Flash Vaporization) curve from ASTM distillation curve. First, relations and parameters values as given by Riazi and Daubert [1] [2] will be presented and the Mathcad version of the mentioned procedure will subsequently be described in detail. The given Mathcad version is relying mainly on composition of functions and allows a simple and direct utilization, by a mere call of a function whose argument is the initial (given) distillation curve to be converted.

Several versions of Mathcad transcription of Daubert-API procedure [3a] [4] for ASTM-TBP (True Boiling Point) distillation temperatures interconversion have been documented in previous parts [5].

Since experimental setup and procedure for EFV data measurement are difficult, several methods for EFV curve prediction have been developed, such as those of : Edmister & Okamoto [6-9] [16], Nelson [10] [11] [16], Maxwell [9] [12] [16], Obreadcikov & Smidov, or of Piroomov and Beiswenger [8] [13-16], to mention some of the most frequently used. The first method, of Edmister & Okamoto, is basically using ASTM curve, that of Nelson may use ASTM or TBP curves, while the last three are starting from TBP data. Unfortunately, all these

older methods are using graphical correlations and hence are not amenable to a direct utilization on computers. Subsequently, some of these methods were adapted for computer use [17] or improved correlations [2] allowed their direct use in computer programs.

Correlations for bubble point pressure [18-21] or dew point pressure [22-23] may be also undertaken for the estimation of the EFV curve.

The procedure of Riazi and Daubert cited above [2] was included in API 5th ed. [3a], while latest editions of API-TDB (the 6th and 7th, [3b, 3c]) does no more contain some convenient correlation between EFV curve and the other types of distillation curves, being argued that the tedious experimental procedures for EFV made its determination quite rare presently. EFV data are instead determined in [3b, c] (Ch. 8D, Procedure 8D1.6) by an iterative calculation, based on fugacities in liquid and vapor phases computed from SRK (Soave-Redlich-Kwong) equation of state applied on the entire fraction or crude or on pseudo components and using acentric factors from the Lee & Kesler correlation [24]. Nevertheless, such an approach implies several pages of program lines which may not be available or are cumbersome for estimative purposes or field conditions.

Similar detailed approach for LVE calculation, based on equilibrium constants (or equilibrium ratios, $K_i = y_i / x_i$) values alone or in combination with equations of state for liquid and vapor phases, may be found in several textbooks [16] [25-34]. The detailed calculation can be also carried out with dedicated software packages (Pro/II, Hysys-Aspen, ChemCAD), but their prices and demands in computer resources may not always be profitable to the gain in accuracy of predicted EFV curve or data.

However, in our current practice availability of handy and simple correlations for a fast estimation of EVF points proved often valuable. Enjoying particular features of Mathcad environment like natural syntax and interactivity, the herein presented Mathcad version of Riazi-Daubert procedure is thus providing an easy-to-use method for EFV curve estimation.

Brief Presentation of Riazi-Daubert Procedure for ASTM-EFV Distillation Curves Interconversion [1]

The procedure set forth by Riazi and Daubert [1] [2] uses the following simple relation between the ASTM temperatures ($T_{ip(ASTM)}$, K) and EFV temperatures ($T_{ip(EFV)}$, K) :

$$T_{ip(EFV)} = a_{Rip} \cdot T_{ip(ASTM)}^{\ b_{Rip}} \cdot SG^{c_{Rip}} \qquad (1)$$

where *ip* denotes the selected points on the two curves, corresponding to 0, 10, 30, 50, 70, 90 and 100% vol. distilled, and a_{Rip} , b_{Rip} , c_{Rip} empirical parameters with the values given in Table 1. Same table also gives (last column) the temperature ranges of petroleum cuts analyzed by Riazi and Daubert when developing their correlation (1), that is use of the correlations (1) outside the given ranges can cause large errors in predicted temperatures. It is claimed that the procedure of Riazi and Daubert offers a better accuracy for all EFV points than other methods (*e.g.* of Edmister & Okamoto [6-9] [16]). Supplementary information on the accuracy or on drawbacks of the procedure may be found in the original works of Riazi and Daubert [1] [2].

The ASTM – EFV correlation of Riazi & Daubert is also quoted in [35], with some values of coefficients eventually slightly different from those given in Table 1, $a_{R0} = 2.9748$; $a_{R6} = 7.9950$; $c_{R0} = 0.4208$ to be more specific, that is the values initially published by Riazi & Daubert in [2].

It's worth to remind that such correlation is valid for crude stocks and petroleum fractions, with many components having close boiling temperatures spread over the whole boiling range (quasi-continuous composition).

