Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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INTRODUCTION

The ASTM D2502[1] standard test method uses kinematic viscosity measurements[2] in cSt of a petroleum oil at 100 °F (V100, V1) and 210°F (V210, V2) to estimate its molecular weight. The method requires looking up an "H" function (H100=870*Log(Log(V1+0.6)+154)) from a table based on the viscosity at 100°F. The table H100 function is then located on the vertical y ordinate axis of a chart. Following that value horizontally across the chart until it intersects with the line of viscosity V210 for the oil and then dropping vertically down to the horizontal x abscissa axis, the molecular weight (MW) can be read for the oil.

PROBLEM

The H100 function value in the ASTM D2502 table, its point on the chart ordinate, the lines of constant viscosity (isostoke) at 210°F and the MW on the abscissa may all require interpolate or estimating their locations. The H100 function and spacing of the lines of V210 isostokes are inherently nonlinear making their estimation even more problematic. These issues make the method tedious, time-consuming and prone to error.

The procedure is only valid when using the large chart ASTM developed for the method. This implies using the small chart supplied with the method is not appropriate, as "the precision statements given in the method will not apply". Obtaining the large chart and the difficulties in handling it are additional annoyances that distract from getting correct reading.

A method to calculate the molecular weight from the viscosities would eliminate these errors.

SOLUTION

Calculation

The following original calculation algorithm[3] models the entire ASTM chart. Lines in this paper with alphabetic character(s) in parentheses, an alternate typeface and indented lines designate program calculation code. The code only lists the lines needed for the calculation and not any GW-BASIC definition statements (DEFINT, DEFSNG, DIM), line numbers or input and output statements. Comments precede sections of the calculations to describe their purpose in the computation.

At the end of the paper is the molecular weight calculation coded in GW-BASIC and in Excel VBA that uses viscosities in cSt at 100°F and 210°F. Those viscosities are the ones used in the ASTM method. The Excel VBA has an option to check if the viscosities are valid and within the range of the chart. Since viscosities at these temperatures is less common, an additional VBA function is available that will convert viscosities from 40°C and 100°C for use in the calculation.

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Caution, the logarithmic function has inconsistent naming formats in various programming languages. The same format can reference different bases for the logarithm. Table 1 has the format and base for GW-Basic, Excel VBA and Excel worksheets. Any code listings are in the format used by that language so there is minimal editing when copied.

Table 1 Logarithmic Name Formats in this Paper and Codes

Format	Base	Used in
Ln	***e***	Excel Worksheets, body of this paper, traditional form
Log	10	Excel Worksheets, body of this paper, traditional form
Log	***e***	GW-BASIC, Excel VBA, C++

The calculation lines (a) through (ag) are in GW-BASIC. Throughout the paper, "H" function uses the Log base 10 while the "F" functions use Ln base ***e***.

This is the main polynomial fit using generalized H100 and H210 functions defined as F1 and F2 along with a generalized difference function of F1 and F2 (F12).

```
F1=LOG(LOG(V1+C(1)))                                      (a)
F2=LOG(LOG(V2+C(2)))                                      (b)
F12=LOG(F1-C(3)*F2-C(4))                                  (c)
MW0=C(5)+C(6)*F12+C(7)*F12*F2^2+C(8)*F1^4+C(9)*F1*F2*F12  (d)
```

MWS (molecular weight scaled) is the scaled primary molecular weight (MW0) for use in elliptically skewed normal distribution fits to correct for patterns seen in the residues from (d).

```
MWS=MW0*0.01                                              (e)
```

There were 2 areas that had a pattern of residuals from fitting (d) to the data. One area had negative residuals and the other positive residuals. Figure 3 is an example of the pattern seen for the Hirschler model defined by equation [7]. The model (d) has a similar pattern of residuals. Additional calculations corrected for these patterns. The correction terms for both areas are elliptically skewed normal distribution fits with axis rotation and translation. Below is the listing (g) to (s) for the first correction term used to model the area of negative residuals.

```
SI1=SIN(C(10))                                            (g)
CO1=COS(C(10))                                            (h)
X1=(MWS*CO1+F2*SI1-C(11)*CO1-C(12)*SI1)/C(13)             (i)
X12=X1*X1                                                 (j)
Y1=(F2*CO1-C(12)*CO1-MWS*SI1+C(11)*SI1)/C(14)             (k)
Y12=Y1*Y1                                                 (l)
EL1=X12+Y12                                               (m)
```

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```
SG1=TAN(C(10))*(-C(11)+MWS)+C(12)-F2                    (n)
IF SG1<0 THEN SG12=-1 ELSE SG12=1                       (o)
EX1=SG12*EL1                                            (p)
EX11=EX1*(C(19)+EX1*C(20))                              (q)
EX12=EX1*(C(17)+EX1*(C(18)+EX11))                       (r)
MW1=C(15)*EXP(-(C(16)+EX12))                            (s)
```

Calculation lines (t) to (af) below is the listing for a second correction term for modeling the area of positive residuals. It is the same as (g) to (s) but with variable names altered to define it as the second term.

```
SI2=SIN(C(21))                                          (t)
CO2=COS(C(21))                                          (u)
X2=(MWS*CO2+F2*SI2-C(22)*CO2-C(23)*SI2)/C(24)           (v)
X22=X2*X2                                               (w)
Y2=(F2*CO2-C(23)*CO2-MWS*SI2+C(22)*SI2)/C(25)           (x)
Y22=Y2*Y2                                               (y)
EL2=X22+Y22                                             (z)
SG2=TAN(C(21))*(-C(22)+MWS)+C(23)-F2                    (aa)
IF SG2<0 THEN SG22=-1 ELSE SG22=1                       (ab)
EX2=SG22*EL2                                            (ac)
EX21=EX2*(C(30)+EX2*C(31))                              (ad)
EX22=EX2*(C(28)+EX2*(C(29)+EX21))                       (ae)
MW2=C(26)*EXP(-(C(27)+EX22))                            (af)
```

The main polynomial molecule weight, the 2 correction terms and an offset are summed to give the final MWC.

```
MWC=MW0+MW1+MW2+C(32)                                   (ag)
```

Definitions

Table 2 is a listing of the coefficients. C1, C2, …C32 are alternate references to these coefficients used elsewhere in the paper. Table 3 lists major variables and GW-BASIC reserved words used.

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Table 2 ASTM D2502 Model Coefficients

C(1)=4.11	C(12)=2.356	C(23)=-4.326
C(2)=1.358	C(13)=1.07	C(24)=6.223
C(3)=1.5414	C(14)=1.446	C(25)=300
C(4)=-0.4106	C(15)=-31.5	C(26)=-0.00326
C(5)=197.6	C(16)=-0.64	C(27)=19.54
C(6)=-592.944	C(17)=0.069	C(28)=-30.387
C(7)=-96.08	C(18)=0.31	C(29)=-12.02
C(8)=0.8759	C(19)=-0.032	C(30)=7.276
C(9)=154.29	C(20)=0.002	C(31)=6.498
C(10)=-1.513	C(21)=-1.267	C(32)=52.3
C(11)=4.126	C(22)=8.05	

Table 3 Listing of Important Variables and GW-BASIC Reserved Words

Term	Description	Type
C(#)	Coefficients in the model	Array variable
V1	Viscosity of the oil at 100°F variable	Variable
V2	Viscosity of the oil at 210°F variable	Variable
MWC	Calculated molecular weight	Variable
IF THEN ELSE	Conditional execution statement	Reserved words
LOG	Natural logarithm function (base ***e***)	Reserved word
COS	Cosine function in radians	Reserved word
SIN	Sine function in radians	Reserved word
TAN	Tangent function in radians	Reserved word
DEF*type*, DIM	Examples of a variable definition statements in GW-BASIC with italics as the type of variable	Reserved words

RESULTS

Optimization of the coefficients in the model used one hundred and sixty two data points for fitting. The raw information for the data points was H100, V210 and MW. Testing the model used 40 pairs of randomly generated V100 and V210 values. The H100 value calculated from V100 and the V210 viscosity allowed finding the MW from the chart. Table 4 has the statistics comparing the MWC's to the MW's for the 2 sets of data along with ASTM precision data.

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Table 4 Model Fit to ASTM D2502 and Validation Statistics

Statistic	Fit	Test	ASTM Repeatability	ASTM Reproducibility
Sum of Squares	867	202		
Coefficient of Correlation (Pearson's r)	0.99987	0.99985		
Coefficient of Determination (R^2)	0.99974	0.99970		
F-Ratio	16234	870		
Probability	<0.00001	<0.00001		
Residual Standard Deviation (SD)	2.3	2.3	1.1 S_r	9 S_R
Residual SD 95% Confidence Limits	4.6	4.6	2.1	18
Slope	1.000	0.995		
Slope (95% Confidence)	±0.002	±0.005		
Intercept	0	2		
Intercept (95% Confidence)	±1	±2		
Minimum Residual	-6.8	-5.5		
Maximum Residual	6.4	3.4		
Data Points	162	40		
ASTM Precision (g/mole)	6	6	3 (r)	25 (R)

ASTM D2502-92 (Reapproved 1996) has a 3 g/mole repeatability (r) and a 25 g/mole reproducibility (R) but it was not obtained in accordance with R:D02-1007, "Manual on Determining Precision Data for ASTM Methods on Petroleum Products and Lubricants." Assuming laboratories received pairs of viscosity values and they determined the molecular weights, the repeatability (r) and reproducibility (R) can be calculated from the reported MW's. The relationship to the standard deviation (SD) for r and R (S_r and S_R) is assumed to be S= (r or R)/(Z*sqrt(2)) with the Z score of 1.96. The model has about twice the fit error as the repeatability of reading the chart using duplicate data by a single person in a single laboratory and 1/4 of the reproducibility error between laboratories. The calculation is much better for comparisons between laboratories. The initial fit of 110 data points showed around 15-20 points with large differences between MW and MWC. Rechecking the data to eliminate any that were outliers caused by inadvertent estimation and reading errors showed ten were inaccurate. If this is typical, then 10% of values determined from the chart will be in error.

The conclusion is the model reasonably estimates the values from the ASTM D2502 chart. The avoidance of inadvertent estimation errors is a better trade off as the loss in precision is smaller than the potentially larger errors during the estimation process. As it will be shown later, the loss in precision is small compared to the actual variation of the experimental data.

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DISCUSSION

Data Modeling and Testing

The initial work used 110 data points selected from the 22x28 inch chart offered by ASTM. Comparing these to the one hundred and three points reported in the original paper by Hirschler[4] (page 158, Table XI) showed fifty-one of them to be duplicates. Because the H100 had to be estimated, there were differences in the H100 values between the duplicate sets with the largest being 4. For the duplicate data, Hirschler's data took precedence over the data read from the chart. This gave one hundred and sixty two data points to determine the coefficients for the model (fifty-nine taken from the 22x28 inch chart offered by ASTM and one hundred and three from Hirschler).

These additional points were chosen from the chart to extended the extremes of the H100 function, to extend the extremes of the molecular weights, to fill in gaps on the original data (450, 550 and 650 molecular weight) and to included points on the 15 cSt at 210 °F isostoke. This gave a uniform coverage of the chart. The points chosen are where the H100 lines crossed isostokes of the 210 °F viscosities defined on the chart. This allowed for a more consistent linear interpolation of the axis values of the molecular weight, as the spacing between the 210 °F isostokes is non-linear. These points along with 40 additional test points used to determine the coefficients in the model are in Figure 1 along with their distributions in Figure 2.

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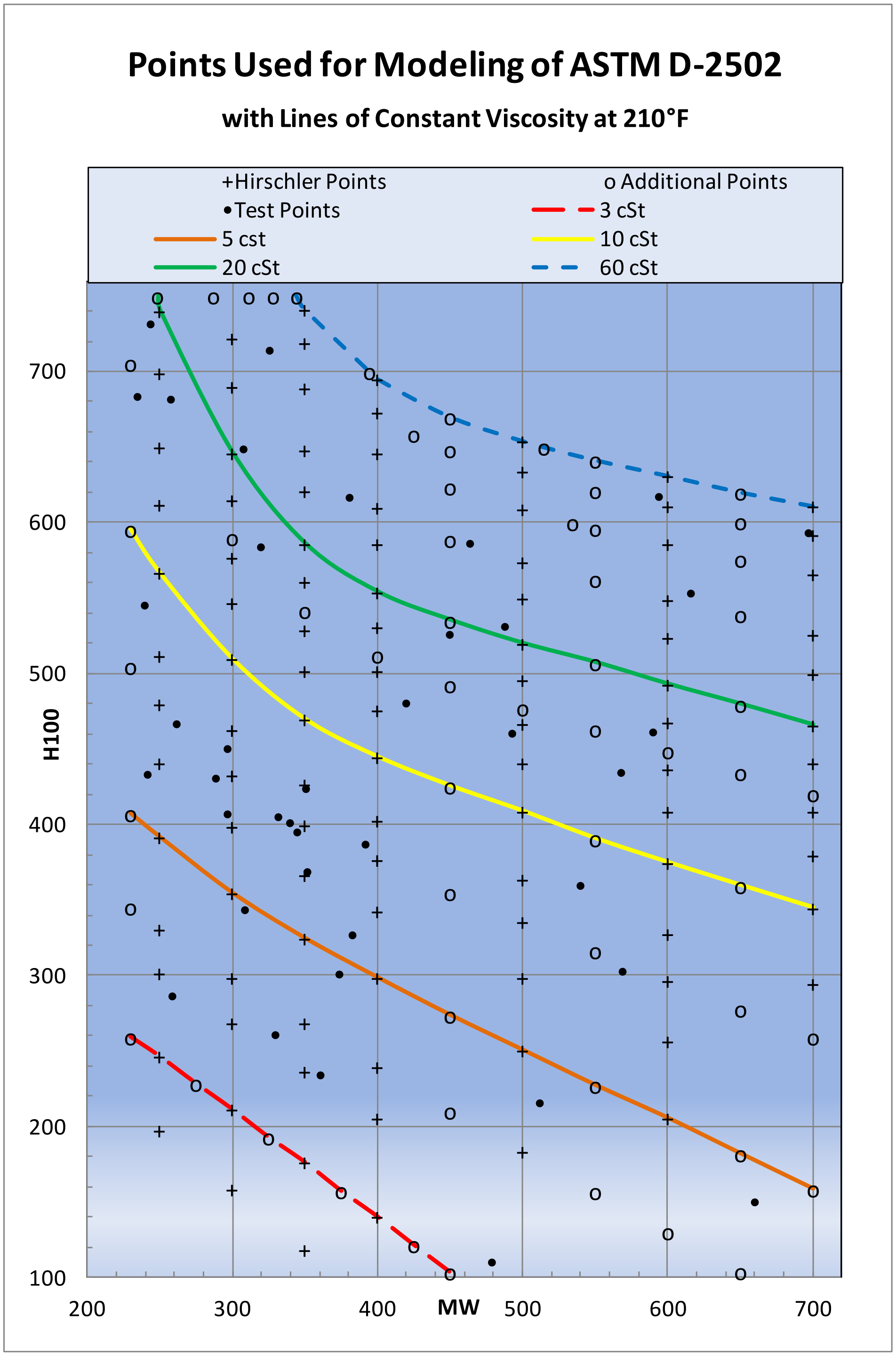

Figure 1 Data Points Used in Modeling ASTM D2502

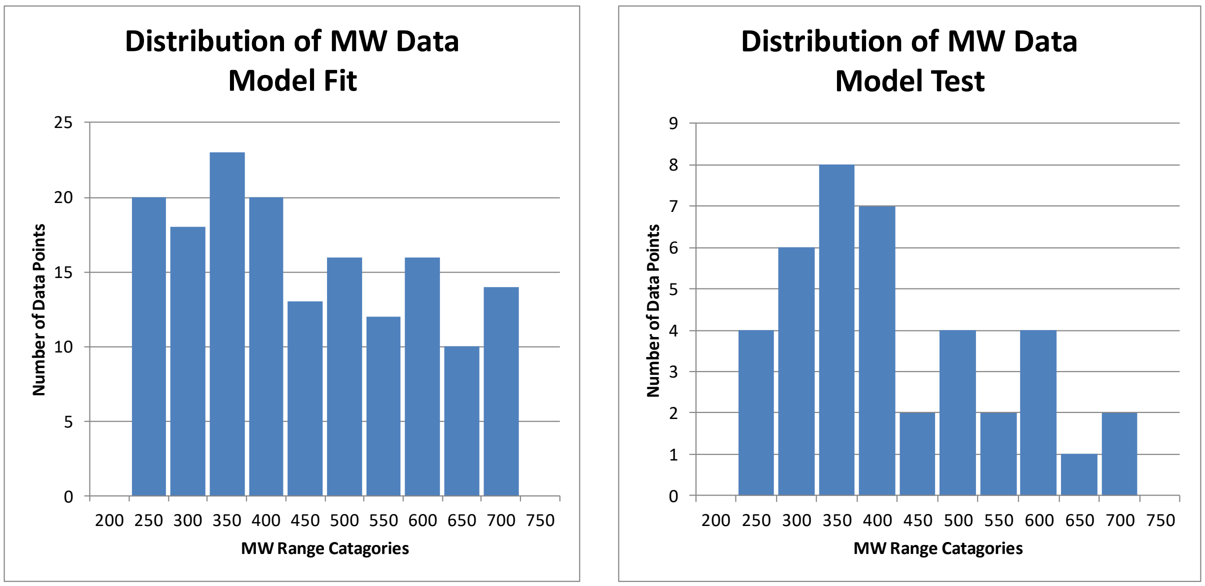

Figure 2 Distribution of MW Data used for Fitting and Testing ASTM D2502 Model

Modeling

Hirschler's equation [1], referenced in his paper as (5), defined the "H" function as a modified version with 0.6 in place of 0.8 used by Bell and Sharp[5].

$$H_t = 870\text{Log}\,(\text{Log}\,(V_t + 0.6)) + 154 \qquad [1]$$

where in [1]

H_t = the "H" function at temperature t
V_t = the kinematic viscosity in cSt at temperature t
Log = logarithm to base 10.

The inverse of the of H_t equation [1] is [2] and referenced as invH_t is

$$V_t = 10\text{^}(10\text{^}((H_t - 154)/870)) - 0.6 \qquad [2]$$

For determining the coefficients for the model, equation [2] converted Hirschler's data and the chart H100 data to V100. V100 is one of the inputs for the model.

Equation [3], given by Hirschler as (6), to calculate the molecular weight of an oil

$$MW = 180 + S(H_{100} + 60) \qquad [3]$$

where

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$$S = 4.146-1.733Log(VSF - 145) \quad [4]$$

$$VSF=H_{100}-H_{210} \quad [5]$$

and VSF is the viscosity slope factor as defined by Bell and Sharp[5].

Through simple algebraic substitution and rearrangement, equations [1], [3], [4] and [5], the MW calculation reduces to the form of [6]

$$MW = [180+4.146(154 + 60)] + [4.146*870]*F1 + [-1.733*870]*F1*F12 + [-1.733 (154+60)]*F12 \quad [6]$$

and generalized to [7]

$$MW= C5+C6*F1+C7*F1*F12+C8*F12 \quad [7]$$

where

$$F1=Log(Log (V1+C1)) \quad [8]$$

$$F2=Log(Log(V2+C2)) \quad [9]$$

$$F12=Log(F1-C3*F2-C4) \quad [10]$$

C1 to C8 = Coefficients.

Although Hirschler's paper used log to the base 10, the fit in GW-BASIC uses *Log* to the base ***e***. There is no issue in replacing Log base 10 with log base ***e*** (Ln) as they are linearly related by a constant (Log=2.3025*Ln). References to a Hirschler model in this paper denotes equation [7] using Ln.

Using the initial 110 data points from the chart before the Hirschler data was available from his paper gave the statistics in Table 6 and the C1 to C8 coefficients in Table 5. A self-written nonlinear least square (NLLSQ) program written in GW-BASIC[6] determined the coefficients. After entering a set of initial guesses for the coefficients, the program used a sequential simplex[7] to modify the coefficients to find a minimum residual sum of the squares. Eventually, a set of initial guesses led to a set of "optimized" coefficients, where no other set of initial guesses seemed to lead to a set of coefficients with a lower residual sum of squares.

Although, the coefficient set yielded a model with good regression statistics (Table 5) the standard deviation for the residuals were higher than desired.

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Table 5 Fit Statistics to Hirschler Model

Statistic	Value
Coefficient of Correlation	0.996
Standard Deviation of the Residuals	9.1
Number of points	110
F-Ratio (7/102 DF)	3457

Table 6 Hirschler Model Coefficients

Coefficient	Value	Coefficient	Value
C1	8.1206	C5	-56.638
C2	3.0463	C6	132.97
C3	1.802	C7	404.92
C4	-0.63234	C8	-1057.8

Figure 3 is a plot of the residuals (MW-MWC) from fitting the coefficients using Lotus[8] 1-2-3 with residual value as data labels. Lines of constant residuals are hand drawn. The negative values indicate the MWC was higher than the MW from the chart. The negative residuals delineate a "peak" or area of higher observed values at the coordinate at MW=400 and H100=400, 600 and a "valley" or area of low observed values at MW=600 and H100=500 with somewhat elliptical contours. Figure 4 is the same plot as Figure 3 but updated to include all 162 fit data points. It confirms the original contour plot.

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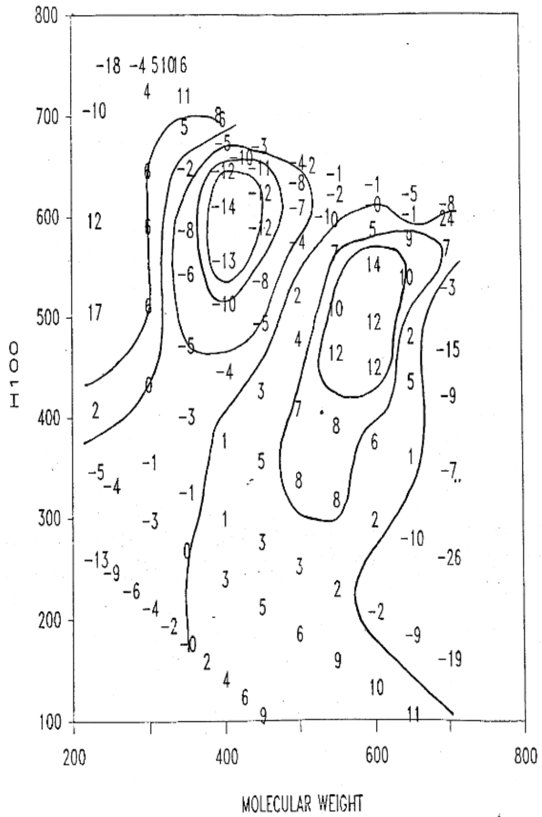

Figure 3 Contour Map of Residuals from Initial Fit of Calculation [7] Using Lotus 123 to Plot the Data and Hand Drawn Contours

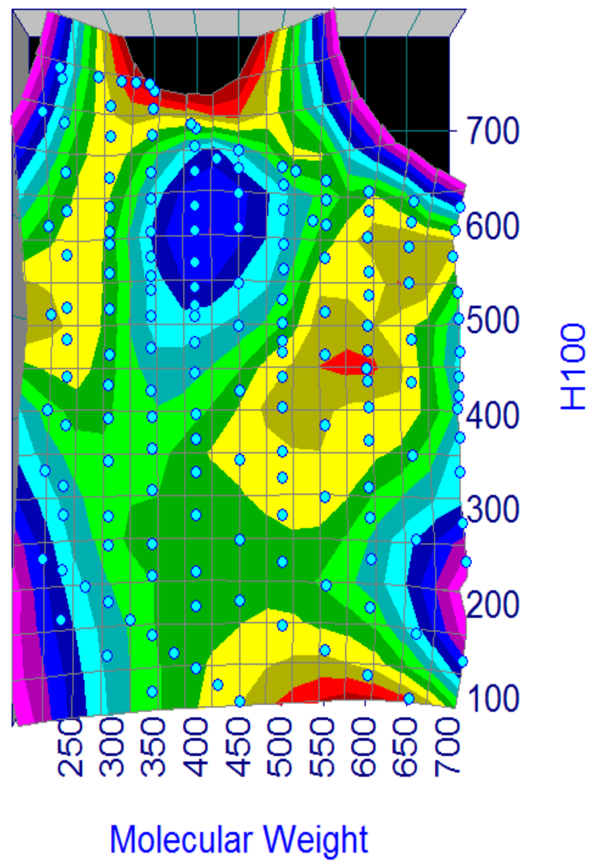

Figure 4 Contour Map of Residuals from Initial Fit of Calculation [7] Using TC3D to Plot the Data

To find an improvement to the fit, higher polynomial terms for F1, F2 and F12 were added to the initial Hirschler model. All 34 (combinations with replication) of the first through the fourth order terms and second through fourth order cross function terms of F1, F2 and F12 (i. e. (F12, (F1)^2, (F1)^4, (F12)^2*(F1)*(F2), (F12)*(F1)*(F2), (F1)^2*F3^3 etc...) were generated. An online computational service[9] with access to a stepwise multiple linear regression program[10] was used to select the most significant terms for inclusion in the model based on r^2 and F-ratio. Equation [11] and the calculation algorithm line (d) shows the terms chosen and used in the model.

$$MW=C5+C6*F12+C7*F12*F2^2+C8*F1^4+C9*F1*F2*F12 \quad [11]$$

This model has a residual pattern similar to Figure 3 so it was further modified to include corrections for the high and low residual areas. Since the residual areas appeared elliptic, skewed and only local deviations needed modeled, a normal distribution was used to model each area. The modification to the normal distribution included translation from the origin, rotation of the axis, making it pseudo-bivariate with elliptic contours and skewing of the distribution. Calculation lines (g) through (s) and (t) through (af) are these modifications. A more detailed explanation of the modifications is in the MODEL AND CALCULATION DETAILS below. The 2 corrections, MW1 (s) and MW2 (af), are added to the initially calculated molecular weight MW0 along with the bias coefficient C(32) to give the final molecular weight MWC (ag).

Coefficients

The model fit in GW-BASIC used double precision calculations. This calculation gave the coefficients 15 significant digits, an amount that would be tedious to use and masked any calculation sensitivity. The number of significant digits was reduced for each coefficient until any calculated molecular weights changed by 0.1. That digit was then added back with rounding to the coefficient. The sum of the square for the single and double precision sets of coefficients was 867. Table 7 lists the coefficients.

Table 7 Coefficients for Calculation to Model ASTM D2502

Coefficients	Reduced Precision	Double Precision
C(1)	4.11	4.11003181783568
C(2)	1.358	1.35799089025327
C(3)	1.5414	1.54140420525662
C(4)	-0.4106	-0.410607700098579
C(5)	197.6	197.600419071304
C(6)	-592.944	-592.943872205857
C(7)	-96.08	-96.0805030676248
C(8)	0.8759	0.875915324179165
C(9)	154.29	154.290212912789
C(10)	-1.513	-1.51300844635545
C(11)	4.126	4.12601795064831