Table 1. Parameters for the Riazi-Daubert correlation (1) between ASTM distillation and EFV temperatures (from [1])

ip	% vol.	a_R	b_R	c_R	Allowed range (on ASTM), ℃
0	0	2.9747	0.8466	0.4209	10 – 265
1	10	1.4459	0.9511	0.1287	60 – 320
2	30	0.8506	1.0315	0.0817	90 – 340
3	50	3.2680	0.8274	0.6214	110 – 355
4	70	8.2873	0.6871	0.9340	130 – 400
5	90	10.6266	0.6529	1.1025	160 – 520
6	100	7.9952	0.6949	1.0737	190 – 430

It is obvious from relation (1) that the specific gravity (*SG*) is needed when Riazi-Daubert procedure is employed for prediction EFV points, while other methods, like that of Edmister and Okamoto are relying on (ASTM) distillation data alone. Nevertheless, when the relative density (d_{60F}^{60F} or specific gravity, *SG*) of the crude or of the petroleum fraction is not available, a workaround is its approximation by the next correlation (2) with the ASTM temperatures, *K*, for 10% and 50% vol.:

$$SG\_A = a_{dA} \cdot T_{10\%}^{b_{dA}} \cdot T_{50\%}^{c_{dA}} \qquad (2)$$

as recommended by the authors of the procedure [1] [2]. The coefficients have the following values: $a_{dA} = 0.08342$, $b_{dA} = 0.10731$, $c_{dA} = 0.26288$ and correlation (2) is valid when the temperatures $T_{10\%}$, $T_{50\%}$ of ASTM distillation are within the ranges 308 – 568 *K* (35 – 295 ℃) and 333 – 638 *K* (60 – 365 ℃), respectively, and *SG* (*SG_A*) between 0.70 and 1.00 . Previous correlation (2) for approximation of *SG* (*SG_A*) is to be used only within the Riazi-Daubert procedure for EFV curve prediction. The authors of the procedure also give in [1] [2] values of the coefficients when the correlation (2) for specific gravity is applied to temperatures $T_{10\%}$, $T_{50\%}$ of a TBP or an EFV curve.

Moreover, relations analogous to (1) and (2) are given by Riazi and Daubert [1] for the interconversion of ASTM and TBP distillation curves. Using these relations, one may readily predict EFV curve starting from TBPs, too.

Mathcad Implementation of Riazi-Daubert Procedure for ASTM – EFV Distillation Curves Interconversion.

The part of the Mathcad worksheet with the procedure for the direct conversion, from ASTM distillation curve to EFV curve, is shown in Figure 1.

The input distillation curve (argument «DC») as well as the output, computed EFV curve, are represented in the same format as in previous parts of our work [5], *i.e.* 7 rows × 2 columns matrix, where the first column elements are volume percentages (0, 10, 30, 50, 70, 90 and 100) of distillate and the second column elements are the corresponding seven temperatures (℃ or *K*) on the (ASTM or EFV) distillation curve.

Text is written in our original Mathcad worksheet with characters (Book Antiqua 9, in blue color) which are different from those employed for calculations (Times New Roman, in black), in order to easier differentiate text regions from math regions.

Parameters : coefficients a_R, b_R, c_R of relation (1) (method of Riazi & Daubert [1, 2]) :

$$a_R := \begin{pmatrix} 2.9747 \\ 1.4459 \\ 0.8506 \\ 3.2680 \\ 8.2873 \\ 10.6266 \\ 7.9952 \end{pmatrix} \quad b_R := \begin{pmatrix} 0.8466 \\ 0.9511 \\ 1.0315 \\ 0.8274 \\ 0.6871 \\ 0.6529 \\ 0.6949 \end{pmatrix} \quad c_R := \begin{pmatrix} 0.4209 \\ 0.1287 \\ 0.0817 \\ 0.6214 \\ 0.9340 \\ 1.1025 \\ 1.0737 \end{pmatrix} \quad \%vol := \begin{pmatrix} 0 \\ 10 \\ 30 \\ 50 \\ 70 \\ 90 \\ 100 \end{pmatrix}$$

$Np := rows(\%vol)$

$Np = 7$

$ip := 0, 1 .. Np - 1$

USING COMPOSITE FUNCTIONS

A. ASTM ---> EFV Conversion

DEFINITIONS - GENERAL

a) SG known

- the function for EFV curve estimation (both ASTM and EFV [$\%vol.$; K]) is :

$$ASTMtoEFV\_K(SG,DC) := augment\left(DC^{\langle 0 \rangle}, \overrightarrow{\left[a_R \cdot SG^{c_R} \cdot \left(DC^{\langle 1 \rangle}\right)^{b_R}\right]}\right) \qquad \text{(MC-1)}$$

- if both distillation curves in [$\%vol.$; $°C$], ASTMtoEFV_C function is to be used :

$$ASTMtoEFV\_C(SG,DC) := augment\left(DC^{\langle 0 \rangle}, \overrightarrow{\left[a_R \cdot SG^{c_R} \cdot \left(DC^{\langle 1 \rangle} + 273.15\right)^{b_R} - 273.15\right]}\right) \qquad \text{(MC-2)}$$

Next "CtoKM" function may alternatively be used for conversion of a distillation curve "DC" from [$\%vol.$; $°C$] to [$\%vol.$; K] before employing (MC-1) :

$$CtoKM(DC) := augment\left(DC^{\langle 0 \rangle}, DC^{\langle 1 \rangle} + 273.15\right) \qquad \text{(MC-3)}$$

b) if SG unknown

it can be estimated with : $SGf\_A(DC) := a_{dA} \cdot \left[\left(DC^{\langle 1 \rangle}\right)_1\right]^{b_{dA}} \cdot \left[\left(DC^{\langle 1 \rangle}\right)_3\right]^{c_{dA}} \qquad \text{(MC-4)}$

where $\left(DC^{\langle 1 \rangle}\right)_1$ and $\left(DC^{\langle 1 \rangle}\right)_3$ provide T10% and T50% [K] (of the input ASTM curve), respecively, and values of the coefficients are : $a_{dA} \equiv 0.08342$, $b_{dA} \equiv 0.10731$ and $c_{dA} \equiv 0.26288$.

Then EFV curve, [$\%vol.$; K], is given by the function ASTMtoEFV_K1 :

$$ASTMtoEFV\_K1(DC) := ASTMtoEFV\_K(SGf\_A(DC),DC) \qquad \text{(MC-5)}$$

(with reuse of the previous definition of function ASTMtoEFV_K).

- or if both distillation curves, given ASTM and computed EFV, are [$\%vol.$; $°C$], then :

$$ASTMtoEFV\_C1(DC) := ASTMtoEFV\_C(SGf\_A(CtoKM(DC)),DC) \qquad \text{(MC-6)}$$

Fig. 1. Part of Mathcad worksheet with the parameters and functions needed for conversion of ASTM distillation curve into EFV curve according Riazi-Daubert procedure

First part of the worksheet (fig. 1) contains the assignments of numerical values (Table 1) to parameters needed subsequently in the procedure. Parameters are given as the three vectors «a_R», «b_R», «c_R». There is also definition of range variable «ip» for „counting" (indexing) the seven selected points on the distillation curve.

If input (given) ASTM curve is with absolute temperatures, prediction of EFV curve according Riazi-Daubert procedure is to be made with the function « ASTMtoEFV_K » defined in (MC-1) (fig. 1). Function « ASTMtoEFV_K » picks up temperatures of the initial ASTM distillation curve, that is second column of input matrix « DC » (« $DC^{<1>}$ »), applies on them relation (1), joins side by side the vector of %vol. and the vector with computed EFV temperatures and finally delivers the determined EFV curve under the standard matrix format (see also the glossary with the relevant Mathcad built-in functions at the end of the paper). The vectorize operator (arrow above) ensures that calculation is made element-wise, that is:

$$(a_R)_{ip} \cdot \left[(SG)_{ip}\right]^{(c_R)_{ip}} \cdot \left[(column2 - of - DC)_{ip}\right]^{(b_R)_{ip}} \tag{3}$$

for all the five vectors (of seven elements each). Reader may see examples in Part 2 and 3 [5b, c] of a calculation written in Mathcad with vectors elements carrying indexes instead using vectorize operator and producing vector-valued result too.

Function « ASTMtoEFV_C » (definition (MC-2) in fig. 1) has a similar aim, but it is to be used when temperatures of the two curves are expressed in degrees Celsius, ^oC. Since relation (1) of Riazi-Daubert procedure is for absolute temperatures, K, in definition (MC-2) input temperatures are first converted to degrees *Kelvin* before applying (1). Finally, 273.15 is subtracted from all the seven computed values, in order to carry out the reversed transformation, from K to ^oC, thus providing the predicted EFV points with temperatures in degrees centigrade (^oC).