C(12)	2.356	2.35600791224956
C(13)	1.07	1.07000402687307
C(14)	1.446	1.44600458596197
C(15)	-31.5	-31.5001241626557
C(16)	-0.64	-0.640003598408545
C(17)	0.069	0.0690004006643367
C(18)	0.31	0.310001621809348
C(19)	-0.032	-0.0320001858216837
C(20)	0.002	0.00200001326614021
C(21)	-1.267	-1.26700221200910

Coefficients	Reduced Precision	Double Precision
C(22)	8.05	8.05005427214987
C(23)	-4.326	-4.32611209469543
C(24)	6.223	6.22299707029742
C(25)	300	300.002223760980
C(26)	-0.00326	-0.00326001357002592
C(27)	19.54	19.5401315086669
C(28)	-30.387	-30.3870376632138
C(29)	-12.02	-12.0200603392125
C(30)	7.276	7.27605505433662
C(31)	6.498	6.49803836482097
C(32)	52.3	52.3002253063886

Results

Figure 5 shows the calculated V210 isostokes from the fitted model along with the data points from the ASTM chart.

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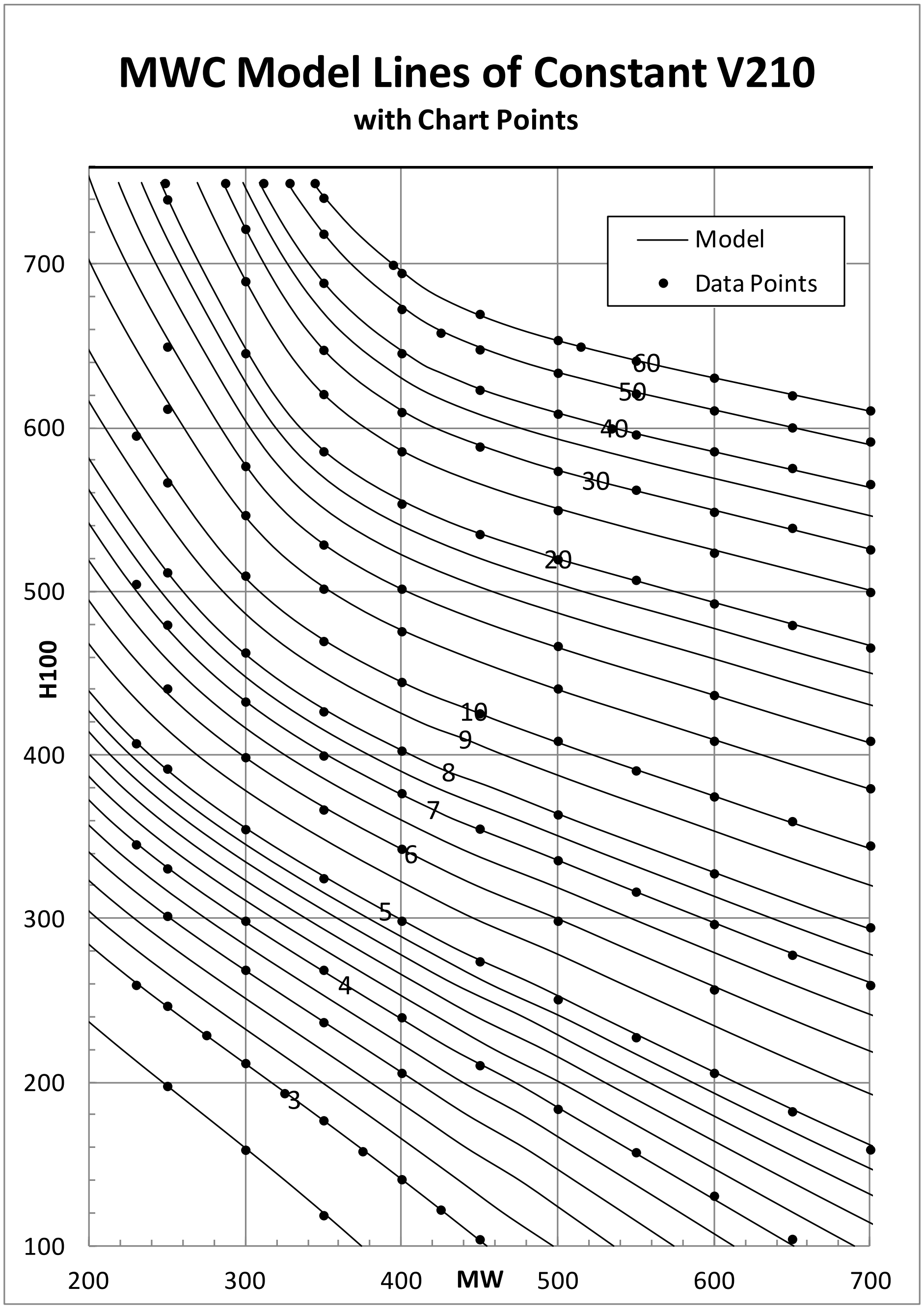

Figure 5 Calculated Isostokes (cSt) at 210°F from Model Fit Along with Data Points from ASTM Chart

Table 8 is the statistical information or the final fit.

Table 8 ASTM D2502 Model Fit Statistics

Statistic	Value
Correlation coefficient	0.99987
F-ratio	16237
Residual sum of square	867
Residual standard deviation	2.3
Coefficients	32
Data points	162

Figure 6, Figure 7 and Figure 8 are the corresponding line plot, residual distribution and residual normal probability plot respectively.

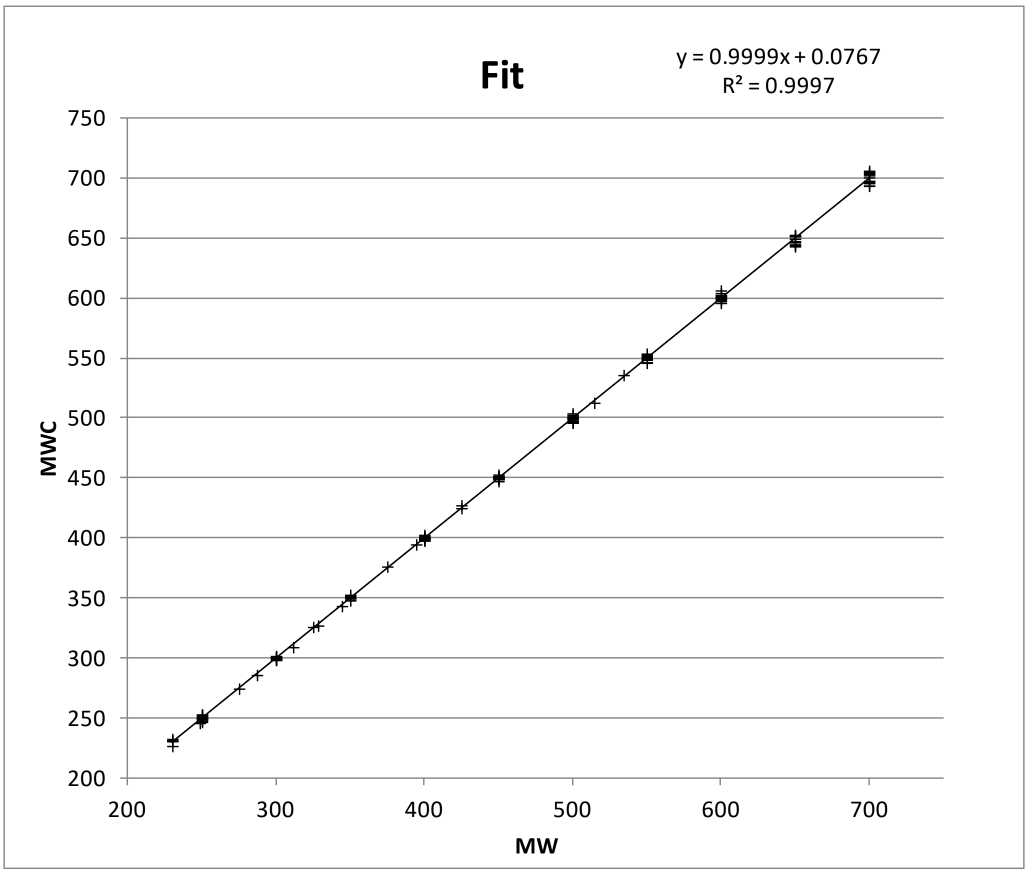

Figure 6 Line Plot of ASTM D2502 Model Fit

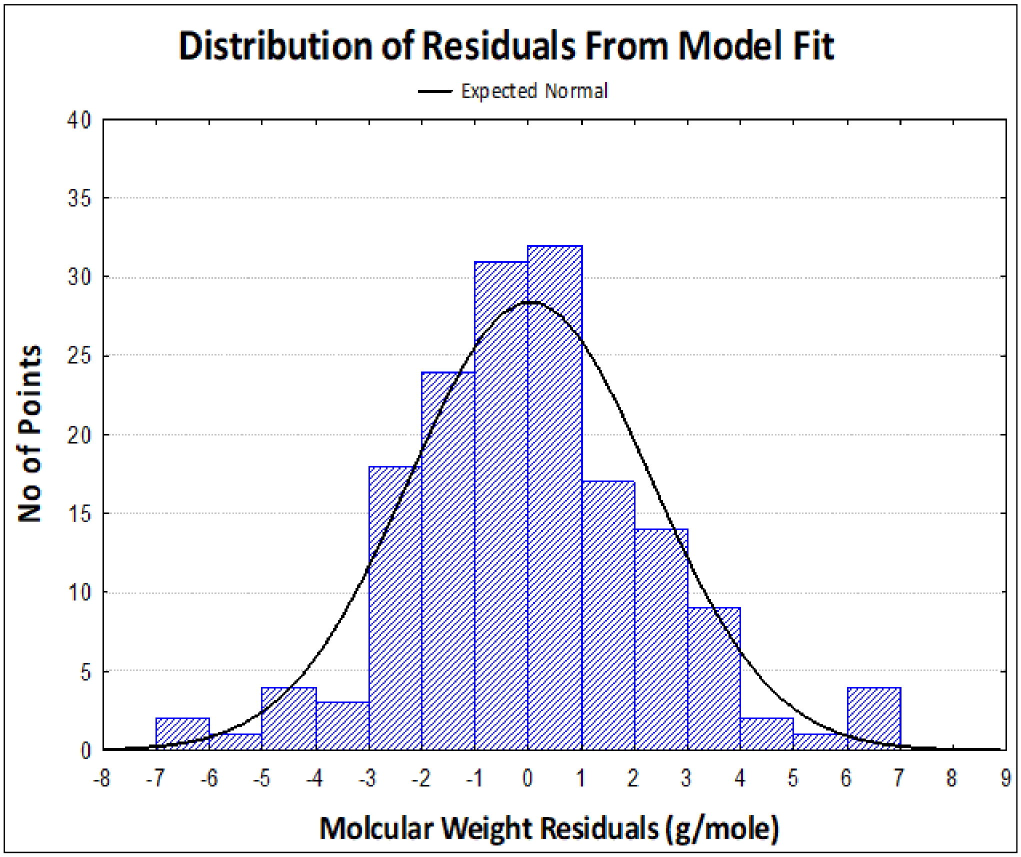

Figure 7 Residuals from ASTM D2502 Model Fit

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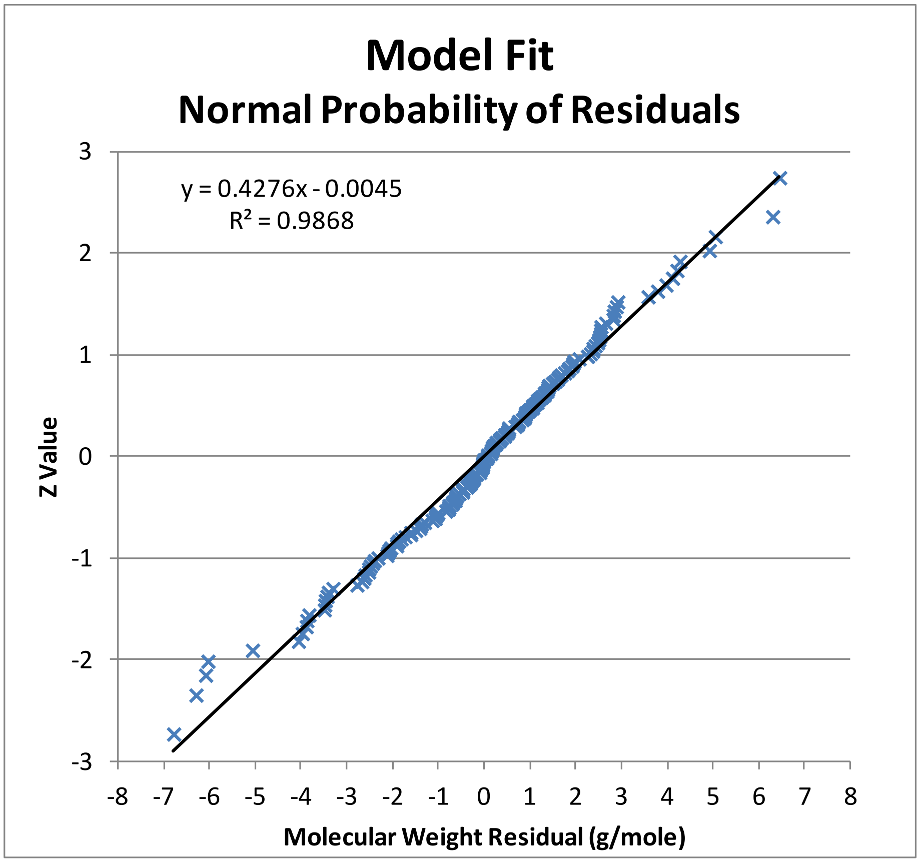

Figure 8 Normal Probability Plot of Residuals from the Model Fit to ASTM D2502

Figure 9 plots the data points labeled with the residual (MW-MWC) from the fit. Points that have a residual >±4 are highlighted in a white circle. These are clustered on the right edge and upper right corner. A recent recalculating the results in Excel using the original data and the reduced precision coefficients verified the model. The Excel VBA code for the calculation is at the end of the paper.

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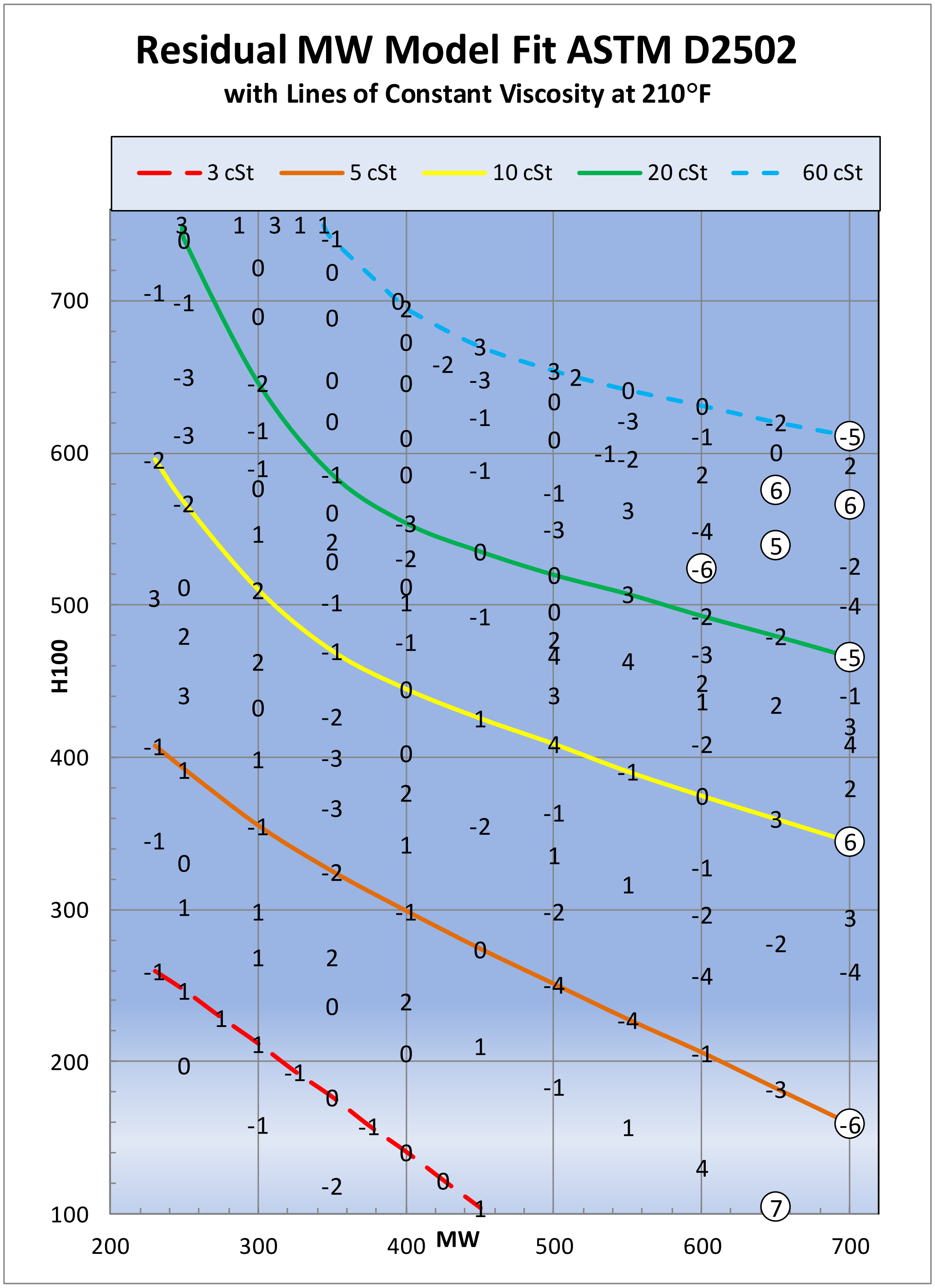

Figure 9 Final Fit Residuals ASTM D2502

The figures 5 through 9 show how well the model represents the chart.

There were no distinct patterns in the residuals when plotted against the independent input viscosities. There did seem to be a possible "rocket nozzle" like pattern for the residuals versus the MW. The variation in the residuals was slightly wider at low MW's and even wider at higher MW's. This may suggest a transform of the MW may be useful or it could be an artifact that the curves drawn by Hirschler are more variable in their placement because the low and high MW areas have little or no experiment data to estimate the curve drawing. Additional work later in this paper fitting MW and MWE to the viscosity data using Table Curve 3D[11] shows many of the fits used an inverse or Ln transform of the molecular weight. Figure 10 shows the pattern.

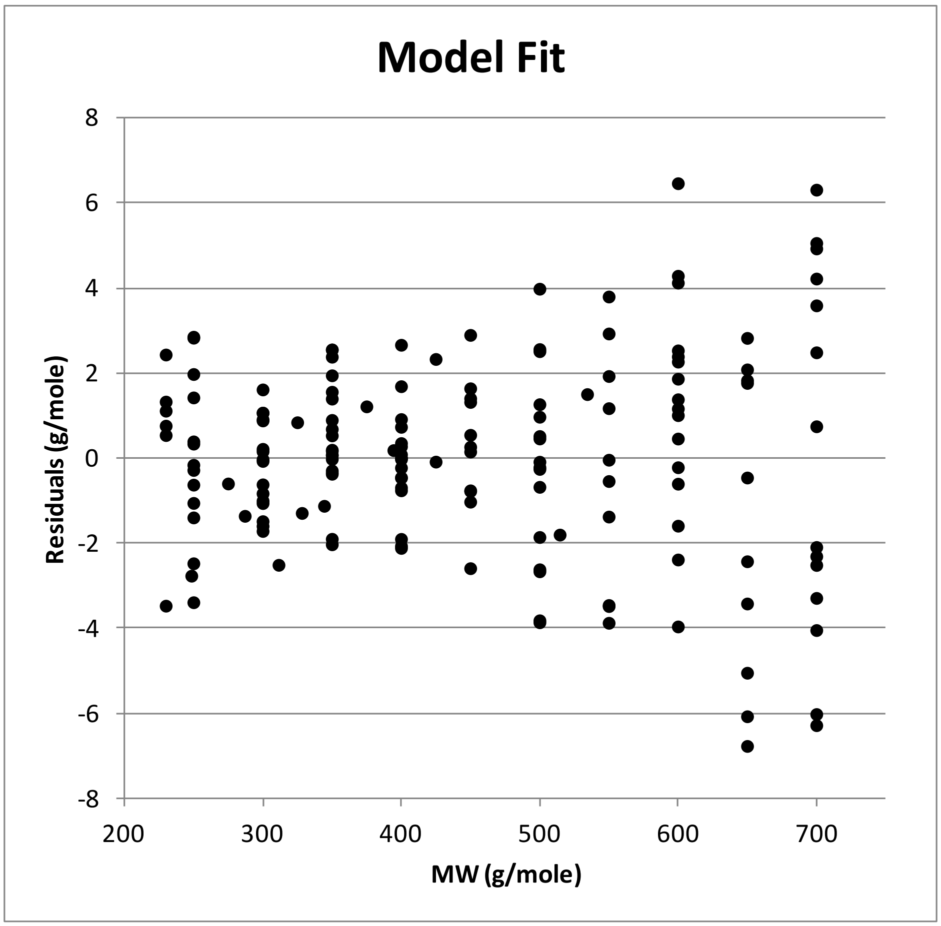

Figure 10 Model Fit Residuals Pattern with MW

Experimental Data

Review

Hirschler's paper[4] examined available data from 9 sources and chose what he considered the most reliable results and gave that data "paramount consideration" when designing the chart.

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These are the reference 26, 27 and 24 with the same major author, same molecular weight determination method and same oil but somewhat different extraction, distillation and hydrogenation treatments. This will bias them to be similar but also lends itself to comparing the molecular weight data with samples of similar viscosities. The ASTM chart is a modification of a chart in reference 18 page 462. The chart in this reference has straight isostoke lines and Hirschler considered the correlation inaccurate. Table 9 lists the references and comments about them. The comments in italics are this paper's author. One issue that adds more variability beyond the variability between the molecular weight methods and viscosity instrument accuracy is the conversion of SUS[12] to cSt by Hirschler and this paper's author. References 9 and 10 has SUS viscosities listed in SUS and cSt that did not convert using ASTM D2161-93 Reapproved 1992)[ε2].

Table 9 Literature Data Used by Hirschler to Make ASTM D2502 Chart

Referenced by Hirschler pp. 134 (160-161)	Number of Experimental Data Points	Chart Code	MW Method[13]	Viscosity Method	Comments
26	43	2	ebullioscopic	cSt	Considered most accurate and given "paramount consideration"
27	15	3	ebullioscopic	cSt	Considered most accurate and given "paramount consideration"
24	28	4	ebullioscopic	cSt	Considered most accurate and given "paramount consideration"
9	48	5	cryoscopic	cSt	*Viscosity as cSt; SUS given does not agree with current ASTM D 2161 calculations*
18	37	6	cryoscopic	SUS	*Converted to cSt by ASTM D 2161*; Considered correlation not satisfactory and modified the given straight line chart
38	9	7	cryoscopic	SUS	*Converted to cSt by ASTM D 2161; viscosity method not defined but appears to be SUS*; MW method undefined and Hirschler believed it was cryoscopic
5	20	8	cryoscopic	SUS	*Converted to cSt by ASTM D 2161*
10	14	9	thermal	cSt	*Used cSt listed; SUS listed does not agree with current ASTM D 2161; Table IV shows 6 samples have different MW's by thermal and cryogenic methods*
12	19	A,a	cryoscopic	cSt	*Light distillates; only 3 samples (250, 251, 308 = A)would be in the ASTM Chart Range, 1 data point*

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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Referenced by Hirschler pp. 134 (160-161)	Number of Experimental Data Points	Chart Code	MW Method[13]	Viscosity Method	Comments
					suspect, no data points used in fitting model

There were 233 experimental points. Only 217 are in the area covered by the chart. Sixteen from reference 12 have H100's or MWE's too low to be put on the chart. Figure 11 shows the distribution of all the experimental data with labels from Table 9 indicating the Hirschler reference. The point "a" at MWE=172.5 and H100=230.2 is considered suspect (see Erratum). Figure 12 displays the experimental data covered by the same area as in the ASTM chart. Data labeled 2, 3 and 4 are from references 26, 27, and 24 and were the ones given the most weight by Hirschler. It is evident from Figure 12 that the ASTM chart has sparse experimental data in the lower and upper right quadrants. There is also limited data below a 250 MWE.

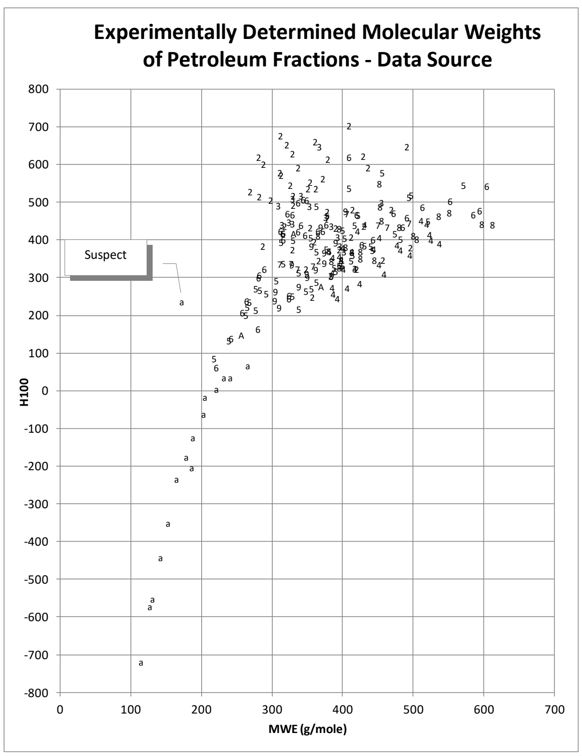

Figure 11 Experimental Data

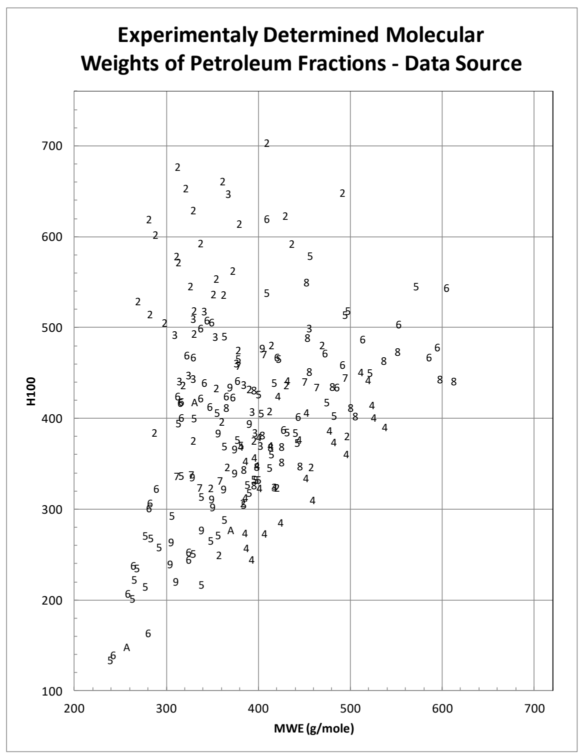

Figure 12 Experimental Data with ASTM D2502 Chart Limits

Figure 13 has the experimental points color coded to emphasize the methods used to determine the molecular weights. Figure 14 is similar for viscosity methods. The color-coding is to show visually any area that might have a data bias based on methods. The methods are distributed across the chart.

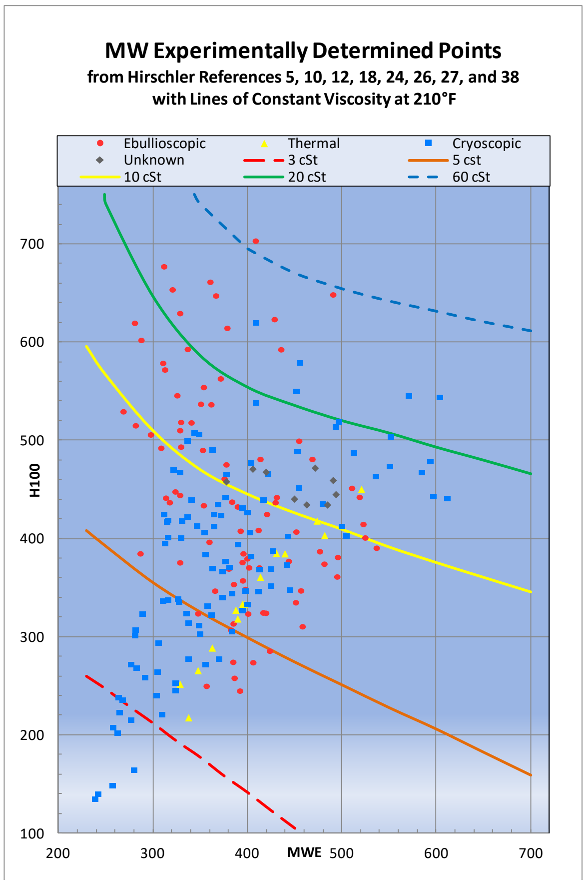

Figure 13 Experimental Data MW Method

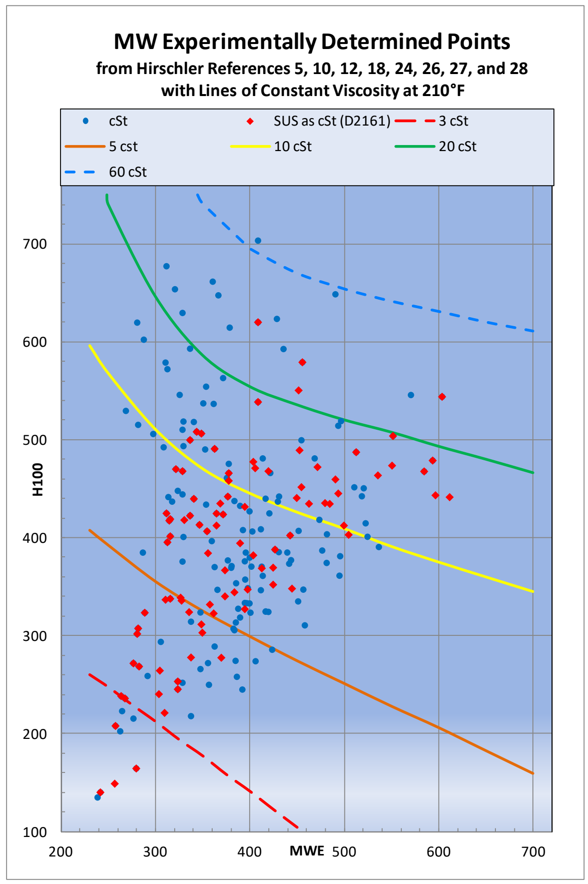

Figure 14 Experimental Data Viscosity Method

The relationship of the 2 viscosities for the experimental samples is shown in Figure 15 and the distribution of the determined MWE is in Figure 16. The MWE centers on a 400 MW.

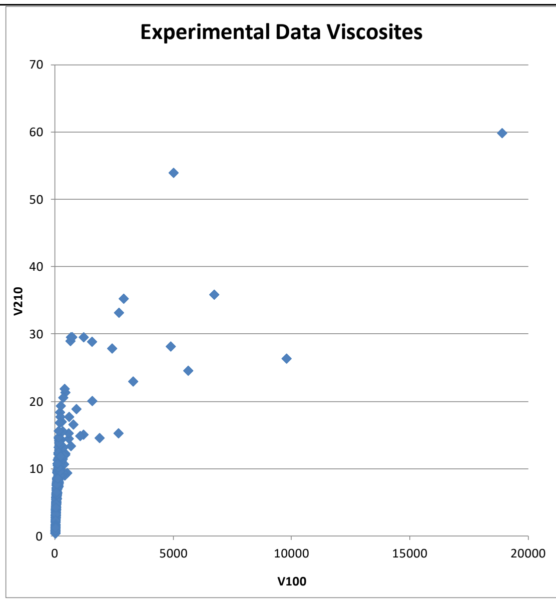

Figure 15 Viscosities of Experimental Samples

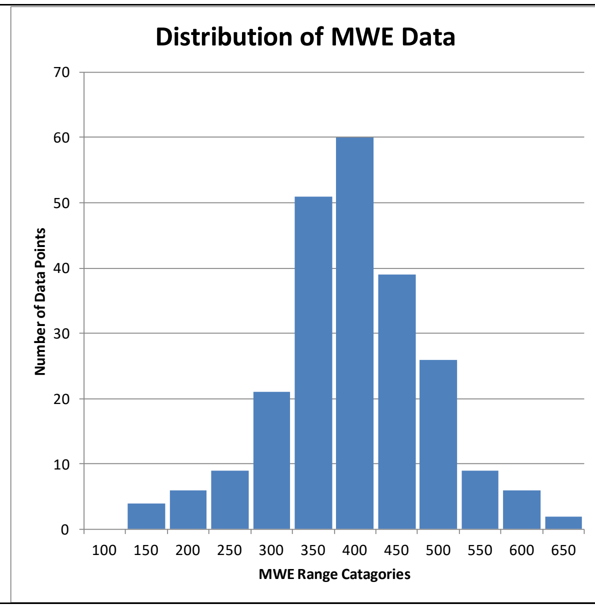

Figure 16 Distribution of Molecular Weights (MWE) for Experimental Samples

The format of the ASTM chart and a plot of the raw viscosities can mask the high degree of collinearity of the viscosities that is more evident when the viscosities are plotted as H functions as in Figure 17.

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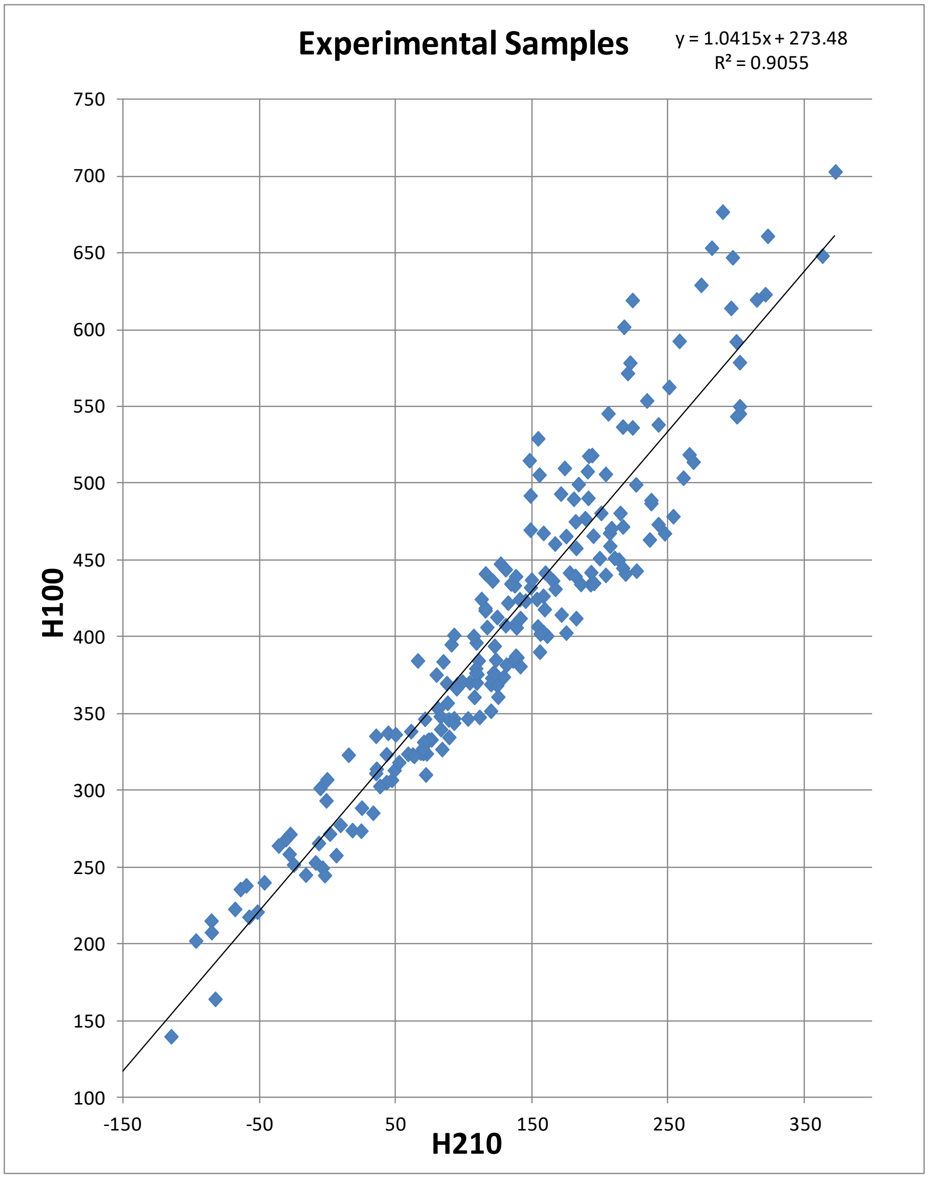

Figure 17 Experimental Samples Viscosities Collinearity

When the axes ranges are limited to the central area in Figure 17, the MWE labels are less cluttered and more readable (Figure 18). Figure 18 begins to hint of a molecular weight trend perpendicular to the relationship of H100 to H210.

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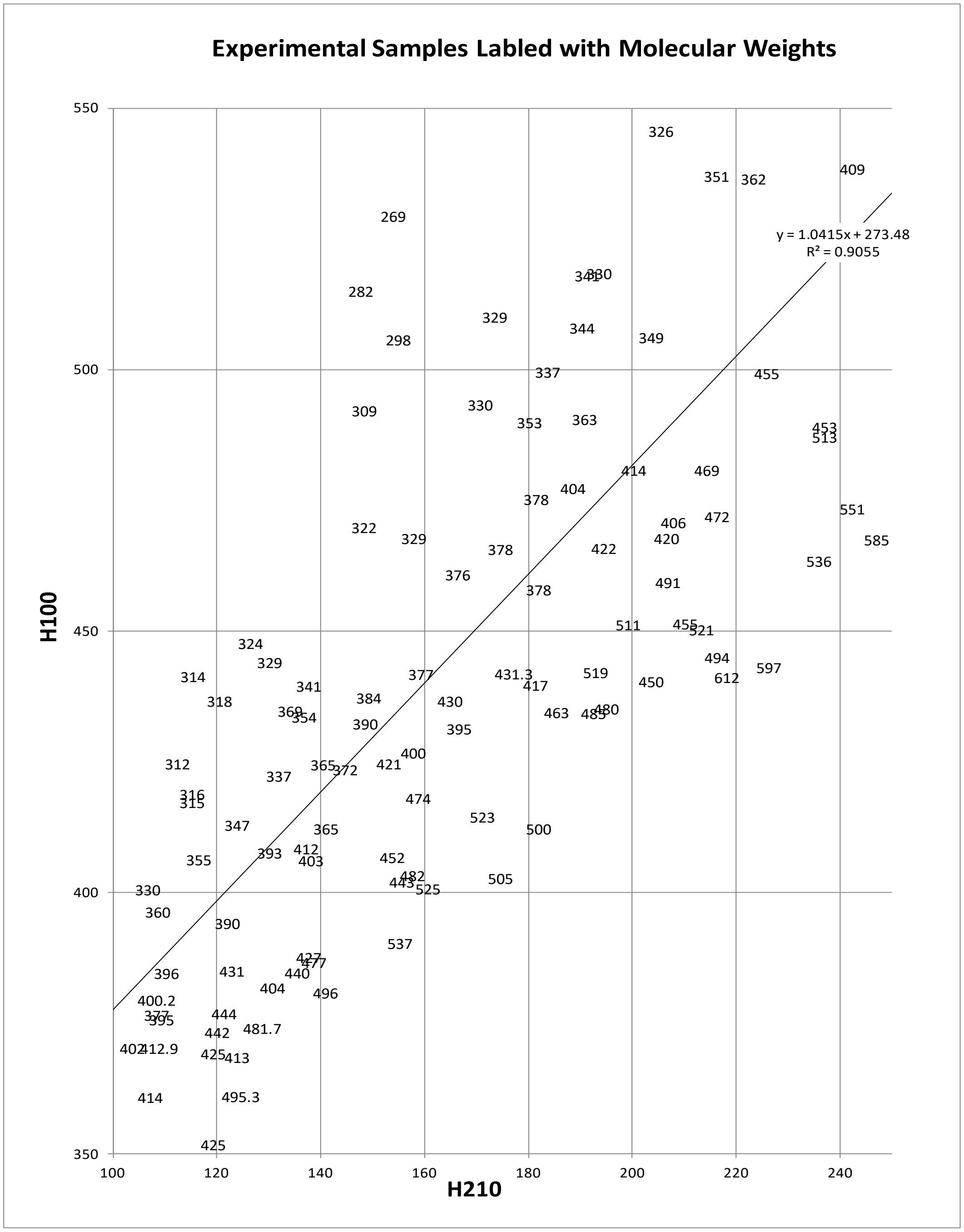

Figure 18 Experimental Samples Molecular Weights

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Experimental Best Case (MWE) vs. the Chart (MW)

The purpose of reviewing the experimental data is to understand how well it compares to the ASTM chart.

Table 10 has 25 experimental points (MWE) selected from the set of 86 points in references 24, 26 and 27. The 86 points are from those given "paramount importance" by Hirschler. This subset of the total experimental data (214 from 9 references) is a best-case comparison of the data to the chart. Table 10 also has the corresponding molecular weight data from the chart (MW) and chart model (MWC) as well as the differences between the various molecular weights.

The comparison of the chart and calculated MW's (MW-MWC) has a SD of 3.6. This is higher than the 2.1 in Table 4 found during the fitting of the model to the chart. The points selected for fitting the model were on the well defined integer crossing points of the H100 and the V210 line. Only the MW needed interpolation. For the experimental data, the H100 and viscosity were non-integer and required estimating where the point was on the chart. The higher SD of this data reflects this and supports the problem outlined in the INTRODUCTION.

Table 10 shows, expectedly, that the chart and calculation (MW-MWC) are in better agreement than the MWE-MW and MWE-MWC differences. The SD for this best case is better than the SD's (22, 27) in Table 13, which is fitting the model to the experimental data. This supports that the chart is biased toward the data in the first 3 references.

Table 10 Comparison of Reference's MWE's to Chart MW's and MWC's

	H100	MWE	MW	MWC	MWE-MW	MWE-MWC	MW-MWC
Average	415	398	402	399	-3.2	-0.5	2.7
SD					8.0	8.6	3.6
95% CF					±17	±18	±7
Min	307	281	280	284	-18.7	-18.9	-4.3
Max	703	477	474	474	19.0	18.7	8.2
Point Number		Exp.	Chart	Calc.	Difference	Difference	Difference
6	648.2	491.0	480.0	478.6	11.0	12.4	1.4
9	505.6	298.0	296.0	290.9	2.0	7.1	5.1
12	323.4	348.0	353.0	351.2	-5.0	-3.2	1.8
14	619.3	281.0	280.0	284.3	1.0	-3.3	-4.3
21	396.3	360.0	371.0	365.5	-11.0	-5.5	5.5
23	306.8	383.0	388.0	391.4	-5.0	-8.4	-3.4
30	475.2	378.0	385.0	381.1	-7.0	-3.1	3.9
32	375.7	395.0	409.5	409.7	-14.5	-14.7	-0.2
34	324.0	420.0	423.0	421.9	-3.0	-1.9	1.1
37	480.7	414.0	422.0	418.0	-8.0	-4.0	4.0

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	H100	MWE	MW	MWC	MWE-MW	MWE-MWC	MW-MWC
40	703.0	409.0	390.0	390.3	19.0	18.7	-0.3
42	480.7	469.0	470.0	464.1	-1.0	4.9	5.9
50	489.8	353.0	359.0	351.6	-6.0	1.4	7.4
51	460.7	376.0	378.0	374.2	-2.0	1.8	3.8
54	384.5	396.0	398.5	393.1	-2.5	2.9	5.4
55	370.2	402.0	413.0	406.6	-11.0	-4.6	6.4
56	324.3	417.0	419.0	414.5	-2.0	2.5	4.5
61	313.2	385.5	383.0	383.8	2.5	1.7	-0.8
67	323.2	401.0	400.0	397.0	1.0	4.0	3.0
69	379.4	400.2	406.0	399.0	-5.8	1.2	7.0
74	376.8	444.0	449.0	440.8	-5.0	3.2	8.2
76	310.3	458.6	456.0	449.8	2.6	8.8	6.2
77	441.8	431.3	450.0	450.2	-18.7	-18.9	-0.2
78	406.7	452.0	466.5	469.5	-14.5	-17.5	-3.0
79	386.7	477.0	473.5	474.1	3.5	2.9	-0.6

The correlation of the molecular weight data in Table 11 exemplifies that the chart and model are more closely related than they are to the experimental data. The relationship of the chart and model to the experimental data is similar. The regression plot in Figure 19 is a plot of the experiment molecular weight and chart data in Table 10. The regression has a slope of 0.99±0.03 and an intercept of 9±14 and affirms the relationship of the experimental data to the chart. Figure 20 is the pattern of the experimental points for the data in Table 10. Since the pattern covers most of the chart, it is not biased to any region.

Table 11 Correlations of Molecular Weight Data

Correlation Matrix Pearson r		
	MW	MWC
MWE	0.988	0.985
MW		0.997

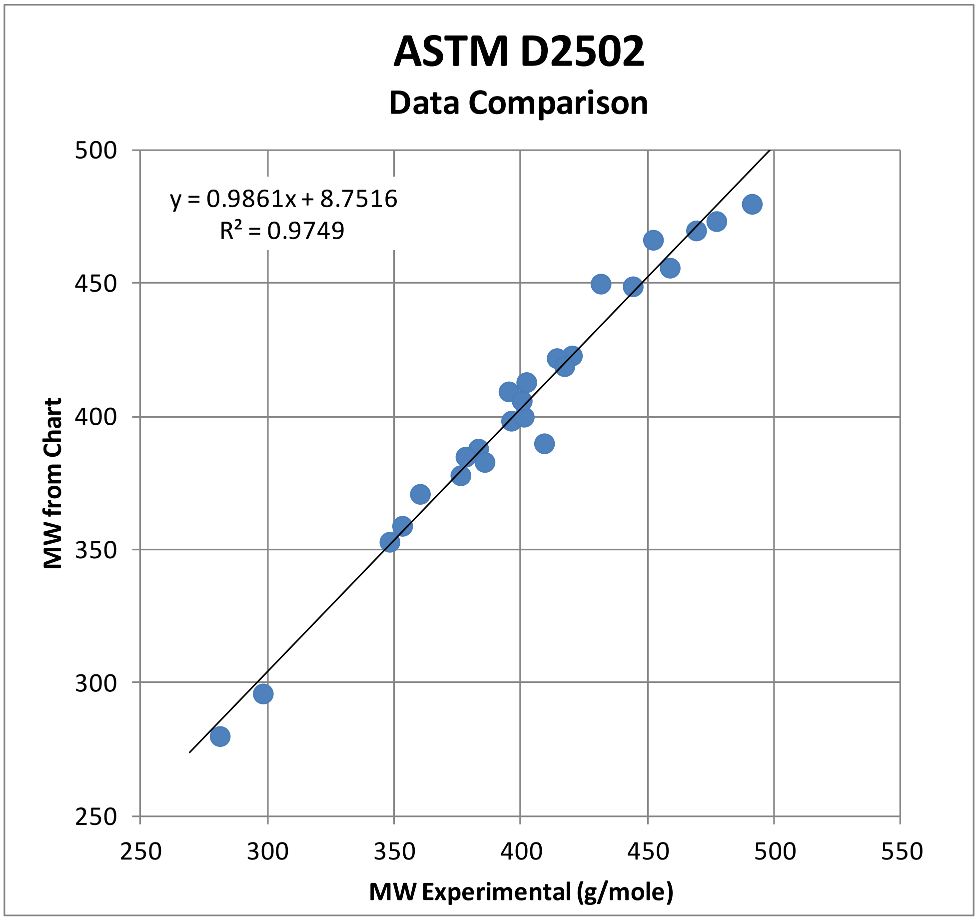

Figure 19 Comparison of MWE with MW

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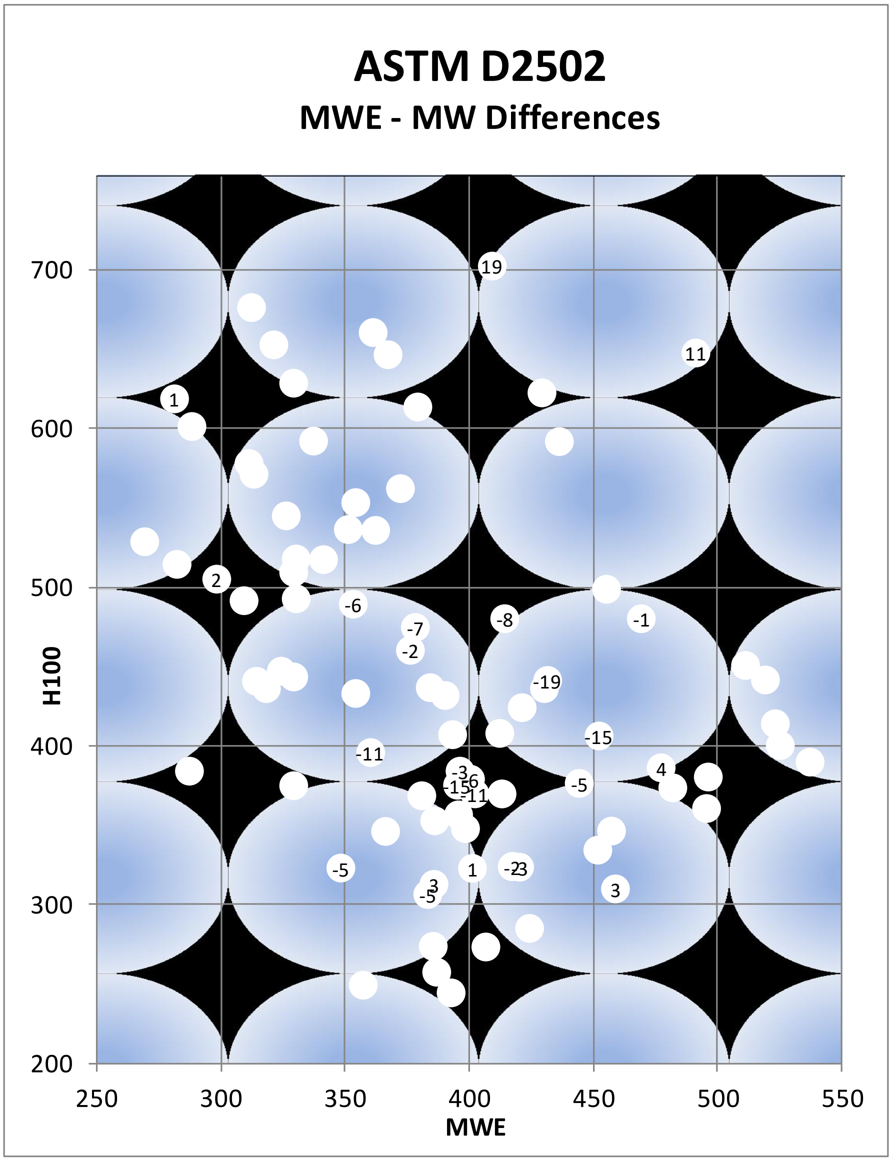

Figure 20 MWE-MW Differences for Data and Chart in ASTM D2502

Model Predictions