Alternatively, function « CtoK » defined in (MC-3) may be employed for conversion of distillation data set from temperatures expressed in ^oC into data set with absolute temperatures (in K) (regardless the number of data points). We recall that in Mathcad a vector is by convention a single column matrix, convention which is also adopted in the present work since more natural (at least in the Mathcad environment). Moreover, several simple common operations between vectors and scalars (such as addition, multiplication with a scalar, linear combinations, ..., but not power) or implying vectors alone (logarithm, trigonometric, ...) are by default applying on all elements of the vector. For such operations (like in the definition (MC-3)) vectorize operator is obviously superfluous.

If the specific gravity (*SG*) is not available, correlation (2) must be included in the procedure calculations for the ASTM-to-EFV conversion, as described in previous chapter. *SG* is thus estimated with function « SGf_A » defined by expression (MC-4) (fig. 1). The function « SGf_A » of one argument, the input matrix « DC » with the distillation points, picks up the second element of the second column, « $[DC^{<1>}]_1$ », and the fourth element of the same column, « $[DC^{<1>}]_3$ », of the matrix « DC », that is temperatures $T_{10\%}$ and $T_{50\%}$, respectively, and applies on them relation (2).

Assignments of values to the three parameters needed in function « SGf_A » are made with global definition (« ≡ », triple equal) in math regions, but which are inserted in text area (below definition (MC-4), fig. 1). Global definitions prevail in the usual order of evaluations in the Mathcad worksheet on common definitions made with colon-equal (« := ») operator, that is a variable defined with global definition is evaluated before any variables defined with the usual colon-equal assignment. In our case, assignments of corresponding values to parameters « a_{dA} », « b_{dA} », « c_{dA} » are effective from the beginning of the worksheet, before the first colon-equal definition (*i.e.* before definition of vector « a_R »), and thus available to all colon-equal expressions (function « SGf_A » included) and calculations in the worksheet.

Global definitions are used here just for worksheet layout convenience, since they allow to display the assignments of parameters values *after* definition of function « SGf_A » which is including the three mentioned parameters.
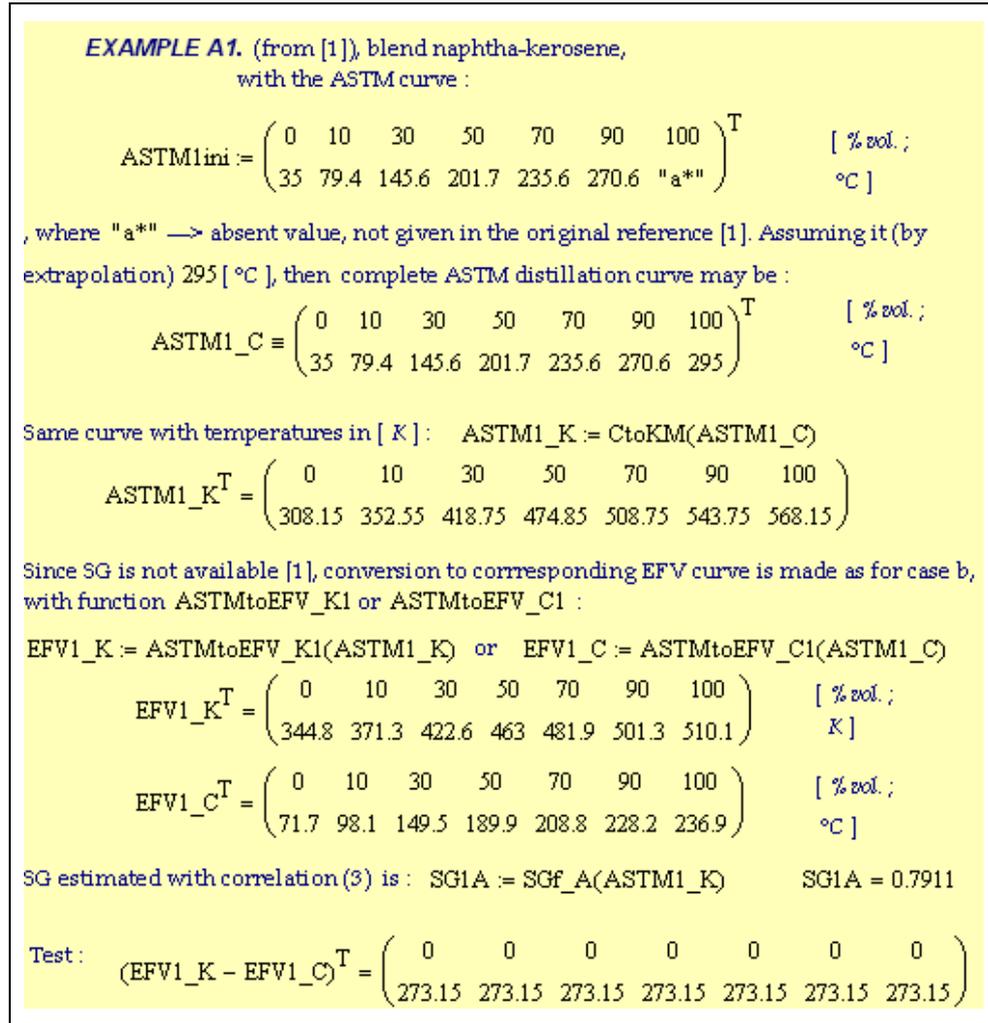
Fig. 2. Part of Mathcad worksheet containing an example of ASTM-to-EFV distillation data conversion with the Riazi-Daubert procedure

Function « ASTMtoEFV_K1 », which is then defined in relation (MC-5) (fig. 1), is aimed to carry out the computation of the EFV curve. Function « ASTMtoEFV_K1 » is obtained by composition of the two-variable function « ASTMtoEFV_K » with the one-variable function « SG_Af », both functions being previously defined in the Mathcad worksheet. Composition is made by replacement of the first variable (« SG ») of function « ASTMtoEFV_K » by the value of function « SGf_A ». Since argument of function « SGf_A » is the distillation data matrix « DC », and the second variable of function « ASTMtoEFV_K » remains the same « DC », the resulted composite function « ASTMtoEFV_K1 » is obviously of a single variable, same generic variable « DC » standing for the matrix of the initial ASTM distillation curve.

Definitions of composite functions such as « ASTMtoEFV_K », « ASTMtoEFV_C », « CtoK » or even like « ASTMtoEFV_K1 » or « ASTMtoEFV_C1 » in Fig. 1 can also be easily written in Mathcad employing the tree operator (see example of tree operator use in Part 3 [5c]).

Composite function « ASTMtoEFV_K1 » (case b, *SG* not available, absolute temperatures) may be rewritten more explicitly, always in a single line, as in the next definition (4) of « ASTMtoEFV_K1c » which provides same result (same 7 × 2 matrix) like « ASTMtoEFV_K1 » of (MC-5), Figure 1:

$$\text{ASTMtoEFV\_K1c(DC)} := \text{augment}\left[\text{DC}^{\langle 0 \rangle}, \begin{vmatrix} \text{for } ip \in 0,1\ldots \text{rows(DC)} - 1 \\ T_{EFV_{ip}} \leftarrow \left[{}^a R_{ip} \cdot \left[\left(\text{DC}^{\langle 1 \rangle} \right)_{ip} \right]^{{}^b R_{ip}} \cdot \text{SGf\_A(DC)}^{{}^c R_{ip}} \right] \\ T_{EFV} \end{vmatrix}\right] \tag{4}$$

The programming module in (4) in the second argument of « augment » is needed in order to provide a vector, since otherwise direct calculation with the variables and the parameters indexed with the range variable « ip » like in the following expression (5)

$${}^a R_{ip} \cdot \left[\left(\text{DC}^{\langle 1 \rangle} + 273.15 \right)_{ip} \right]^{{}^b R_{ip}} \cdot \text{SGf\_A(CtoKM(DC))}^{{}^c R_{ip}} \tag{5}$$

is generating an array of (seven) values which is not a vector and hence it is not suitable as argument for « augment » function (leading on evaluation to error message and turning into red ; see also p. 171 in [5b] or [36] for supplementary explanations on this issue).

Utilization of the Riazi-Daubert procedure transcribed into Mathcad as described above is illustrated in Figure 2. Input ASTM distillation data (« ASTM1ini ») has been taken from [1], in order to be able to check our Mathcad version of the procedure. The EFV data computed in Figure 2 (« EFV1_C ») are thus identical with those determined with the same procedure in [1].

Relation (1) can be readily rearranged in order to use it for the reversed conversion, that is from EFV temperatures to ASTM distillation data :

$$T_{(ASTM)ip} = a_{Rip}^{-\frac{1}{b_{Rip}}} \cdot T_{(EFV)ip}^{\frac{1}{b_{Rip}}} \cdot SG^{-\frac{c_{Rip}}{b_{Rip}}} \tag{6}$$