A complete comparison of the difference between the MWE's and MWC's are in the data Table 35 at the end of the paper. The precision of the raw data listed in the table is that from the references. Graphically the differences are shown as point labels in Figure 21.

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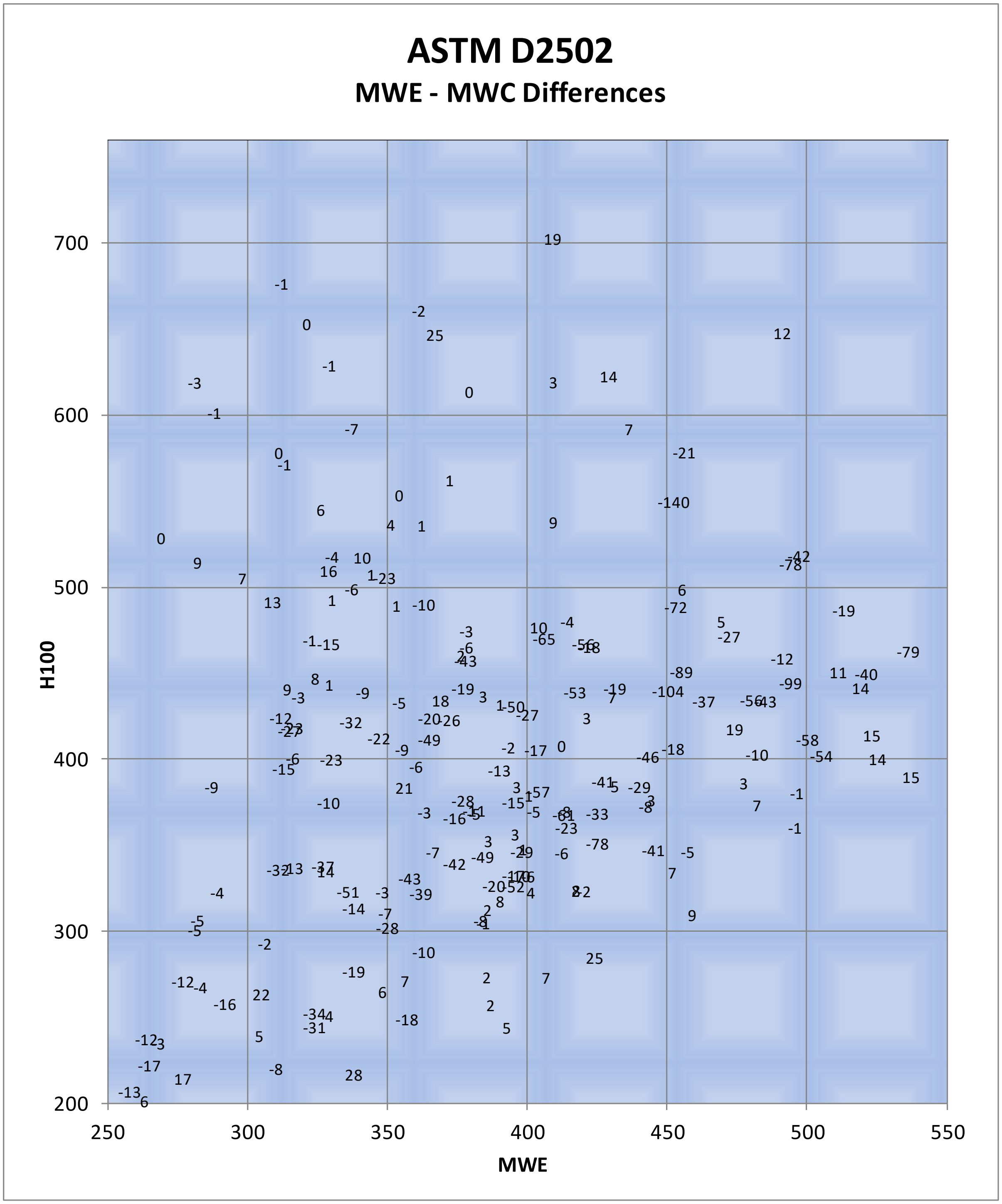

Figure 21 Comparison of Differences Between MWC and MWE

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Table 12 compares the molecular weights calculated (MWC) from the experimental viscosity data using the method in this paper and the experimentally determined molecular weights (MWE) for each of the Hirschler references. The model fit has repeatability worse than reading the chart (6 vs. 3). Its reproducibility is much better (6 vs. 25). The model and the chart are equal in representing the experimental data. A model should not be more precise than the experimental data. In this case the model is better than the data because the idealized chart is modeled and not the data. The standard deviations for the model fit to references 24, 26 and 27 are about one-half to one-third the other data sources. The experimental data is likely more consistent for these references as they are by the same main author, on similar oils using the same molecular weight method and Hirschler gave them more importance in making the chart.

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Table 12 Details of Molecular Weight Model Fit to Data from Hirschler, ASTM D2502 Chart and Experimental Results

Statistic	ASTM Repeat.	ASTM Reprod.	Model Fit	Model Test	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data	Exp. Data
Hirschler Reference pp.134 (160-161)					All	All But 12	26*	27*	24*	9	18	38	5	10	12**
Data Points															
Number			162	40	233	214	43	15	28	48	37	9	20	14	19
Minimum Molecular Weight			230	235	115	218	269	309	381	218	221	311	365	304	115
Average Molecular Weight			447	399	372	387	364	366	439	374	374	391	460	351	205
Maximum Molecular Weight			700	697	612	612	496	455	537	571	604	494	612	404	370
Molecular Weight Method							Ebul.	Ebul.	Ebul.	Cryo.	Cryo.	Cryo.	Cryo.	Therm.	Cryo.
Viscosity Method							cSt	cSt	cSt	cSt	SUS	SUS	SUS	cSt	cSt
Fit															
F-Ratio			16234												
Probability			<0.00001												
Coefficient of Correlation (Pearson's r)			0.99987	0.9999	0.94	0.95	0.99	0.99	0.98	0.98	0.98	0.98	0.93	0.87	0.97
Coefficient of Determination (R^2)			0.99974	0.9997	0.89	0.91	0.99	0.98	0.97	0.97	0.95	0.95	0.86	0.76	0.94
Slope			1.000	0.995	1.33	1.08	0.97	1.07	0.93	1.15	1.01	1.3	0.9	1.2	2.27
Slope ±(95% Confidence)			0.002	0.005	0.06	0.05	0.04	0.09	0.06	0.06	0.07	0.22	0.2	0.4	0.07
Intercept			0	2	-119	-17	11	-34	28	-44	21	-58	82	-59	-380
Intercept ±(95% Confidence)			1	2	23	18	13	33	28	24	28	86	81	133	12
Residuals															
Sum of Squares (SS)			867	202	630659	194597	2062	1398	2777	24070	42590	35007	80162	6530	436062
SS/Number of Points			5	5	2707	909	48	93	99	501	1151	3890	4008	466	22951
Standard Deviation	1	6	2	2	52	27	7	8	9	20	23	27	27	22	95
95% Confidence Limits	2	9	5	5	103	53	14	16	19	40	46	63	57	47	199
Minimum			-6.8	-5.5	-275	-28	-18.7	-24.8	-25.4	-27.9	-3	32	2	-21.7	-275
Average			0.01	0.00	3	14	0.6	-6.3	-4.1	10.5	26	57	58	5.8	-120
Maximum			6.4	3.4	140	140	18.1	4.6	18.9	77.8	104	104	140	42.0	66
ASTM Precision (g/mole)	3	25	6	6	144	74	19	21	26	55	62	75	75	60	263

* Hirschler considered most accurate and given "paramount consideration"

** Cracked Distillates, only 3 point in range of ASTM D2502, 10 of 19 had MW <=200, 1 data point suspect

Repeat.=Repeatability, Reprod.=Reproducibility, Ebul.=ebullioscopic, Cryo.=cryoscopic, Therm.=thermal

Determining the best coefficients to fit the model to the 214 experimental data points (excluding data in reference 12) showed major shifts in them that would indicate a much better local or global optimum for the experimental data was possible. It did reduce the sum of the squares but there was only a moderate change in the standard deviation of the residuals. Expectedly with the refit, the minimum residual became more negative and the maximum became less positive for the refitted model. The average of the residuals became close to zero as would be expected. Residuals for a good model fit have a normal distribution centered on zero.

Table 13 Residuals for Fitting Model Coefficients to Experimental Data

Statistic	Model	Model Refit
Sum of Squares	194597	102019
Number of Residuals	214	214
Standard Deviation	27	22
Minimum	-28	-57
Maximum	140	84.2
Average	14	-0.45

Whether there would be value in attempting to model actual experimental determined molecular weights to get a better model fit would depend on the variation of the MWE's.

Variation of Experimental Molecular Weight (MWE) Data

Using a cluster analysis of the samples' viscosities to determine which ones were most similar, gave those listed in Table 15. Those selected for this list would depend on the clustering method, how to define the "same" viscosity and the precision of the viscosities and molecular weight determinations.

There are many forms of cluster analysis. Points visually close to each other were selected from a chart of H100, MWE and V210 isostokes. These were compared to a cluster analysis using Euclidean distance measurement with single linkage amalgamation. The visual proximity of a single pair of points did not match the cluster amalgamation. The discrepancy seemed related to using the linearization V100 (H100) versus the non-linear nature of the V210 lines. After conversion of the viscosity data to F1 and F2 functions that are analogous to the H100 and H210 function, the cluster analysis gave samples more reasonably similar for both viscosities. The F1 and F2 functions used were the Ln Ln of the corresponding viscosity and its corresponding coefficient from the model (as exampled in calculations (a) and (b)).

The second item is determining the "same" viscosities. ASTM D445 has a repeatability of 0.0011% of the sample's viscosity for base oils at both viscosity temperatures. If the viscosities fall within the repeatability then they are not considered different.

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The initial thrust was to find a set of similar samples from the same reference and a set from different references to get some understanding of the impact of the analytical methods and reproducibility between laboratories. The data analyzed consisted of only amalgamated sample pairs. There were no triplicate or higher amalgamations used. Using the ASTM repeatability gave no set of samples where both viscosities would be the "same". To get a minimum of 5 samples preferably for both sets of samples (same and different references), the repeatability range was widened. It was not possible to get at least 5 samples for each set.

The closest 10 pairs of samples are in Table 15. Calculations include values that give the range of molecular weights for the sample pairs using their maximum and minimum viscosities. The molecular weight with the maximum V100 and minimum V210 would give the lowest MWC while the minimum V210 and maximum V100 would give the highest.

Table 14 shows the comparison of the standard deviations (SDs) for selected sample pairs and that of the MWC. Not included were those having large percent differences in V100 unless they were from the same reference. Sample pair 5 had a V100 difference of 1.9% yet the molecular weight difference was only 1.0. One would expect the molecular weight difference to be more if the molecular weight analysis and correlation of viscosities to molecular weights are reliable. The difference in standard deviation for sample pairs from different sources, which could also include different molecular weight methods, compared to the standard deviation for sample pairs from the same reference was extreme at 22 vs. 1.4.

Table 14 Sample Pair Standard Deviations

	SD	Sample Pair
Same Ref.	1.4	1,5
Diff Ref	22	2, 3, 4, 6
MWC	2.5	All

Table 15 Experimental Samples with Similar Viscosities

Pair	Sample #	V100	V210	MWE	Ref.	V100 Diff.	V210 Diff.	ASTM Repeat V100	ASTM Repeat V210	V100 % Diff.	V210 % Diff.	MWE Diff.	Same Ref.	MWC (Max, Min.) (Min., Max)	Diff.
1-1	99	39.73	5.84	397.0	9									405.8	
1-2	103	39.63	5.82	400.0	9	0.10	0.02	0.04	0.006	0.25	0.34	3.0	Yes	408.0	2.2
2-1	67	36.12	5.48	401.0	24									397.0	
2-2	204	35.85	5.51	362.0	10	0.27	0.03	0.04	0.006	0.75	0.55	39.0	No	401.2	4.1
3-1	32	62.20	7.14	395.0	26									405.2	
3-2	114	62.81	7.10	377.0	9	0.61	0.04	0.07	0.008	0.98	0.56	18.0	No	409.7	4.5
4-1	79	70.37	8.53	477.0	24									468.3	
4-2	136	71.14	8.48	427.0	18	0.77	0.05	0.08	0.009	1.09	0.63	50.0	No	474.1	5.8
5-1	156	100.98	7.39	315.0	18									339.3	
5-2	159	102.93	7.39	316.0	18	1.94	0.00	0.11	0.008	1.93	0.00	1.0	Yes	341.9	2.6
6-1	56	36.50	5.71	417.0	27									409.0	
6-2	71	36.57	5.65	417.2	24	0.07	0.06	0.04	0.006	0.19	1.06	0.2	No	414.5	5.5
7-1	141	259.04	17.01	513.0	18									525.3	
7-2	192	266.59	17.01	453.0	5	7.56	0.00	0.29	0.019	2.92	0.00	60.0	No	532.4	7.0
8-1	97	85.32	9.63	482.0	9									485.4	
8-2	140	84.12	9.50	443.0	18	1.20	0.13	0.09	0.010	1.43	1.34	39.0	No	495.9	10.6
9-1	19	419.00	12.30	330.0	26									330.2	
9-2	49	416.00	12.10	341.0	27	3.00	0.20	0.46	0.013	0.72	1.65	11.0	No	334.6	4.4
10-1	33	90.70	8.45	412.0	26									411.7	
10-2	119	88.28	8.50	403.0	9	2.42	0.05	0.10	0.009	2.74	0.59	9.0	No	419.5	7.8

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Comparison

ASTM D445 Viscosity Measurements

Viscosity measurements will affect the calculated oil's molecular weight. This is not a rigorous attempt at the propagation of error.

The repeatability and reproducibility of the method for base oils given in ASTM D445 is in Table 16. Both values are a percent (0.0011 = 0.11%) of the measured value. The measured value is x in Table 16. The precision values for base oils are the lowest for the types of oils listed in the method so represent a best-case scenario.

Table 16 ASTM D445 Percent Repeatability and Reproducibility for Base Oils

Repeatability	0.0011 x
Reproducibility	0.0065 x

Three H100 values were chosen that represent the bottom, middle and top of the chart (100, 400 and 620). These represent viscosities of 6.759, 82.18 and 2707.5. Eight V210 viscosities that intersected the V100 viscosities were selected; two for the bottom, three for the middle and three for the top. Table 17 has the repeatability and Table 18 has the reproducibility. The viscosity values highlighted in yellow are in pairs with the second in the pair having the repeatability or reproducibility value added.

For a given V100, a higher V210 viscosity will give a higher MWC. For a given V210, a higher V100 viscosity will give a lower the MWC. Given a set of high and low viscosities for both V100 and V210, the maximum MWC for this set is when the low V100 and high V210 are used. The minimum is when the high V100 and low V210 are used. Table 19 illustrates this.

The SD for the Max-Min. of the reproducibility is 1.8. As it is unlikely that both measurements would be at extreme values, the more reasonable value 1.4 = (0.6^2+1.3^2)^0.5 will be used for comparison. The SD for the model fit is 2.3 (Table 4). The variation in the viscosity measurement can approach 60-80% of the model fit.

Table 17 ASTM D445 Repeatability Affect on MWC

H100	Varying V100	V210	MWC	MWC Diff	V100	Varying V210	MWC	MWC Diff	MWC Max-Min.	Diff
100	6.759	2.6	374.3		6.759	2.6	374.3		374.9	
100	6.767	2.6	374.1	0.2	6.759	2.60286	374.9	-0.59	374.1	0.8
100	6.759	4	651.3		6.759	4	651.3		652.2	
100	6.767	4	651.0	0.3	6.759	4.0044	652.2	-0.85	651.0	1.2
400	82.12	5	239.0		82.12	5	239.0		239.3	

400	82.21	5	238.9	0.1	82.12	5.0055	239.3	-0.34	238.9	0.4
400	82.12	8	406.6		82.12	8	406.6		407.1	
400	82.21	8	406.4	0.2	82.12	8.0088	407.1	-0.48	406.4	0.7
400	82.12	10	523.1		82.12	10	523.1		523.7	
400	82.21	10	522.8	0.3	82.12	10.011	523.7	-0.63	522.8	0.9
620	2707.54	12	247.7		2707.54	12	247.7		247.9	
620	2710.52	12	247.6	0.0	2707.54	12.0132	247.9	-0.18	247.6	0.2
620	2707.54	35	419.8		2707.54	35	419.8		420.1	
620	2710.52	35	419.7	0.1	2707.54	35.0385	420.1	-0.31	419.7	0.4
620	2707.54	60	652.7		2707.54	60	652.7		653.2	
620	2710.52	60	652.4	0.2	2707.54	60.066	653.2	-0.55	652.4	0.8
Ave.				**0.2**				**-0.5**		**0.7**
SD				**0.1**				**0.2**		**0.3**

Table 18 ASTM D445 Reproducibility Affect on MWC