The part of Mathcad worksheet with functions definitions needed for this reversed conversion is given in Figure 3. These definitions have been written following same lines as those detailed above for the direct conversion. Coefficients for *SG* estimation according correlation (2) when applied to EFV temperatures have the following values : $a_{dE} = 0.09138$, $b_{dE} = -0.0153$, $c_{dE} = 0.36844$, which are valid for EFV temperatures $T_{10\%}$ and $T_{50\%}$ within the ranges 352 – 623 *K* (79 – 350 ^oC) and 378 – 638 *K* (105 – 365 ^oC), respectively. An example illustrating the use of mentioned functions for the EFV-to-ASTM conversion is provided by the part of Mathcad worksheet given in Figure 4 (« *EXAMPLE B1* »). As shown in the latter figure, when using the same *SG* as that estimated based on ASTM data (« SG1A », = 0.7911), the ASTM temperatures computed with the reversed procedure (and given in matrices « ASTM1a_C » or « ASTM1a_K », temperatures in ^oC, *K*, respectively) are, as expected, identical with the initial ones (« ASTM1_C » or « ASTM1_K »), taken as input in example A1 of the direct procedure. Differences in some of the last *displayed* decimal may be noticed, *i.e.* for computed $T_{50\%}$ and $T_{70\%}$ in « ASTM1a_K » of Figure 4 when compared to same temperatures in the initial « ASTM1_K » of Figure 2, but explanation for these differences is left to the reader's care (The reason for the noticed differences is not obvious ..., some hints may be found at [37]).

Correlations of same form with (1) and (2) have been also established by Riazi & Daubert [1] for TBP – ASTM distillation data interconversion or for estimation of ASTM distillation curve based on SD (Simulated Distillation, by gas-chromatography, according ASTM D 2887 standard). Using as a model the worksheet previously described, Mathcad files (worksheets) with Riazi-Daubert procedures for interconversion of the various distillation data or prediction based on SD curve may be readily written too.

We currently use the Mathcad version of the Riazi-Daubert procedure for EFV curve prediction as one of the tools in the design and computation of operating parameters (temperatures, pressure drops) of transportation pipes or of fired heaters tubes for crude or petroleum fractions.

For such equipment, where biphasic liquid-vapor flow occurs frequently, availability of a simple and yet of adequate accuracy method for EFV data prediction proved to be very useful.

Fig. 3. Part of Mathcad worksheet with the parameters and functions needed for conversion of EFV data into ASTM distillation curve according the Riazi-Daubert procedure

Conclusion

After a first part with a brief review of the most ever used methods for EFV prediction, procedure developed by Riazi and Daubert [1] [2] for interconversion of ASTM and EFV distillation curves and the Mathcad-written version of the procedure are described in detail in the rest of the paper. The Mathcad worksheet containing the Riazi-Daubert procedure is presented at full length and provides a convenient tool for a fast prediction of the EFV temperatures, all the more so it enjoys some of particular features of Mathcad environment, such as natural syntax and readability or numerous built-in functions.

Once the Mathcad worksheet written as presented herein, the EFV curve may be then determined based on ASTM distillation data by a simple call of a single-variable function in the Mathcad worksheet, *i.e.* of that named « ASTMtoEFV_K » or « ASTMtoEFV_K1 » (temperatures in K ; « ASTMtoEFV_C » or « ASTMtoEFV_C1 » when temperatures in ^{o}C) in Figure 1 or in the example of Figure 2.

EXAMPLE B1. (adapted from [1]), same blend naphtha-kerosene, with a given EFV curve same as that computed in EXAMPLE A1 (Fig. 2)

$$EFV1\_C^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 71.7 & 98.1 & 149.5 & 189.9 & 208.8 & 228.2 & 236.9 \end{pmatrix} \quad [\%\,vol.; \; ^{\circ}C]$$

or with temperatures in [K] :

$$EFV1\_K^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 344.8 & 371.3 & 422.6 & 463 & 481.9 & 501.3 & 510.1 \end{pmatrix} \quad [\%\,vol.; \; K]$$

- SG of the blend not known => conversion to corresponding ASTM curve with the function EFVtoASTM_K1 :

ASTM1b_K := EFVtoASTM_K1(EFV1_K)

$$ASTM1b\_K^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 306.24 & 351.95 & 418.34 & 470.41 & 500.17 & 532.39 & 557.28 \end{pmatrix} \quad [\%\,vol.; \; K]$$

or with function EFVtoASTM_C1 :

ASTM1b_C := EFVtoASTM_C1(EFV1_C)

$$ASTM1b\_C^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 33.09 & 78.8 & 145.19 & 197.26 & 227.02 & 259.24 & 284.13 \end{pmatrix} \quad [\%\,vol.; \; ^{\circ}C]$$

SG estimated based on input EFV curve is :   SG1b_E := SGf_E(ASTM1b_K)   SG1b_E = 0.8064

Test :

$$ASTM1b\_K^T - ASTM1b\_C^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 273.15 & 273.15 & 273.15 & 273.15 & 273.15 & 273.15 & 273.15 \end{pmatrix}$$