H100	Varying V100	V210	MWC	MWC Diff	V100	Varying V210	MWC	MWC Diff	MWC Max-Min.	Diff
100	6.759	2.6	374.3		6.759	2.6	374.3		377.8	
100	6.803	2.6	373.0	1.3	6.759	2.6169	377.8	-3.50	373.0	4.8
100	6.759	4	651.3		6.759	4	651.3		656.3	
100	6.803	4	649.3	2.0	6.759	4.026	656.3	-5.02	649.3	7.0
400	82.12	5	239.0		82.12	5	239.0		241.0	
400	82.65	5	238.4	0.6	82.12	5.0325	241.0	-2.01	238.4	2.7
400	82.12	8	406.6		82.12	8	406.6		409.4	
400	82.65	8	405.4	1.2	82.12	8.052	409.4	-2.84	405.4	4.1
400	82.12	10	523.1		82.12	10	523.1		526.8	
400	82.65	10	521.4	1.7	82.12	10.065	526.8	-3.72	521.4	5.4
620	2707.54	12	247.7		2707.54	12	247.7		248.7	
620	2725.14	12	247.5	0.2	2707.54	12.078	248.7	-1.05	247.5	1.2
620	2707.54	35	419.8		2707.54	35	419.8		421.6	
620	2725.14	35	419.1	0.7	2707.54	35.2275	421.6	-1.82	419.1	2.5
620	2707.54	60	652.7		2707.54	60	652.7		655.9	
620	2725.14	60	651.2	1.4	2707.54	60.39	655.9	-3.25	651.2	4.7
Ave.				**1.2**				**-2.9**		**4.1**
SD				**0.6**				**1.3**		**1.8**

Table 19 MWC Max-Min. Relation to Viscosities

V100	V210	V100	V210	MWC	Diff
6.759	2.603	Low	High	374.9	
6.767	2.600	High	Low	374.1	0.8

Maroto and de las Nieves[14]

This paper details a refinement in the molecular weight calculation by Hirschler where a cubic polynomial of the VSF function replaces the S function in equation [4].

Doing the various algebraic substitutions led to the generalized equation for MWC of [12].

$$MWC=\underline{a}+\underline{b}\eta^4+\underline{c}\eta^3+\underline{d}\eta^2+\underline{e}\eta+\underline{f}\eta H+\underline{g}\eta H^2+\underline{h}\eta H^3+\underline{i}\eta^2 H+\underline{j}\eta^2 H^2+\underline{k}\eta^3 H+\underline{l}H+\underline{m}H^2+\underline{o}H^3 \qquad [12]$$

where

Table 20 Coefficients of the Generalized Calculation in the Maroto Paper

MWC= Molecular weight calculated of a petroleum oil					
a=	180	$\underline{a}$=	(a+bf)	H_t=	870Log(Log(V_t+0.6))+154
b=	60	$\underline{b}$=	i	H_t=	jLog(Log(V_t+k))+l
c=	4.146	$\underline{c}$=	(-h+bi)	t=	temperature in °F
d=	1.733	$\underline{d}$=	(-g-bh)	η=	H_{100} (Greek h)
e=	145	$\underline{e}$=	(f-bg)	H=	H_{210}
f=	3.562	$\underline{f}$=	(-g+2bh)	VSF=	H_{100}-H_{210}
g=	0.01129	$\underline{g}$=	(-h+3bi)	VSF=	η-H
h=	$1.857*10^{-5}$	$\underline{h}$=	-i		
i=	$6.843*10^{-8}$	$\underline{i}$=	(2h-3bi)		
j=	870	$\underline{j}$=	3i		
k=	0.6	$\underline{k}$=	-3i		
l=	154	$\underline{l}$=	-bg		
		$\underline{m}$=	-bh		
		$\underline{n}$=	not used		
		$\underline{o}$=	-bi		

The Maroto paper used the H function with the standard j, k and l coefficients. In this paper, the H functions were a generalized version at 100°F and 210°F referred to as F1 and F2 where the H function coefficients were optimizable parameters. The S function has a Log function of the VSF. Using the cubic modification of the VSF for S, there is no longer a Log function of the VSF. In this paper, keeping the Log function of the VSF causes the generation of the F12 function, which is a Log function of the combined F1 and F2. There is no corresponding H12 in the Hirschler-Maroto equations.

A matrix of the 14 terms in equation [12] shows the powers (order) of the H_{100} function, the H_{210} function and the cross-product terms (X's).

Table 21 Matrix of Terms in the Hirschler-Maroto Model

H\η	0	1	2	3	4
0	X	X	X	X	X
1	X	X	X	X	
2	X	X	X		
3	X	X			
4					

Table 22 shows a comparison of the H or F polynomials used in the calculations in this paper and in the Maroto paper. The 3 tuples in the table indicate the power of the cross-term functions. The tuple 0,2,1 represents $F1^0 * F2^2 * F12^1$. The Hirschler-Maroto equations have more polynomial terms than the calculation in this paper. However, the elliptic and skewed normal functions required 22 coefficients (11 for each of the 2 elliptics) for modeling areas of the residuals but it also resulted in modeling a much wider area of the chart.

Table 22 Model Terms

Polynomial bi-elliptic		**Hirschler-Maroto**	
F1,F2,F12	Order	*η, H,* H12	Order
0,0,0	0	0,0,0	0
0,0,1	1	1,0,0	1
0,2,1	3	2,0,0	2
4,0,0	4	3,0,0	3
1,1,1	3	4,0,0	4
		0,1,0	1
		1,1,0	2
		2,1,0	3
		3,1,0	4
		0,2,0	2
		1,2,0	3
		2,2,0	4
		0,3,0	3
		1,3,0	4

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What was interesting about the Maroto paper was how the area of the results compared to the actual experimental data. Figure 22 has the experimental data shown in Figure 12 bounded by an irregular decagon. The area centered on the H100=590 and Relative Molecular Mass=380 area are points from Hirschler reference 26 which he considered "paramount". In Figure 12, these points have the label 2. The Maroto modification does not model this area of the ASTM chart.

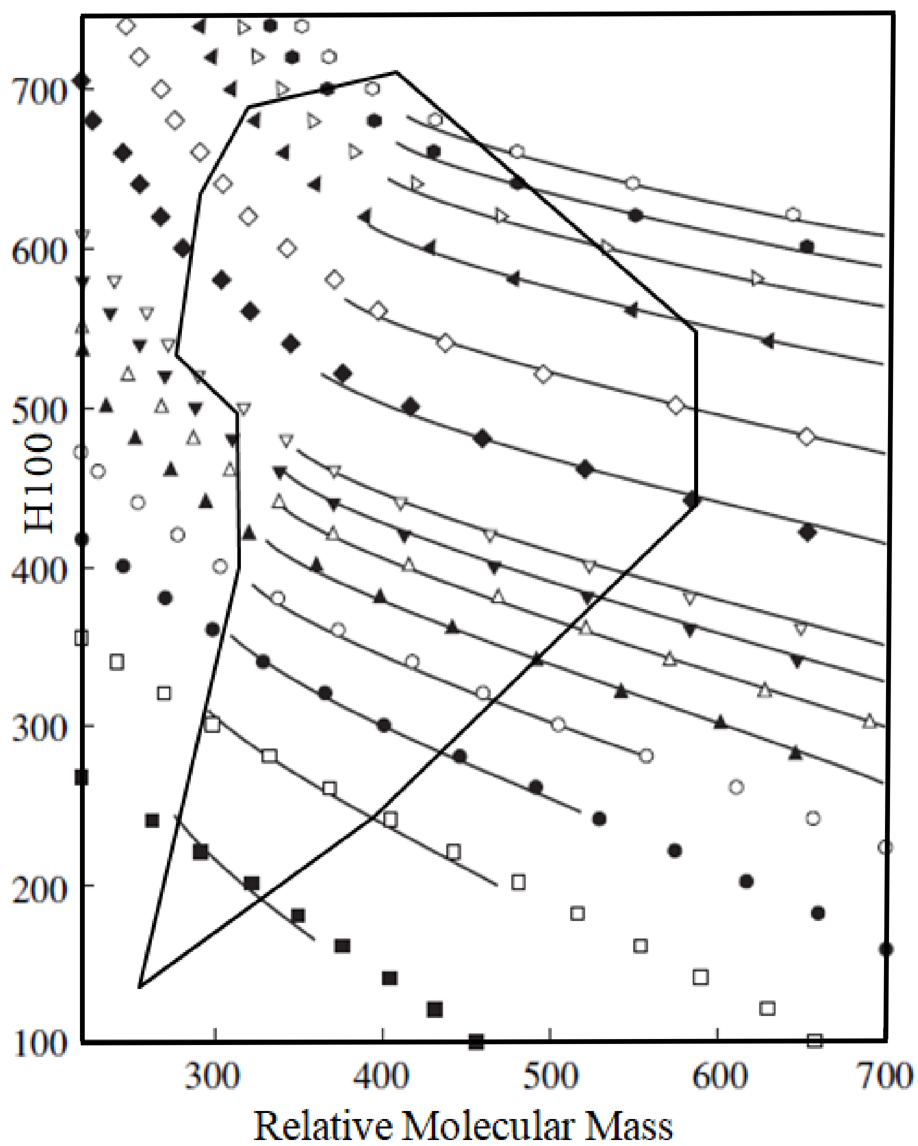

Figure 22 Hirschler Experiment Data Outlined on the Restricted Maroto Chart (Fig. 3. in their paper)

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Criticisms

ASTM

This calculation was presented to C. L. Stuckey chairman of ASTM Committee D02.04 in 1991. At the June meeting, Rinus Daane of Shell Research, Europe commented that:

1. The data was a mix of actual and artificial data, and a correlation of a correlation.
2. Thirty-two coefficients did not qualify as a good correlation and was "hocus pocus."[15]
3. The viscosities were non-standard and not at the standard temperatures of 40°C and 100°C. He recommended leave the method as is or develop a new correlation.

In response,

1. The data for the fit was not a mix of actual and artificial data. Hirschler gave data in his paper to generate the chart. The calculation used the idealized data from his paper and additional data points were taken from the chart. All the data was of the same type.
2. Thirty-two coefficients would normally be a lot if the calculations were simply using higher order polynomials that generate small differences to make the fit better. They also start to model noise. If this was the reason for the polynomials, I would agree it is "hocus pocus." However, the polynomials showed significance in the Stat II fits. Because the polynomials were significant and the coefficients needed only a limited number of significant digits, I do not believe they represent an example of Runge's phenomenon[16] or the modeling of noise.
3. There was no intent for it to be a replacement with new experimental data or methods but only to model the chart. This work was to avoid the inconvenience and errors of interpolating data from the chart. The work showed that about 10% of the molecular weights read from the chart would be in error. Other ASTM methods have both a chart or table and a calculation associated with them. By example, ASTM D341 has a calculation with 13 coefficients.

Incorporating the calculation into the method was due to the lack of a task force leader that could devote the time needed for the project.

Hydrocarbon Processing

Hydrocarbon Processing rejected the manuscript on calculation of molecular weight because it did not meet their editorial needs at that time (12/12/1985).

Concerns

The only concerns are the molecular weight transition for the EL1 and EL2 elliptic skewed normal distribution sign change. For the EL1, the transitions are modest being less than 5. The transitions for EL2 are much larger but are in areas that are on the extreme edge of the chart where there were no real samples. The section Elliptic Transition with Skewed Normal Distribution discusses this and is shown in Figure 27 and Figure 29.

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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MODEL AND CALCULATION DETAILS

Model Background

The purpose of the NLLSQ program was to become familiar with the modified sequential simplex optimization method and use it to develop formulation mixtures. It would also provide a flexible least squares fitting program for use on other laboratory data. It proved inappropriate for mixtures because of the formulation constraint in that type of design of experiment (DOE[17]). The misuse of sequential simplex for mixture designs are in the literature[18]. The fitting of a model to the ASTM D2502 chart was a method to test the program and possibly avoid the inconvenience of reading the chart.

Hirschler Model F1, F2, F12

F12' equation [13] is a term used in the Hirschler model equation [7] before it was generalized. The following steps detail how F12' was generalized to F12. It also shows how the functions and coefficient from the generalization manifested themselves in the higher order function polynomials of equation [11].

F12' Generalization

F12'=Log(870*F1-870*F2-145) [13]

Algebraic manipulation of [13] yielded [15].

F12'=Log(870*(F1-1*F2-145/870)) [14]
F12'=Log(870) + Log(F1-1*F2-145/870) [15]

The "1" before F2 and the constant 145/870 were generalized by making them C3 and C4 shown in equation [16].

F12'=Log(870) + Log(F1-C3*F2-C4) [16]

The use of F12 simply means the C5 constant in equation [11] will include the constant Log(870) from equation [16].

*F1*F12 Generalization and Reduction*

For the C7*F1*F12 term from equation [7], the generalization of F12' [16] will generate a second F1 term in equation [18]

C7'*F1*F12=C7'*F1*[F12'-Log(870)] [17]
C7'*F1*F12=C7'*F1*F12' -C7'*F1*Log(870)] [18]

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The C6 coefficient in equation [20] for F1 would essentially be a combination of other coefficients and constants of the non-generalized form of F12.

C6*F1= -C7'*Log(870)*F1+C6'*F1 [19]
C6*F1= (-C7'*Log(870)+C6')*F1 [20]

Model Elliptics + Skewed Normal Distribution Adjustments

The residuals from fitting the Hirschler model have a pattern of a high "peak" and of a low "valley" area seen in Figure 3. It seemed that the 2 areas could be modeled by 2 modified normal distributions, a positive and a negated one. They would have a structure where the value at farther distances from the center of the high or low area would go to zero and just be adding correction terms to the initially calculated molecular weight (MW0). The areas also looked possibly elliptic and possibly skewed on the various sides of an elliptic axes. A calculated elliptic contour became the basis of a normal distribution creating a bivariate-like normal distribution from a univariate distribution. Replacing the typical quadratic power of ***e*** with a quartic order polynomial introduced skewing. In crossing the axes, the X value would become negative. Expecting the sign change would cause a possible jump in the value from the distribution, the negative X values were converted to positive values when the axes were crossed. The calculation used two elliptics, EL1 (m) and EL2 (z).

Elliptics

The axes of the ASTM chart are MW and H100. The translation and rotation of the elliptics used the axes of MW0 and F2. Since MW is being calculated, it is not available as data to translate and rotate the axes. Residual contours of H210 and MW were similar to the contour using H100 but appear more uniform so the generalized F2 function was used.

Translation and rotation of a function in Cartesian coordinates from (0, 0) origin to a new origin at (X,Y) are shown in equations [21] and [22][19].

$$X = (x - h)\cos\theta + (y - k)\sin\theta = x*\cos\theta + y*\sin\theta - h*\cos\theta - k*\sin\theta \quad [21]$$
$$Y = -(x - h)\sin\theta + (y - k)\cos\theta = y*\cos\theta - k*\cos\theta - x*\sin\theta + h*\sin\theta \quad [22]$$

Expansion of Equations [21] and [22] with the replacement of X with MWS and Y with F2 gives equations [23] and [24]

X=MWS*CO1+F2*SI1-C(11)*CO1-C(12)*SI1 [23]
Y=F2*CO1-C(12)*CO1-MWS*SI1+C(11)*SI1 [24]

where

X = the translated and rotated coordinate in terms of MWS (x-axis)

Y = the translated and rotated coordinate in terms of F2 (y-axis) – note not F1
MWS = the scaled primary molecular weight MW0 in calculation (e).
SI1 = SIN(C(10))= sine of the rotation angle of the first ellipse
CO1 = COS(C(10))= cosine of the rotation angle of the first ellipse
C(10) = angle of rotation (θ) of the first ellipse determined by regression
C(11) = translation in the x axis (h) determined by regression
C(12) = translation in the y axis (k) determined by regression

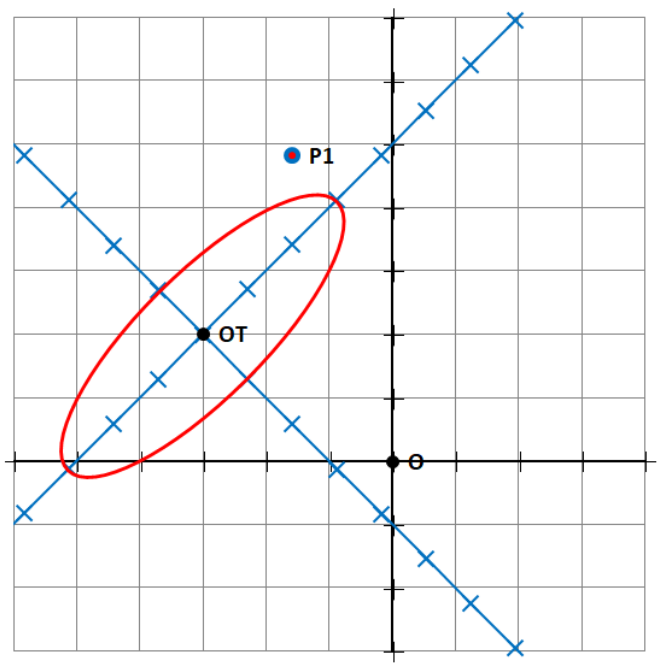

Figure 23 Translation of the Origin and Rotation of Axis with Elliptical Contour

Equation [25] shows the standard elliptical.

$$X^2/b^2+Y^2/a^2=1 \quad [25]$$

Since equations [23] and [24] have the translation and rotation incorporated, there was no need to do the translation to the center point of the ellipse or its rotation. The new origin coordinates (X, Y at point OT) were divided by regression determinable coefficients C(13) and C(14) making them equivalent to equations [26] and [27].

$$X/b=X/(C(13) \quad [26]$$
$$Y/a=Y/(C(14) \quad [27]$$

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Combining [23] with [26] and [24] with [27] gives the form of the calculations for the elliptics. Calculations (i) and (k) shows these the elliptic contour forms EL1 (v) and EL2 (x).

X1 and Y1 were then squared (calculations (j) X12 and (l) Y12) and added together (calculation (m) EL1=X12+Y12) to make an elliptic contour defined as EL1. EL2 used the same calculations but with other coefficients.

A normal distribution used the elliptic contour values to calculate the adjustment in the initially calculated molecular weight (MW0). Equation [33] shows a generalized normal distribution (GND). The modified generalized normal distribution (MGND) equation [35] was the GND altered by having Euler's ***e*** raised to the 4th power of the elliptic contours EX1 or EX2. An issue might occur if the distribution did not have a smooth transition across the elliptic axis and result in jumps in values when the point was on one side of the axis or because of the odd terms in the distribution. Changing the signs of the elliptic values on opposite sides of the axes made them consistent. Using them in the higher order polynomial normal distribution, the coefficients would regress to the appropriate negative or positive values. If the calculation in equation (n) indicated the EL1 (ellipse 1) in equation (m) was negative, it was made positive by multiplying by -1 in equation (p) (EX1, exponent 1).

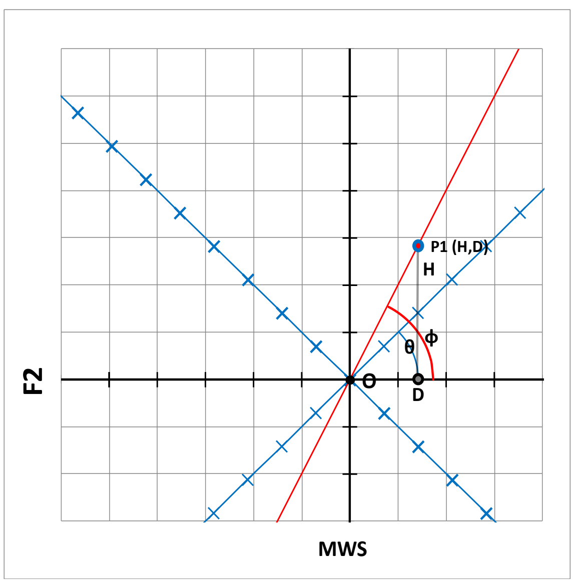

Figure 24 Elliptic Center Translated Back to the Origin

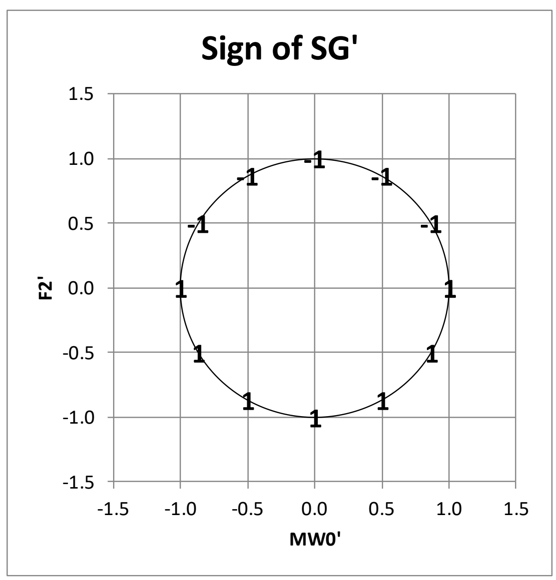

Figure 25 Sign of SG

In the calculation, the coordinates of the center of the ellipse was defined by the coefficients (C(11), C((12)) and the point P1 by the coordinates (MWS,F2). To determine which side of the rotated and translated ellipse a point was on, the coordinates of the point would be used to calculate the angle of the point from the original axes. Figure 24 visualizes putting the center or origin of the ellipse, point OT (origin translated) in Figure 23, superimposed on the original origin. Angle ϕ of the point would be compared to θ, the angle of the rotation of the ellipse (C(10) for ellipse 1). If ϕ> θ or (Tanϕ>Tanθ), it would be considered on one side of the axis. Otherwise, its sign is changed. Tanϕ is the length of H/length of D. In terms of the coordinates of the 2 points (P1 and O) and the coefficients in the model, equation [28] defines Tanϕ.

$$\text{Tan}\phi=(F2-C(12))/(MWS-C(11)) \qquad [28]$$

We are looking for

$$\text{Tan}\phi>\text{Tan}\theta \qquad [29]$$

Substituting in equation [28] and the tan of the axis rotation, Tan(C(10))

$$(F2-C(12))/(MWS-C(11))>\text{Tan}(C(10)) \qquad [30]$$

$$0>\text{Tan}(C(10))*(MWS-C(11))+C(12) -F2 \qquad [31]$$

gives equation [31] which is the form of calculation (n) and (aa) to SG1 and SG2. The algebraic manipulation rules for the multiplication or division of an inequality were not necessary, as the absolute value of the sign is not important. For the calculation, it is only important to know if they are on the same side of the axis and if they are not then the sign is made the same. Figure 25 uses the tangent calculation equation to determine the sign on either side of an ellipse axis. The x and y values are representative data. The labels on the axes and title are the actual data name or calculated intermediate used in making the model but are appended with an apostrophe (’) to indicate the use of representative data in making the figure.

Skewed Normal Distribution

Starting with a normal distribution equation [32], generalizing to give the generalized normal distribution (GND) [33] by consolidating constants and expanding the exponential term, and then replacing the exponential term with a higher order polynomial [34] gave a modified generalized normal distribution (MGND) equation [35]. Recent literature has referred to this as a flexible skew-symmetric distribution[20,21,22,23].

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \qquad [32]$$

$$\text{GND}=a\boldsymbol{e}^{-(b+cX+dX\text{^}2)} \qquad [33]$$

$$(b+cX+dX^2+eX^3+fX^4) \qquad [34]$$

$$\text{MGND}=a\boldsymbol{e}^{-(b+cX+dX\text{^}2+eX\text{^}3+fX\text{^}4)} \qquad [35]$$

X in equation [35] represents EX1 in calculation (p) and EX2 in calculation (ac). The polynomial [34] is written in the Horner[24] nested polynomial format to avoid generating large numbers with the higher polynomials. It was also broken into parts for easier coding and represented by calculation (q), (r), and part of (s) and calculations (ad), (ae) and part of (af) for the 2 elliptic skewed normal distribution adjustments. Calculations (s) and (af) yield the elliptic skewed normal distribution adjustments to the molecular weight. Equation 36 represents the full function calculation of adjustment 1 with the coefficients being represented without the array parenthesis.

$$MW1=C15e\text{^}(-(C16+C17*EX1+C18*EX1^2+C19*EX1^3+C20*EX1^4) \quad [36]$$

Figure 26 shows some of the various forms that can be generated by higher order polynomials in a normal distribution and
Table 23 has some description details with the coefficients used to generate the curves.

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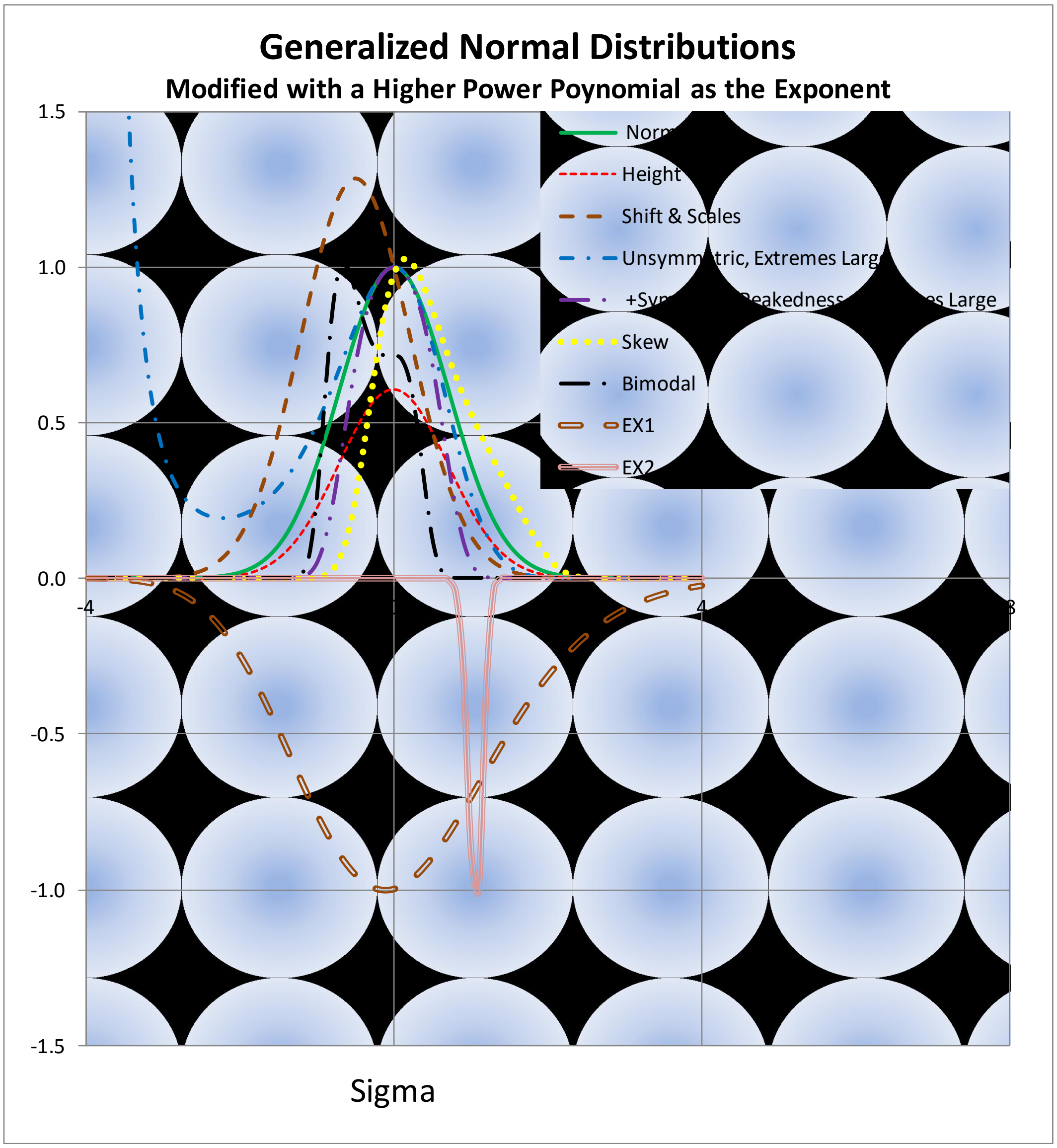

Figure 26 Examples of Higher Order Normal Distributions

Table 23 Chart with Explanation of the Various Curves and the Coefficients of the Powers of X

Chart Legend	Normal	Height	Shift & Scales	Unsymmetric, Extremes Large	+Symmetric Peakedness, - Extremes Large	Bimodal	Skew	EX1	EX2
X powers	2	0,2	1,2	2,3	2,4	2,3,4	0,1,2,3,4	0,1,2,3,4	0,1,2,3,4

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Chart Legend	Normal	Height	Shift & Scales	Unsymmetric, Extremes Large	+Symmetric Peakedness, -Extremes Large	Bimodal	Skew	EX1	EX2
Affect		+b Smaller -b Higher	+c Shifts left -c Shifts right Both Higher	+e Larger left -e Larger Right	+f Narrows -f Widens & >>Max				
Rescale	1	1	1	1	1	0.72	1	-0.53	-9.79E-05
a	1	1	1	1	1	1	1	-31.50	-0.00326
bX^0	0.0	0.5	0.0	0.0	0.0	0.0	0.02	-0.64	19.54
cX^1	0.0	0.0	1.0	0.0	0.0	0.0	-0.70	0.07	-30.387
dX^2	1.0	1.0	1.0	1.0	1.0	1.0	2.78	0.31	-12.02
eX^3	0.0	0.0	0.0	0.3	0.0	8.0	-2.07	-0.03	7.276
fX^4	0.0	0.0	0.0	0.0	2.0	8.0	0.59	0.0020	6.498

The “a” through “f” coefficients in Table 23 are those in equation [35]. EX1 and EX2 are the ellipses from the fit. They were both negative. A rescaling of EX1 and EX2 allowed plotting them in Figure 26. EX1 has a small minimum so rescaled larger. EX2 was massively larger and rescaled considerably smaller to fit on the chart. There is a considerable range of forms for the residuals that adjusting these terms could model.

A second skewed normal distribution calculated (calculations (aa) through (af)) in the same manner as done for the first. This generated a second molecular weight adjustment (MW2)

The base molecular weight MW0, MW1 from the first elliptic and skewed normal distribution and MW2 from the second elliptic and skewed normal distribution are combined to get the final calculated molecular weight (MWC).

Elliptic Transition with Skewed Normal Distribution

One of the concerns was how well this would work. No transition issues were apparent when originally investigated. In preparing the graphic visualization of the transition lines with more granular inputs, they appeared.

Figure 27 to Figure 30 shows the sign transition for both ellipses. The first chart of each pair uses the same axes (H100, MW) as the ASTM chart while the second has axes based on the calculation parameter used for the ellipses (F2, MW0). The use of F2 causes the curved transition lines in Figure 27, Figure 29 and Figure 33. All the figures show smooth transitions but the granularity is the size of the data point on the plot.

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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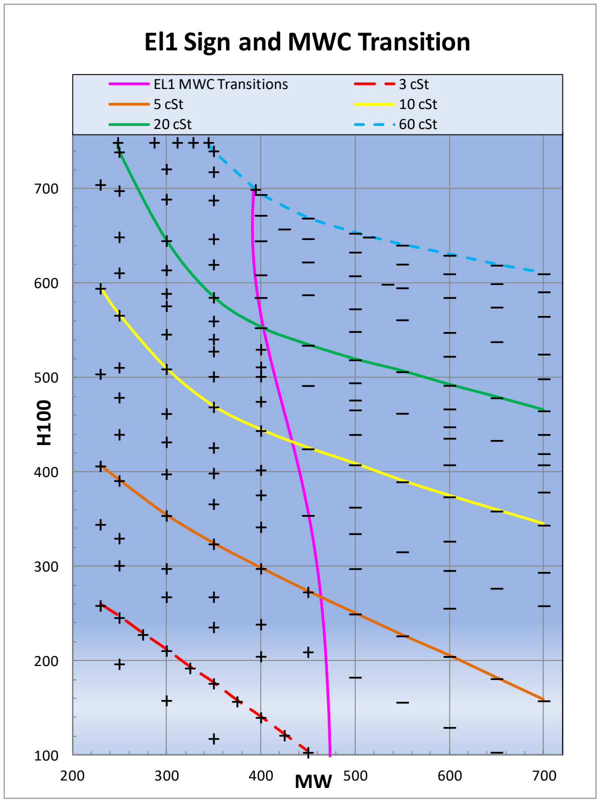

Figure 27 Ellipse 1 Sign Transition

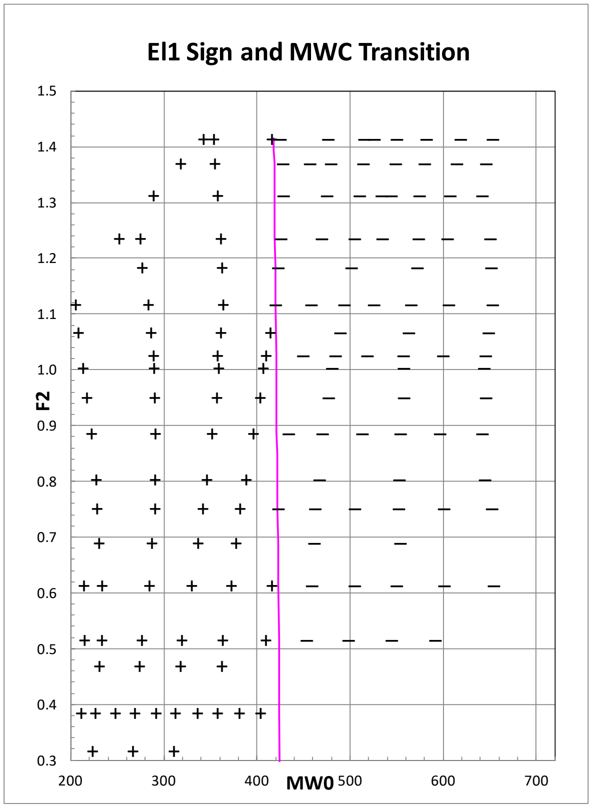

Figure 28 Ellipse 1 Sign Transition

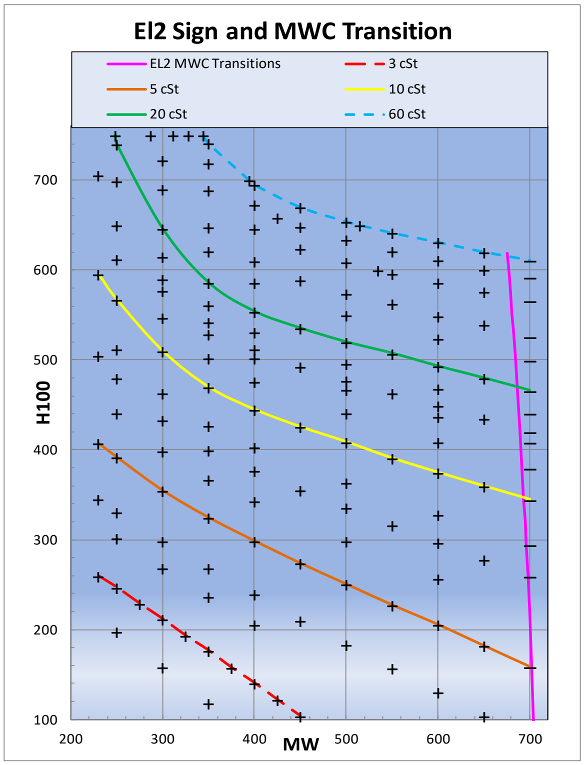

Figure 29 Ellipse 2 Sign Transition

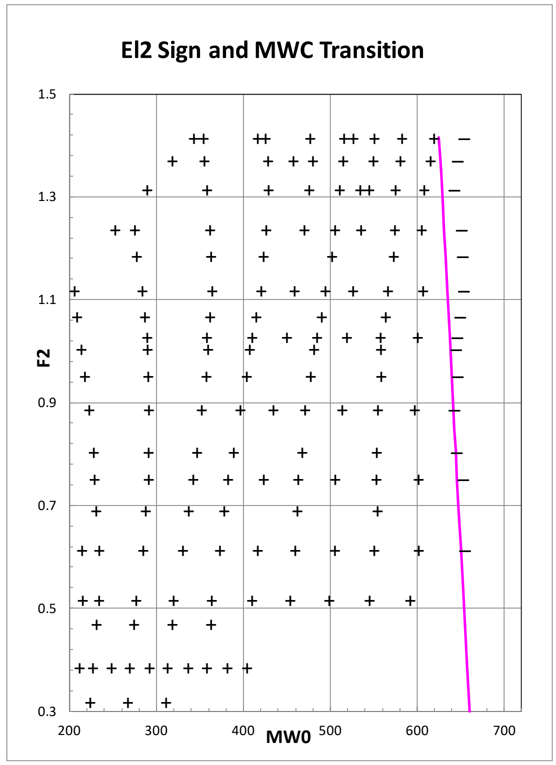

Figure 30 Ellipse 2 Sign Transition

A granularity of <0.05 for the H100 function showed the transition.

Figure 31 and Figure 32 show the magnitude of the effect for EL1 and EL2. Table 24 lists the values for EL1 and EL2 at various V210's. For EL1 the maximum amount is 5 at a V210 of 6 and for EL2 is a maximum of 15 at a V210 of 60. Figure 33 shows the transition for the experimental data. The EL2 transitions are essential in an area devoid of any experimental data and would have a low likelihood of being encountered in practice (Figure 33). The EL1 transition is in an area where there is experimental data close to the middle of the data. Although the amount is higher than desired to match the repeatability of reading the ASTM chart, it is within the reproducibility and similar to the difference seen with experimental samples.

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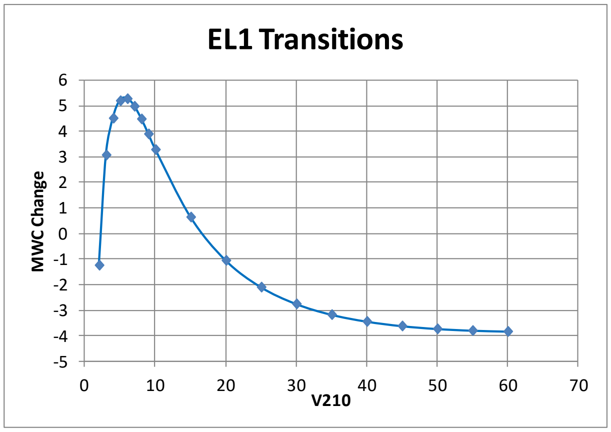

Figure 31 Ellipse 1 MWC Transition Amount

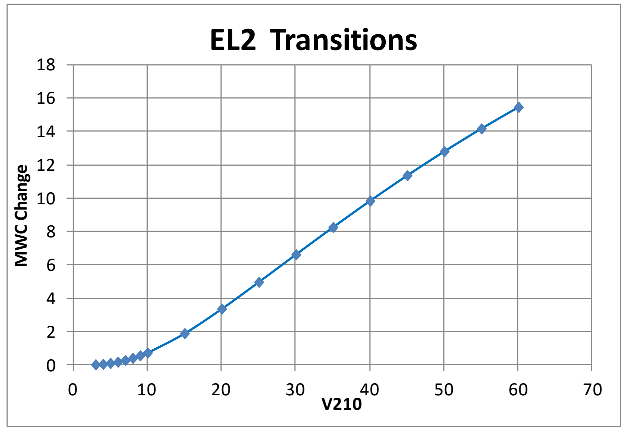

Figure 32 Ellipse 2 MWC Transition Amount

Table 24 Table of MWC Transitions at the Elliptic Axes

EL1					EL2				
V100	H100	V210	MWC	MWC Transition	V100	H100	V210	MWC	MWC Transition
6	88	3	474	3.1	2	-120	3	710	0.0
13	202	4	469	4.5	6	70	4	705	0.0
22	270	5	463	5.2	10	161	5	702	0.1
35	319	6	457	5.3	15	219	6	700	0.2
50	356	7	451	5.0	21	262	7	698	0.3
70	386	8	444	4.5	28	295	8	696	0.4
93	411	9	439	3.9	36	322	9	695	0.5
122	432	10	433	3.3	45	345	10	694	0.7
350	507	15	414	0.7	109	423	15	689	1.9
762	554	20	403	-1.0	206	471	20	687	3.3
1415	588	25	397	-2.1	342	505	25	684	5.0
2361	613	30	394	-2.7	519	531	30	683	6.6
3652	634	35	392	-3.2	741	552	35	681	8.2
5337	651	40	391	-3.4	1011	570	40	680	9.8
7462	666	45	391	-3.6	1331	584	45	679	11.3
10071	678	50	392	-3.7	1704	597	50	678	12.8
13206	689	55	392	-3.8	2131	608	55	677	14.2
16905	699	60	393	-3.8	2616	618	60	676	15.4

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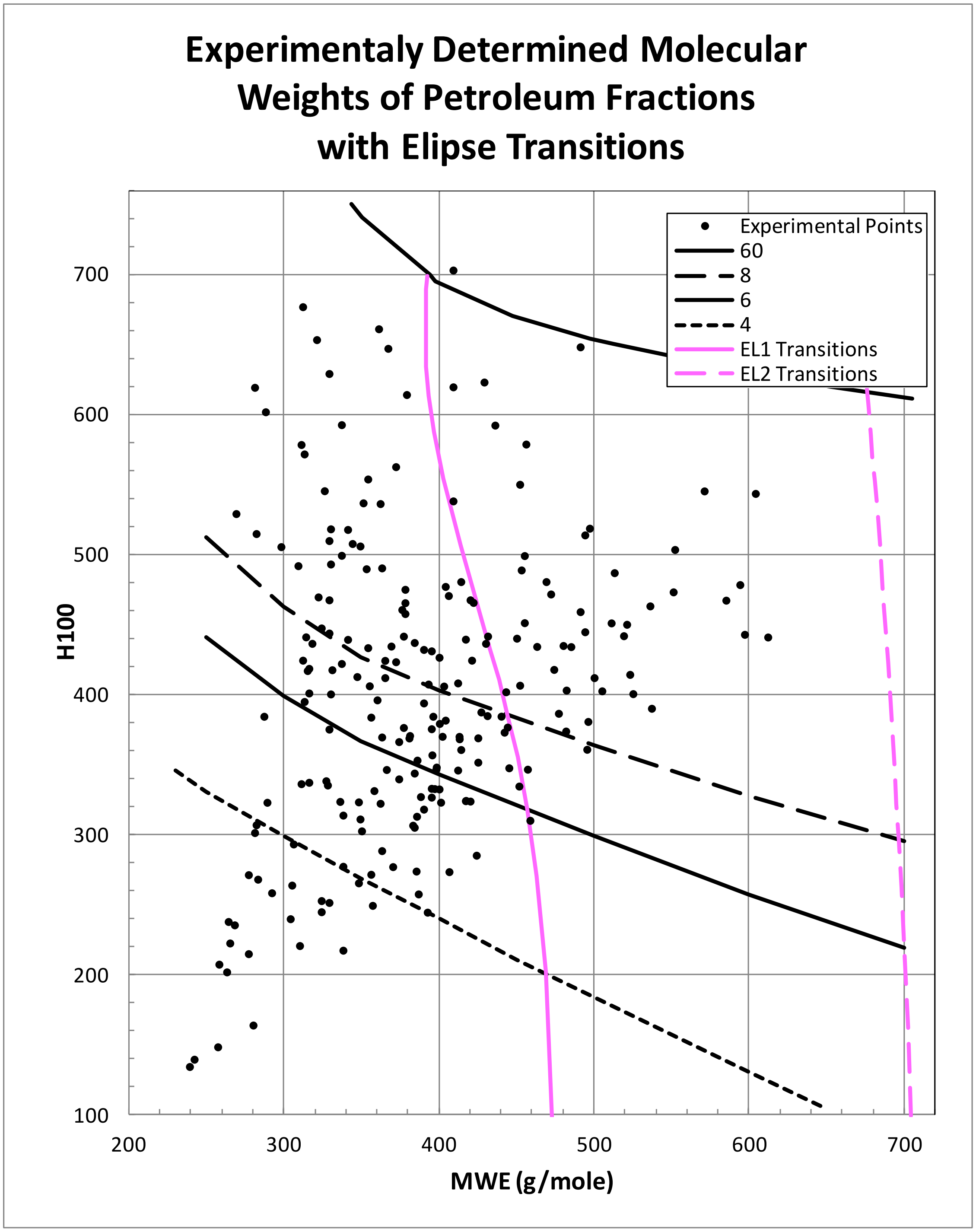

Figure 33 Elliptic Transitions with Experimental Data

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Coefficients Purposes

The coefficients are color-coded indicating their use in the calculation.

Table 25 Coefficients Color-Coded by Function in the Calculation

Main
Polynomial
First Elliptic
First Modified Normal
Second Elliptic
Second Modified Normal

Table 26 Explanation of Model Coefficients

Coefficients	Purpose
C(1)	Walther[25] type shift constant for F1
C(2)	Walther type shift constant for F2
C(3)	Scaling of F1 to F2
C(4)	Offset between F1 and F2 in F12
C(5)	Intercept for the primary MW calculation estimate based on F1, F2 and F12 functions
C(6)	Linear coefficient for F12
C(7)	Linear coefficient for F12*F1^2 cubic polynomial
C(8)	Linear coefficient for F1^4 quartic polynomial
C(9)	Linear coefficient for F1*F2*F12 cubic polynomial
C(10)	Rotation angle (-86.7 Deg) in radians for the first elliptic MW adjustment (MW1)
C(11)	X-axis translation of the center of a residual ellipse 1 in F2 with a scaled MW of MW*0.01
C(12)	Y-axis translation of the center of a residual ellipse 1 in F2 with a scaled MW of MW*0.01
C(13)	Elliptic 1 MW axis contour scaling
C(14)	Elliptic 1 F2 axis contour scaling
C(15)	Scaling of the first MW adjustment from the bivariate ellipse 1
C(16)	Constant for Skewed Gaussian correction MW based on ellipse 1 contour
C(17)	Coefficient for the linear term in a Skewed Gaussian correction MW based on ellipse 1 contour
C(18)	Coefficient for the quadratic term in a Skewed Gaussian correction MW based on ellipse 1 contour
C(19)	Coefficient for the cubic term in a Skewed Gaussian correction MW based on ellipse 1 contour
C(20)	Coefficient for the quartic term in a Skewed Gaussian correction MW based on

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Coefficients	Purpose