- if SG of the naphtha-kerosene blend admitted same as previously determined (SG1A = 0.7911 , Example A1, Fig. 2), two-variable functions, EFVtoASTM_K or EFVtoASTM_C, defined for the case of a known SG, may be used :

ASTM1a_K := EFVtoASTM_K(SG1A, EFV1_K)   ASTM1a_C := EFVtoASTM_C(SG1A, EFV1_C)

$$ASTM1a\_K^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 308.1 & 352.5 & 418.8 & 474.9 & 508.7 & 543.8 & 568.1 \end{pmatrix} \quad [\%\,vol.; \; K]$$

$$ASTM1a\_C^T = \begin{pmatrix} 0 & 10 & 30 & 50 & 70 & 90 & 100 \\ 35 & 79.4 & 145.6 & 201.7 & 235.6 & 270.6 & 295 \end{pmatrix} \quad [\%\,vol.; \; ^{\circ}C]$$

Thus the initial ASTM temperatures (in ASTM1_K or ASTM1_C, Fig. 2) are indeed retrieved.
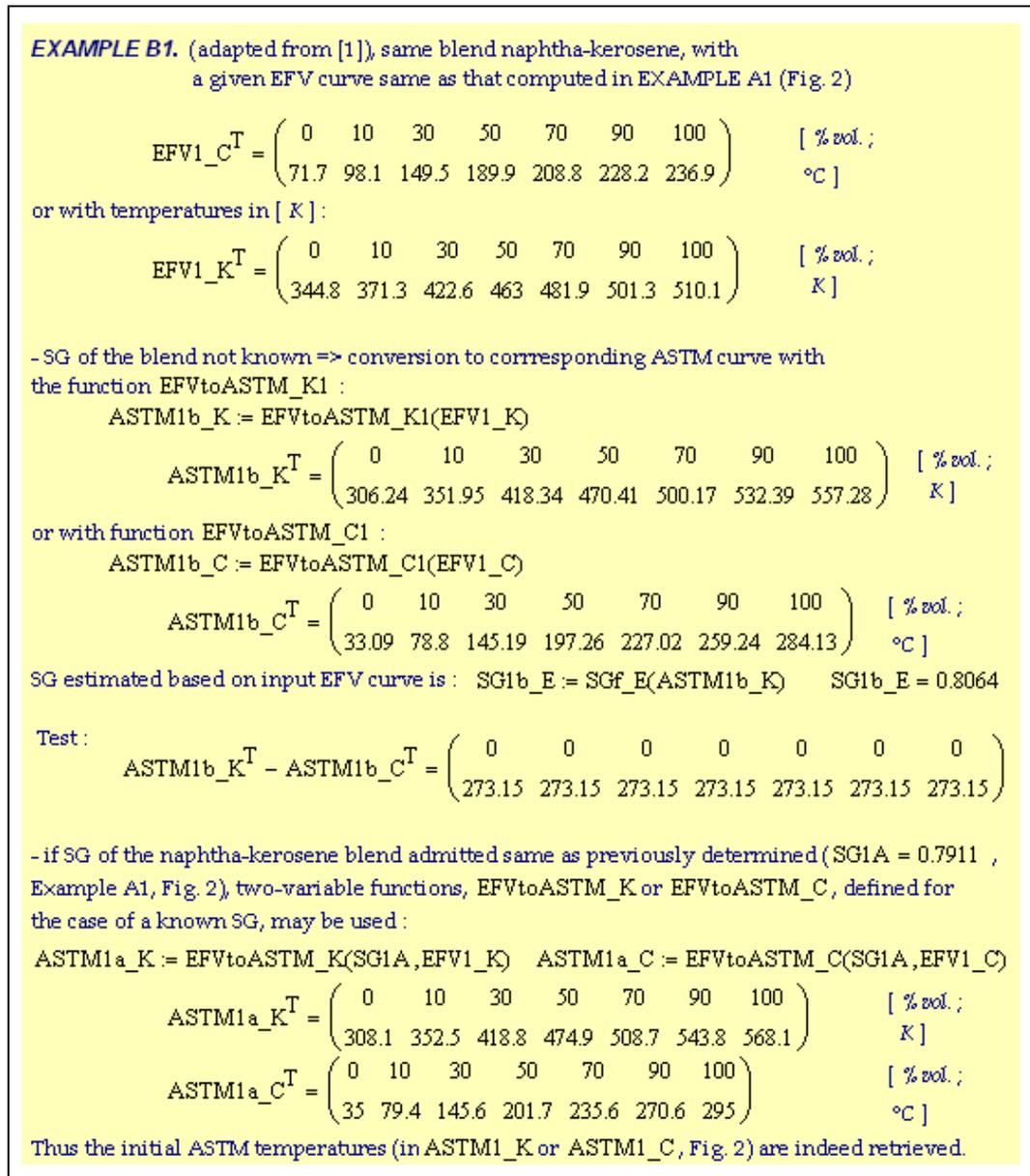
Fig. 4. Part of Mathcad worksheet containing an example of EFV-to-ASTM distillation data conversion