	ellipse 1 contour
C(21)	Rotation angle (-72.6 Deg) in radians for the second elliptic MW adjustment (MW2)
C(22)	X-axis translation of the center of a residual ellipse 2 in F2 with a scaled MW of MW*0.01
C(23)	Y-axis translation of the center of a residual ellipse 2 in F2 with a scaled MW of MW*0.01
C(24)	Elliptic 2 MW axis contour scaling
C(25)	Elliptic 2 F2 axis contour scaling
C(26)	Scaling of the a second MW adjustment from the bivariate ellipse 2
C(27)	Constant for Skewed Gaussian correction MW based on ellipse 2 contour
C(28)	Coefficient for the linear term in a Skewed Gaussian correction MW based on ellipse 2 contour
C(29)	Coefficient for the quadratic term in a Skewed Gaussian correction MW based on ellipse 2 contour
C(30)	Coefficient for the cubic term in a Skewed Gaussian correction MW based on ellipse 2 contour
C(31)	Coefficient for the quartic term in a Skewed Gaussian correction MW based on ellipse 2 contour
C(32)	Offset to the total MW's calculate (primary estimate, normal elliptic 1 adjustment, normal elliptic 2 adjustment)

Viscosity Conversion

Some of the viscosity data in the references is SUS. For use in the calculation, they had to be converted to cSt. The calculation {1} of the SUS from cSt at a temperature T used the formula given in ASTM D2161-93 (Reapproved 1992)$^{\epsilon 2}$ page 2 Equation (6). This equation was used to convert SUS data reported in the references to cSt for input to the model.

SUS is calculation is cell A1

= (1+0.000061*(C1-100))*(4.6324*B1+(1+0.03264*B1)/((3930.2+262.7*B1+23.97*B1^2+1.646*B1^3)*0.00001)) {1}

where the cell references in {1} are defined in Table 27.

Table 27 Cell Content for Calculation SUS from cSt

Excel cell	Content
A1	contains the formula {1} to calculate SUS
B1	cSt viscosity
C1	T, temperature °F

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Some references with viscosity and molecular weight data reported both SUS and cSt viscosity values. Using {1} did not give the same cSt reported. A reverse calculation from cSt to SUS was used to further compare the 2 reported viscosities. Previously a method for doing the reverse (InvSUS) calculation had been developed. It is detailed in the Calculation Codes section. Since it was available, the cSts reported were converted to SUS and reaffirmed the values did not convert equivalently using the current calculation. This adds another element of variability in the experimental data as all of the references that used SUS and converted for use by Hirschler or the reference's authors may not be consistent with the current conversion method.

REVELATIONS

Experimental Data MW Trends

The MWE data follows trends. It increases from samples that have low values of H100 and H210 to those that have high values as shown in Figure 34. This is not a surprising trend, as higher molecular oils would generally have higher viscosities and give higher H functions for both. In Figure 34, the MWE's have only their first digit plotted to make the chart readable. The MWE's vary from 250 to 450 along the dotted regression line of H100 and H210.

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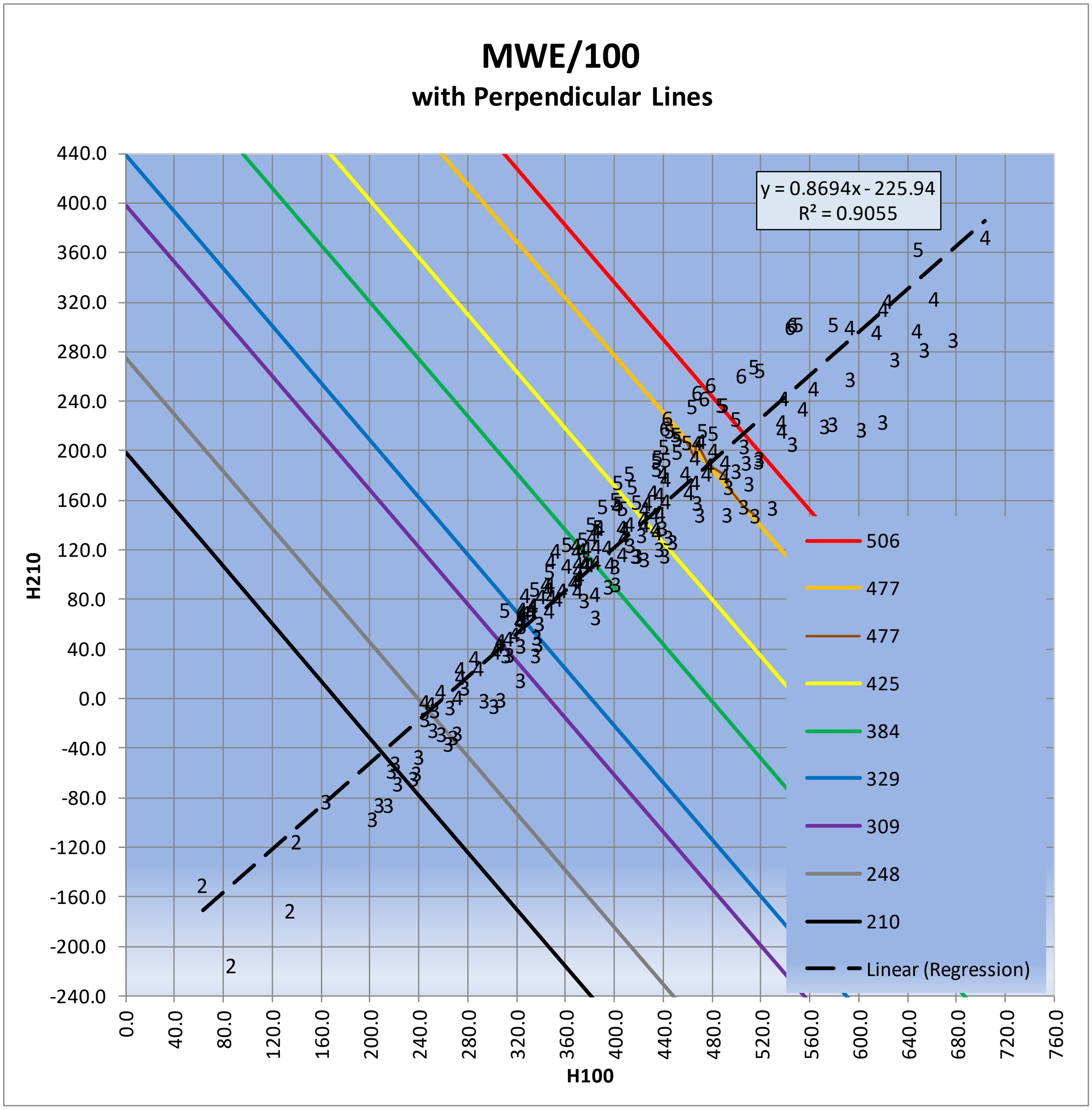

Figure 34 Experiment Molecular Weight Trend Related to H Functions

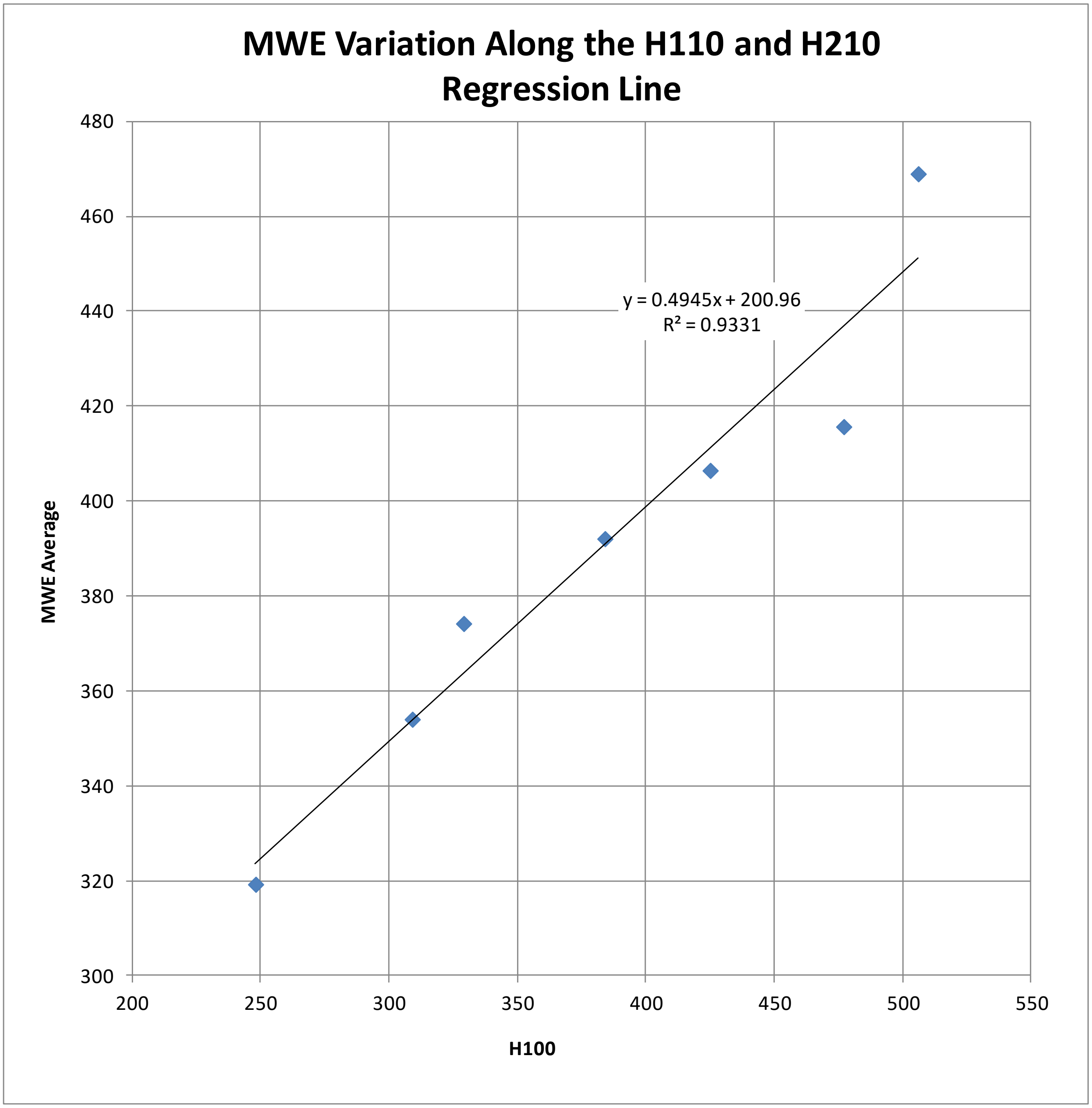

Figure 35 Variation of the Average Molecular Weight along the Regression Line

In addition to this trend, a trend of decreasing molecular weights perpendicular to the H100 and H210 regression line is discernible in Figure 34. Figure 36 using MWE/100 data labels and Figure 37 using data points show the data and trend more clearly. The reason for choosing lines perpendicular to the H100 and H210 regression line was arbitrary based on the appearance of the molecular weights on either side of the trend line. Figure 36 and Figure 37 have points chosen close to several perpendicular lines by calculating the distance from the experiment points to a specific perpendicular line and selecting a subset of the closest ones.

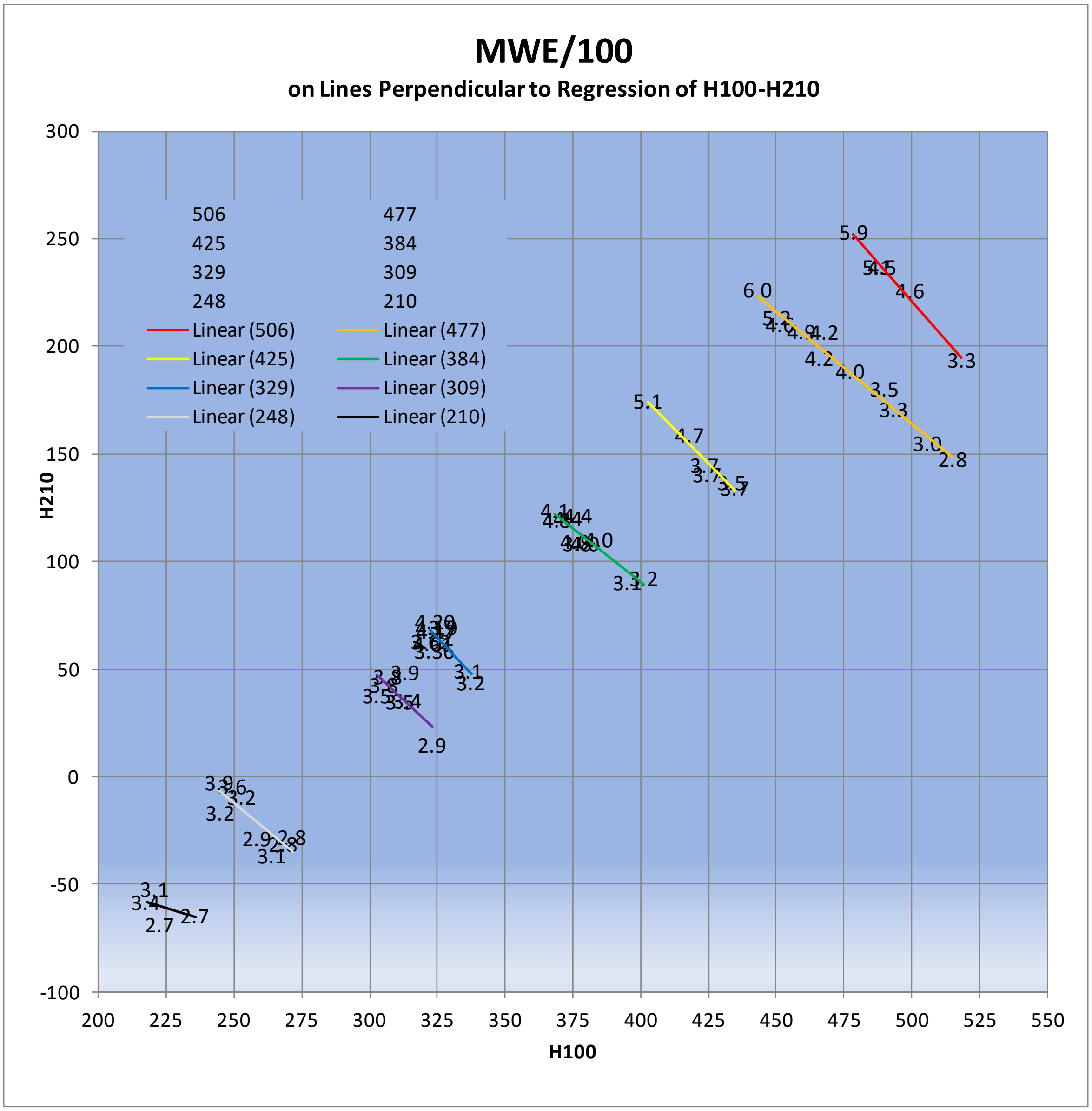

Figure 36 Experiment Molecular Weight Trends Perpendicular to the H100 and H210 Regression Line

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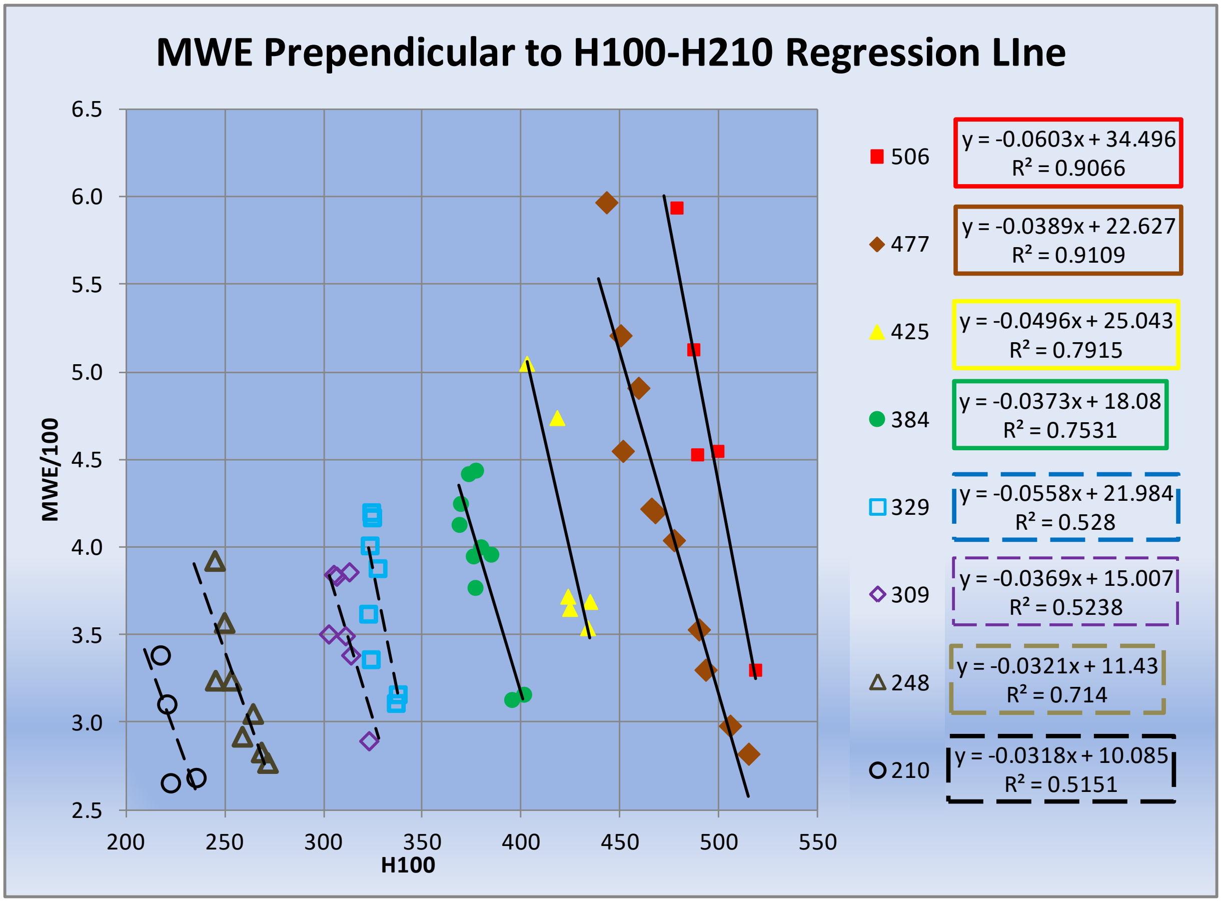

Figure 37 MWE Data Point Proximity to Perpendicular Lines

Other Approaches

The near linear components of the 2 trends in Figure 34 and Figure 37 suggested that other approaches may have interest for both fitting the data to the ASTM chart (MW) and to MWE. These would include:

1. Principal Component Analysis (PCA)
2. Fitting a function to the H100 and H210 relationship and then fitting a function perpendicular to that trend
3. Do the same as described in 2. but in the reverse order
4. Multiple Linear Regression (MLR)
5. Fitting the data with a 3D fitting program like Table Curve 3 D.

PCA selects perpendicular principle components although there might be some variant that fits non-perpendicular components. This was the reason for suggestions 2. and 3. as they could include a parameter to vary the angle off the perpendicular of the lines crossing the molecular weight trend of the H100 and H210 regression line. Some of these approaches may be degenerate and lead to essentially similar types of fits.

MLR and Table Curve 3D

The data H100 as x, H210 as y and either MW or MWE as z was fit to equations using Statistica and Table Curve 3D. These programs report the standard deviation of the fit as the standard error of estimate.

The equation fits of MWE in Table 30 named MLR 1 from Statistica and Best 3 from TC3D had standard deviations (23, 26) similar to the standard deviation of nearly replicate experimental data given in Table 14 (22) indicating that there are unlikely to be any models that will fit the actual experimental data better. Figure 38 is a plot of the TC3D fit Simple 4 and Figure 39 is a plot of the residuals for the Simple 4 fit. They give a visual representation showing how difficult it would be to find a better model due to the points being about equally above and the surface of the fitted plane and being nearly uniformly scattered across it. One of the data points that is considered a possible outlier is clearly evident in Figure 38 as a red dot with a long red line to the equation plane. The residuals plot in Figure 39 shows a second possible suspected outlier. The circles represent the data points with the fill colors representing the size of standard deviation. The color of the lines from the point to the fit plane and the point border color indicates whether it is above or below the plane. Table 28 is a description of the color-coding used in Figures 38 to 40.

Table 28 Legend for TC3D Figure 38, Figure 39, and Figure 40

Point Fill Color	SD		Drop Line and Point Border Color	Location Relative to the Surface
Blue	<1		Blue	Above
Green	>=1, <2		Red	Below
Yellow	>=2, <3			
Red	>3			

For the Statistica data, the standard deviation of fits to MWE and MW appear odd in that the standard deviation for the MW is greater than for the experimental data. The MW data covers a wider area and is not as linear as the MWE data making the error in a simple linear fit to the chart data greater.

For the best TC3D fits (Best 3 of MWE and Best 6 of MW), there is a significant reduction in the standard deviation fit for the MW data. A feature of the Chebyshev[26] polynomial is it generates a smooth and continuous curve. The bivariate form makes a surface. Figure 40 plots Best 6 for the MW data as a visual representation that the data points lay on the smooth continuous equation plane. Because of the smooth and continuous fit, a better fit to the MW data is unlikely. The same is true for the Chebyshev fit to MWE. As typically seen with extrapolated empirical fits,

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areas outside the fit may not realistically represent data in those areas. The Chebyshev fit has a "wall" plane on the right of Figure 40 that would not represent any experimental data in that area. The standard deviation (1.7) for the fit Best 6 was very close to the standard deviation for the fit model in this paper (2.3 Table 8). The "Best" equations and the "Simple" equations are considered limiting cases showing the range of standard deviations for the 2 sets of data.

The Chebyshev Bivariate Polynomial Order 10 is more complex to implement, has 66 coefficients and each coefficient will need at least 6 significant digits (precision) for calculations. Table Curve does not appear to check each coefficient for needed precision but reduces all of them equally starting at 18. The coefficient precision data in Table 29 shows that 6 digits will give a maximum error less than the ASTM repeatability error (Table 4). Coefficients with the next lower precision (5) are significantly worse.

Table Curve 3D has the ability to generate code for the fitted equations. The inputs for the code are the H100 and H210 values of V100 and V210. Code is available for C 64 bit, C 80 bit, Pascal, Basic, Fortran 77, Fortran 90, Java, Matlab and C++ from the author.

The Chebyshev Bivariate 10^{th} Order Polynomial C++ code is at the end of the paper.

Table 29 Table Curve 3D Coefficient Precision Effect on Chebyshev Fit

Coefficient Precision	Average Absolute Error	Minimum Absolute Error	Maximum Absolute Error
5	1.49	5.8	7.5
6	0.07	0.38	3.0

Table 30 Table Curve 3D Equation Fits to MW and MWE

Program	Equation	Data	R^2	SD	F-ratio	Equation Form
Statistica	MLR 1	MWE	0.88	26	798	z=a+bx+cy
Statistica	MLR 2	MW	0.91	44	771	z=a+bx+cy
TC3D	Best 3	MWE	0.95	20	46	Chebyshev X,Y Bivariate Polynomial Order 10
TC3D	Best 6	MW	0.9999	1.7	17156	Chebyshev X,Y Bivariate Polynomial Order 10
TC3D	Simple 4	MWE	0.91	23	1068	Ln(z)=a + bxLn(x)+cy
TC3D	Simple 5	MWE	0.90	24	989	1/z=a+bxLn(x)+cy
TC3D	Simple 7	MW	0.979	21	3796	1/z=a+bxLn(x)+cy

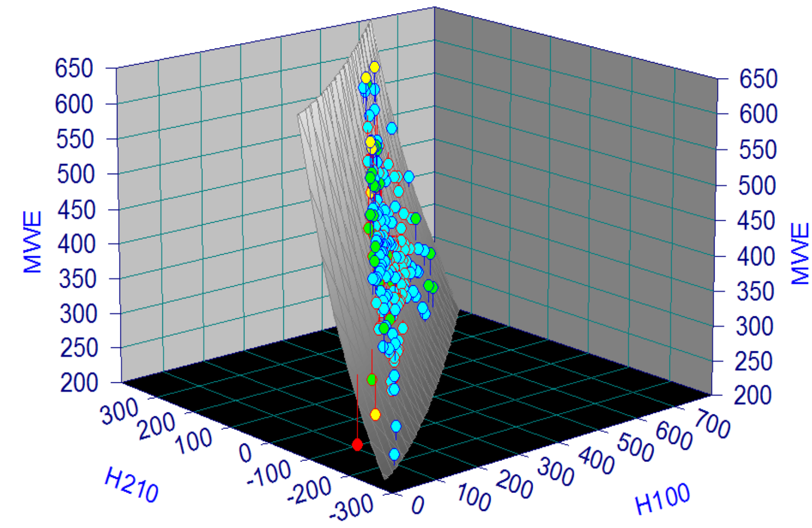

Figure 38 TC3D Equation Simple 4
Ln(MWE)=a + b*H100*Ln(H100)+c*(H210)

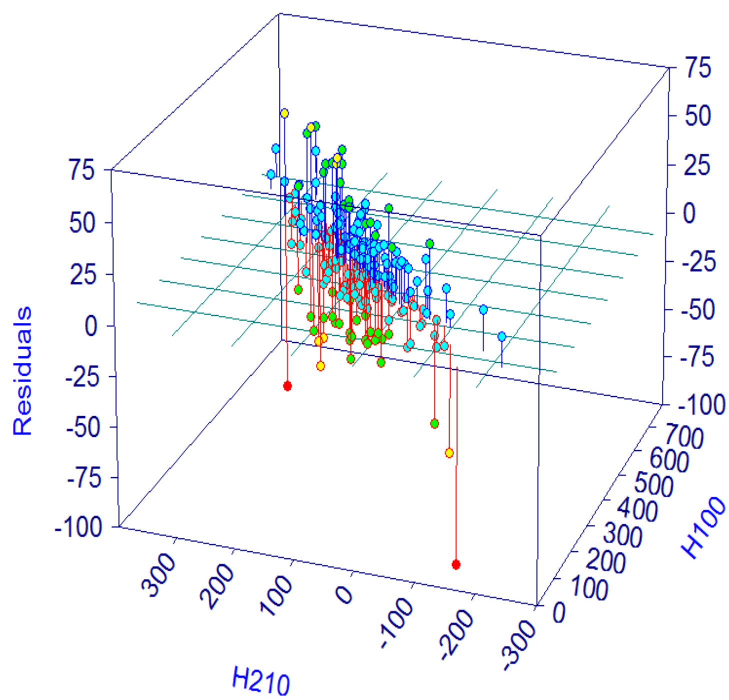

Figure 39 TC3D Equation Simple 4 Residuals
Ln(MWE)=a + b*H100*Ln(H100)+c*(H210)

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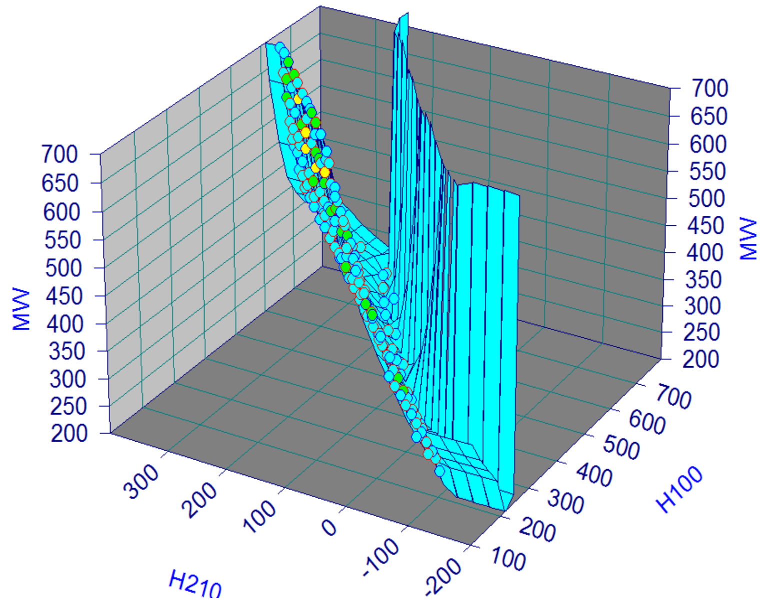

Figure 40 TC3D Best 6

Another interesting aspect of the TC3D fits was that for many of the better fits there were data transforms applied. In particular, H100 had an additional logarithmic transform essential making that data a triple logarithmic transform. The MW and MWE had many fits with an inverse or logarithmic transform.

H100-H210 Relationships

The parameters added to the F1 and F2 functions used in this paper instead of using H100 and H210 would give additional flexibility for attempting to fit a model. Varying the relationship between F1 and F2 in function F12 would give even more flexibility.

The parameter added to the viscosity is limited to those that are greater than one minus the minimum viscosity in the data set (>1-Min(V_t)). This is because the inner Log has to give a value >1 otherwise the outer Log would be the Log of 0 or a negative number and undefined. The other constraint is if the viscosity + the parameter become very small and close to the minimum viscosity, the F function will become extremely negative.

Below are some figures with MWEs that have various constants added to the viscosities. They exclude the low viscosity data from Reference 12 most of which would not be on the chart. The minimum V100 and V210 is 5.5052 and 1.78 respectively. Note that experimental point number 123 with the V210 of 1.78 in reference 9 is not on the chart but has no impact on the concept being exampled. The parameters have to be greater than -4.5052 and -0.78. The figures list the

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F1 and F2 parameters used to generate the charts in the title in the order for F1, F2. The red point in the figures is a suspect data point that was > 3 standard deviations for the fits.

Table 31 is a grid of figures. Figure 41 has the H functions as a reference and Figure 42, Figure 43 and Figure 44 have parameters near the low viscosities for the both the F1 and F2 function. Inspection of Figure 42 shows that the data point, which has low viscosities for both temperatures, is at an extreme distance from the other data point and would cause it to have a very high leverage, if used in any fitting. Similarly, both Figure 43 and Figure 44 have a point that is errant or extreme. This would cause issues in fitting models.