Glossary of main Mathcad operators and built-in functions used
(see also [36])

$\rightarrow$ („vectorize") (placed above expression containing a vector) – operations or function applied to every element of the vector, providing a result-vector of same dimension (may be used for matrices, too)

$^{<n>}$ (as superscript) – returns a vector made from the elements of the $n+1$-th column of a matrix

^{T} (as superscript) – returns the transposed matrix

augment – provides a „larger" matrix by joining side by side two (or several) vectors or matrices with same number of rows (of same „height")

rows – returns the number of rows of the input matrix

Notations and acronyms

_A – meaning applied to ASTM data (as in « SGf_A » in relation (MC-4) of fig. 1)
_C – showing that dealing with temperatures in ^{o}C (when in function name)
_E – meaning : for EFV, or applied to EFV data (like for « SGf_E » in relation (MC-9) of fig. 3)
_K – showing that dealing with absolute temperature, in degrees K (when in function name)
ASTM – distillation curve, according ASTM D 86 (as part of functions or matrices names ; also as subscript)
a, *b*, *c* – coefficients
d – density (relative), or denoting „for density" when subscript
DC – generic matrix with distillation curve (given under the format described in text)
EFV – Equilibrium Flash Vaporization (as part of functions or matrices names ; also as subscript)
F – degrees Fahrenheit, ^{o}F
f – function (in function names, when needed for clarity)
Np – number of points in distillation data (Np = 7)
SD – simulated distillation (by GC, according ASTM D 2887)
SG – specific gravity (d_{60F}^{60F})
TBP – True Boiling Point

Subscripts

ip – range variable, for indexing elements of vectors (ip = 0, 1,..., 6)
A – denoting: applied to ASTM data
E – denoting: applied to EFV data
R – denoting: of Riazi(-Daubert) procedure

Errata

1. in Part 2 [5b], p. 170, row 22, word „six" is to be replaced by „seven" and thus read „the corresponding seven temperatures";
2. in title of Part 3 [5c] (5th row) and some other few places, erroneous term „composed" instead of the correct one, „composite", has slipped in, although the right „composite function(s)" has been used in the rest of occurrences.

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36. * * * – a) Mathcad help; b) Resource Center accompanying Mathcad platform, which can be accessed from Mathcad help menu.
37. * * * – http://communities.ptc.com/message/154834#154834 (Mathcad forum of PTC; accessed June 2011).

Transpuneri în Mathcad uşor de utilizat pe calculator ale metodelor de interconversie a curbelor de distilare ale fracţiunilor petroliere. Partea a 4-a. Proceduri de interconversie a curbelor ASRO („STAS") – VE (vaporizare la echilibru) folosind funcţii compuse

Rezumat

Procedura elaborată de către Riazi şi Daubert [1] [2] pentru predicţia curbei VE (Vaporizare la Echilibru) pe baza curbei de distilare ASRO (cf. SR ISO 3405:1998, în trecut „STAS", cf. STAS 36-1980 ; echivalent cu ASTM D 86) este transpusă în platforma Mathcad. Este astfel prezentată foaia de calcul Mathcad cu care se poate efectua atât conversia directă, de la curba ASRO la curba VE, cât şi conversia inversă, VE - ASRO. Foaia de calcul permite o utilizare comodă, fiind totodată uşor de citit, datorită în particular sintaxei naturale a platformei Mathcad. Ambele curbe de distilare, iniţială şi calculată, sunt reprezentate sub forma unei matrici cu 7 linii şi 2 coloane, prima coloană cuprinzând % volum distilat, iar a 2-a coloană temperaturile corespunzătoare. Corelaţiile Riazi-Daubert folosite de către procedură sunt scrise în Mathcad sub formă de funcţii sau funcţii compuse, ce fac posibilă în final conversia de la un tip la celălalt de curbă printr-o simplă apelare a unei funcţii de o singură variabilă, curba de distilare iniţială (dată). Exemplele furnizate, cu date preluate din literatură [1], pe lângă ilustrarea modului convenabil de utilizare a foii de calcul, au permis verificarea versiunii Mathcad a procedurii.