Table 31 Grid of Reference and F Functions Minimum Viscosities

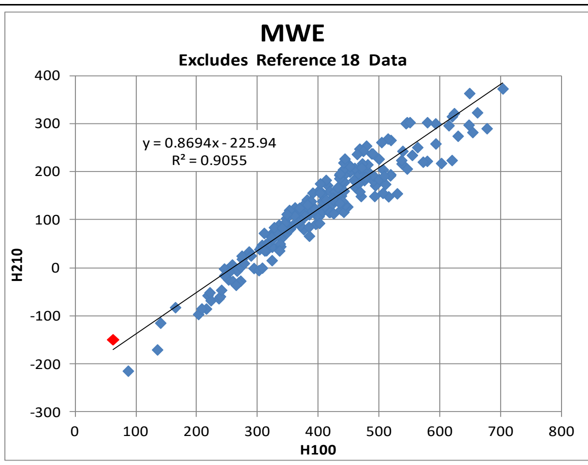

Figure 41 Reference H100 and H210

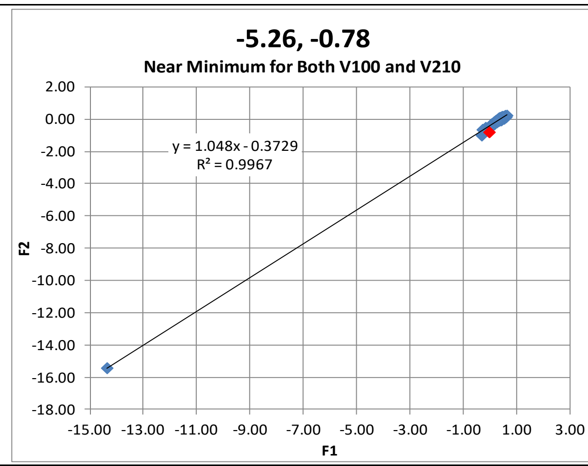

Figure 42 F Parameters Both Near Minimum

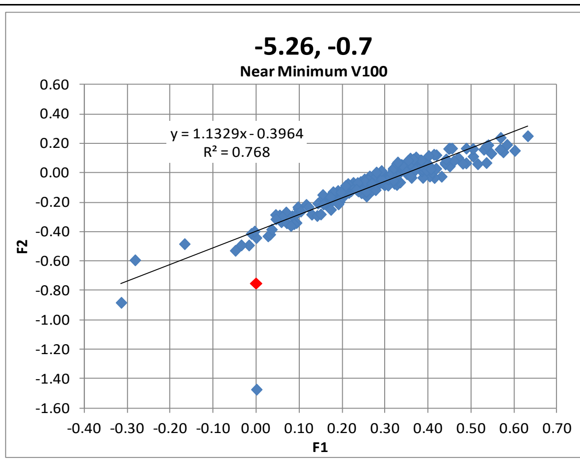

Figure 43 Near Minimum V100

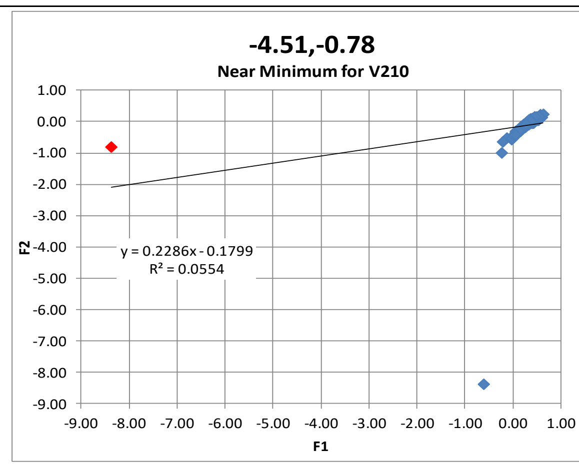

Figure 44 Near Minimum V210

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Table 32 is a grid of the F function parameters to show the different relationships between V100 and V210. Figure 45 with small F1 and F2 parameters (0, 0) not close to the minimum viscosities is essentially the same as Figure 41 but with different axis scaling. The others take various forms and have descriptive names. The more interesting one is Figure 47, the “Fan”. It is interesting because it expands the relationship giving greater variation in the correlation between the viscosities. This is somewhat similar to the belief in PCA that finding a principle component will increase the spread for the next principle component and help in making a model. It also reduces the collinearity. The others might be useful if a more complex function of the relationship of F1 to F1 is used for modeling.

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Table 32 Grid of Low, Medium and Large F Function Parameters

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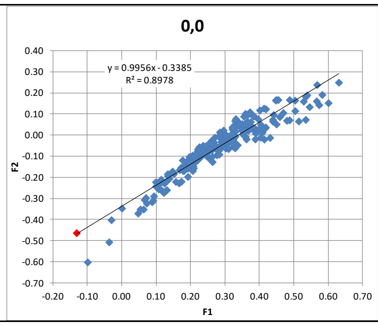
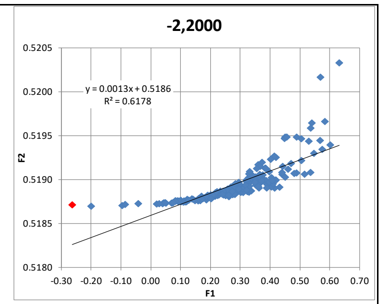
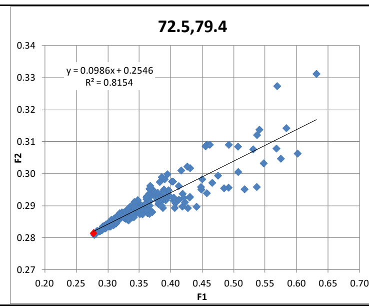
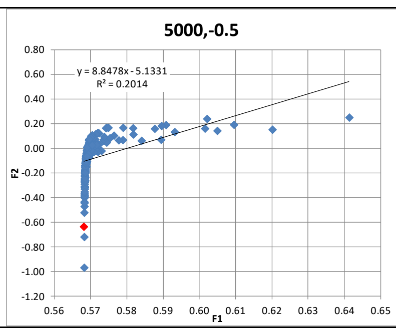
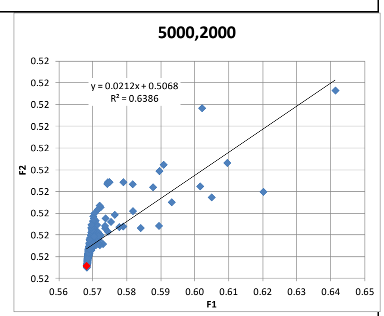
<tr><td></td><td></td><td></td></tr>
<tr><td>Figure 45 “Near Linear”
Low Values</td><td></td><td>Figure 46 “Ski Slope”
Low High Values</td></tr>
<tr><td></td><td></td><td></td></tr>
<tr><td></td><td>Figure 47 “Fan”
Mid. Values</td><td></td></tr>
<tr><td></td><td></td><td></td></tr>
<tr><td>Figure 48 “Left Cliff”
High Low Values</td><td></td><td>Figure 49 “Sneeze”
High Values</td></tr>
</table>

CONCLUSIONS

The calculation models the full range of the ASTM D2502 chart better than any other previously known method. Any differences between the chart and the model do not have any practical significance as the calculated molecular weight matches the chart better than the chart matches the experimental values as shown in Table 11 correlations. Viscosity measurement errors are 60-80% of the fit. The convenience of use, the reduction of interpolation and reading errors, results

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better than the reproducibility of the method, results similar to the repeatability and similar to the measurement errors make the use of the calculation viable.

The Chebyshev X,Y Bivariate Polynomial Order 10 model was found and can be considered for use in modeling the chart. It would not have the sign change transitions as the model in this paper. It offers a modest but likely not significant improvement in the standard deviation of the residuals (1.7 vs. 2.3). It is more complex to implement, has 66 coefficients and each coefficient will need at least 6 significant digits for calculations to give less than an absolute maximum error 0.4 MW.

It is unlikely that a better model to fit the experimental data is possible based on the standard deviations of the experimental data and that models of the current experimental data give nearly the same standard deviations as the data.

FUTURE

Functions that actually model the peaks and valleys as originally seen in Figure 3 and Figure 4 and avoids the molecular weight transition caused by the sign change across the elliptics would be of interest. Some possible refinements mentioned in the REVELATION section. The elliptic skew normal distribution replaced with the bivariate flexible skewed normal distributions detailed in the references (20, 21, 22 and 23) would likely avoid the transitions. The refinements are unlikely to have any practical significance that would merit any significant additional work.

Determining the standard error of the coefficients might make it possible to reduce the number of coefficients and allow refitting of the model to make it simpler.

To get a model that is closer to the experimental data would require a significant amount of work to generate new consistent data. The data would likely show that additional independent factors beyond the 2 viscosities may then be needed. Getting a model that is causal and theoretically based would be the best goal.

DATA: INPUT AND OUTPUT

Model Fitting Data

Table 33 below is the raw data used to generate the coefficients for the model. The V100 Input is calculated from H100 using equation [1]. The source of the data was Hirschler[27] (H) or Chart (C). HC denotes duplicate data given by Hirschler and taken from the chart. Only the Hirschler values were used for the model fit. The duplicate data differed only in the H100 value list in the Not Used column. The Hirschler values for H100 were integers in his paper. The H100 values from the chart had to be estimated from the MW lines and V210 isostokes. This highlights the difficulties in estimating values and the introduction of errors that can occur.

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Table 33 Data and Results for Fitting Model

Fit Point	Raw Data H100 (H)	Raw Data Input V210	Raw Data Input MW	Input V100	Output MWC	Residual	Source	Raw Data Not Used H100 (C) (C-H)
1	198	2.60	250	12.69	249.7	-0.3	H	
2	159	2.60	300	9.71	301.1	1.1	H	
3	119	2.60	350	7.56	351.5	1.5	H	
4	259.8	3	230	20.45	231.3	1.3	C	
5	247	3	250	18.41	248.9	-1.1	HC	246.8(-0.2)
6	229.1	3	275	15.99	274.4	-0.6	C	
7	212	3	300	14.05	299.2	-0.8	HC	211.3(-0.7)
8	193.6	3	325	12.30	325.8	0.8	C	
9	177	3	350	10.95	349.6	-0.4	HC	175.6(-1.4)
10	158.1	3	375	9.65	376.2	1.2	C	
11	141	3	400	8.65	399.8	-0.2	HC	140.3(-0.7)
12	122.4	3	425	7.71	424.9	-0.1	C	
13	104.3	3	450	6.93	449	-1.0	C	
14	302	4	250	29.56	249.4	-0.6	H	
15	269	4	300	22.09	299	-1.0	H	
16	237	4	350	17.01	350.2	0.2	H	
17	206	4	400	13.45	400.3	0.3	H	
18	345.7	4	230	45.20	230.7	0.7	C	
19	331	4	250	38.98	250.4	0.4	HC	331.7(0.7)
20	299	4	300	28.76	298.5	-1.5	HC	297(-2)
21	269	4	350	22.09	348.1	-1.9	HC	267.2(-1.8)
22	240	4	400	17.41	397.9	-2.1	HC	238.5(-1.5)
23	210.7	4	450	13.92	449.2	-0.8	C	
24	184	4	500	11.50	501.3	1.3	HC	183.5(-0.5)
25	157.5	4	550	9.62	548.6	-1.4	C	
26	130.9	4	600	8.12	596	-4.0	C	
27	104.5	4	650	6.94	643.2	-6.8	C	
28	407.5	5	230	89.77	230.5	0.5	C	
29	392	5	250	74.81	248.6	-1.4	H	
30	355	5	300	49.78	300.9	0.9	HC	355.1(0.1)
31	325	5	350	36.76	351.9	1.9	HC	324.7(-0.3)
32	299	5	400	28.76	400.7	0.7	HC	298.3(-0.7)

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Fit Point	Raw Data H100 (H)	Raw Data Input V210	Raw Data Input MW	Input V100	Output MWC	Residual	Source	Raw Data Not Used H100 (C) (C-H)
33	274.2	5	450	23.09	450.3	0.3	C	
34	251	5	500	19.02	504	4.0	HC	250.4(-0.6)
35	227.8	5	550	15.83	553.8	3.8	C	
36	206	5	600	13.45	601	1.0	HC	205.2(-0.8)
37	182.5	5	650	11.38	652.8	2.8	C	
38	159.2	5	700	9.72	706.3	6.3	C	
39	441	6	250	136.61	246.6	-3.4	H	
40	399	6	300	81.16	299.4	-0.6	H	
41	367	6	350	56.58	352.5	2.5	H	
42	343	6	400	43.97	399.3	-0.7	H	
43	299	6	500	28.76	502.5	2.5	H	
44	257	6	600	19.98	604.3	4.3	H	
45	504.9	7	230	339.21	226.5	-3.5	C	
46	480	7	250	233.72	247.5	-2.5	H	
47	433	7	300	123.17	300	0.0	HC	432.5(-0.5)
48	400	7	350	82.12	352.5	2.5	HC	400.2(0.2)
49	377	7	400	63.13	397.9	-2.1	HC	376.1(-0.9)
50	355.3	7	450	49.94	451.6	1.6	C	
51	336	7	500	40.97	499.3	-0.7	HC	335.5(-0.5)
52	316.8	7	550	33.96	549.4	-0.6	C	
53	297	7	600	28.24	601.9	1.9	HC	297(0)
54	278.2	7	650	23.90	652.1	2.1	C	
55	259.7	7	700	20.43	704.2	4.2	C	
56	512	8	250	378.94	249.8	-0.2	H	
57	463	8	300	183.71	298.4	-1.6	H	
58	427	8	350	114.12	352.4	2.4	H	
59	403	8	400	85.08	400	0.0	H	
60	364	8	500	54.78	500.5	0.5	H	
61	328	8	600	37.85	601.4	1.4	H	
62	295	8	700	27.74	696.7	-3.3	H	
63	595.6	10	230	1651.37	232.4	2.4	C	
64	567	10	250	961.92	252	2.0	H	
65	510	10	300	367.22	298.3	-1.7	HC	510.7(0.7)

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	Raw Data	Raw Data	Raw Data					Raw Data
Fit		Input	Input	Input	Output			Not Used
Point	H100 (H)	V210	MW	V100	MWC	Residual	Source	H100 (C) (C-H)
66	470	10	350	202.59	350.9	0.9	HC	470.7(0.7)
67	445	10	400	143.99	399.5	-0.5	HC	444.8(-0.2)
68	425.8	10	450	112.41	449.2	-0.8	C	
69	409	10	500	91.41	496.1	-3.9	HC	407.7(-1.3)
70	390.9	10	550	73.87	551.2	1.2	C	
71	375	10	600	61.75	600.4	0.4	HC	374.9(-0.1)
72	359.9	10	650	52.43	646.6	-3.4	C	
73	345	10	700	44.88	694	-6.0	HC	345.7(0.7)
74	612	12	250	2294.25	252.8	2.8	H	
75	547	12	300	674.85	298.9	-1.1	H	
76	502	12	350	324.40	351.4	1.4	H	
77	476	12	400	220.63	400.9	0.9	H	
78	441	12	500	136.61	497.4	-2.6	H	
79	409	12	600	91.41	602.3	2.3	H	
80	380	12	700	65.28	697.9	-2.1	H	
81	650	14	250	5203.38	252.8	2.8	H	
82	577	14	300	1156.64	300.2	0.2	H	
83	529	14	350	498.23	350.1	0.1	H	
84	502	14	400	324.40	399.2	-0.8	H	
85	467	14	500	194.23	496.2	-3.8	H	
86	437	14	600	129.68	599.4	-0.6	H	
87	409	14	700	91.41	695.9	-4.1	H	
88	705.4	15	230	20100.30	231.1	1.1	C	
89	590.1	15	300	1483.62	300.9	0.9	C	
90	541.9	15	350	618.35	348	-2.0	C	
91	512.4	15	400	381.33	400.3	0.3	C	
92	492.8	15	450	282.19	450.5	0.5	C	
93	477.4	15	500	225.11	498.1	-1.9	C	
94	463.5	15	550	184.99	546.1	-3.9	C	
95	449.1	15	600	152.06	597.6	-2.4	C	
96	434.7	15	650	125.89	647.6	-2.4	C	
97	420.7	15	700	105.47	697.5	-2.5	C	
98	699	17	250	17018.60	251.4	1.4	H	

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	Raw Data	Raw Data	Raw Data					Raw Data
Fit		Input	Input	Input	Output			Not Used
Point	H100 (H)	V210	MW	V100	MWC	Residual	Source	H100 (C) (C-H)
99	615	17	300	2440.27	301.1	1.1	H	
100	561	17	350	863.19	349.7	-0.3	H	
101	531	17	400	514.95	401.7	1.7	H	
102	496	17	500	296.10	500.4	0.4	H	
103	468	17	600	196.97	602.5	2.5	H	
104	441	17	700	136.61	700.7	0.7	H	
105	750.0	20	249	69560.18	245.7	-2.8	C	
106	740	20	250	51985.25	250.3	0.3	H	
107	646	20	300	4754.94	301.6	1.6	HC	644.9(-1.1)
108	586	20	350	1371.13	350.5	0.5	HC	586.2(0.2)
109	554	20	400	762.37	402.7	2.7	HC	555.4(1.4)
110	535.4	20	450	554.08	450.1	0.1	C	
111	520	20	500	430.37	499.9	-0.1	HC	520.7(0.7)
112	507.4	20	550	352.62	546.5	-3.5	C	
113	493	20	600	283.04	602.4	2.4	HC	494(1)
114	479.8	20	650	233.04	651.8	1.8	C	
115	466	20	700	191.53	704.9	4.9	HC	466.3(0.3)
116	690	25	300	13531.02	300.1	0.1	H	
117	621	25	350	2764.86	349.7	-0.3	H	
118	586	25	400	1371.13	400	0.0	H	
119	550	25	500	710.86	502.5	2.5	H	
120	524	25	600	459.11	606.4	6.4	H	
121	500	25	700	314.63	703.6	3.6	H	
122	750.0	30	287	69560.18	285.7	-1.4	C	
123	722	30	300	31367.58	299.9	-0.1	HC	724(2)
124	648	30	350	4973.52	350	0.0	HC	647.5(-0.5)
125	610	30	400	2202.39	400	0.0	HC	609.9(-0.1)
126	588.9	30	450	1449.64	451.3	1.3	C	
127	574	30	500	1093.85	501	1.0	HC	574.2(0.2)
128	562.5	30	550	886.73	546.5	-3.5	C	
129	549	30	600	698.62	604.1	4.1	HC	551.2(2.2)
130	539.2	30	650	590.66	644.9	-5.1	C	
131	526	30	700	474.32	702.5	2.5	HC	527.2(1.2)

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Fit Point	Raw Data H100 (H)	Raw Data Input V210	Raw Data Input MW	Input V100	Output MWC	Residual	Source	Raw Data Not Used H100 (C) (C-H)
132	750.0	40	312	69560.18	309	-2.5	C	
133	689	40	350	13195.02	350.2	0.2	HC	688.9(-0.1)
134	646	40	400	4754.94	400.1	0.1	HC	644.9(-1.1)
135	623.6	40	450	2920.41	451.4	1.4	C	
136	609	40	500	2158.02	499.7	-0.3	HC	608.3(-0.7)
137	600.0	40	534	1801.15	535.9	1.5	C	
138	596.3	40	550	1674.22	551.9	1.9	C	
139	586	40	600	1371.13	598.4	-1.6	HC	585.5(-0.5)
140	575.8	40	650	1131.04	643.9	-6.1	C	
141	566	40	700	944.60	693.7	-6.3	HC	566.3(0.3)
142	750.0	50	328	69560.18	327	-1.3	C	
143	719	50	350	28901.46	350.1	0.1	HC	719.3(0.3)
144	673	50	400	8903.45	399.5	-0.5	HC	672.4(-0.6)
145	658.5	50	425	6321.89	427.3	2.3	C	
146	648.3	50	450	5007.26	452.9	2.9	C	
147	634	50	500	3649.02	499.8	-0.2	HC	633.1(-0.9)
148	621.3	50	550	2782.33	552.9	2.9	C	
149	611	50	600	2247.79	601.2	1.2	HC	610.5(-0.5)
150	600.6	50	650	1822.75	649.5	-0.5	C	
151	592	50	700	1539.28	697.7	-2.3	HC	596.1(4.1)
152	750.0	60	344	69560.18	343.3	-1.1	C	
153	741	60	350	53502.99	350.7	0.7	H	
154	700.0	60	395	17463.73	394.7	0.2	C	
155	695	60	400	15359.15	398.1	-1.9	HC	696.1(1.1)
156	670.0	60	450	8285.54	447.4	-2.6	C	
157	654	60	500	5699.57	497.3	-2.7	HC	653.7(-0.3)
158	650.0	60	515	5203.38	512.8	-1.8	C	
159	641.4	60	550	4291.83	549.9	-0.1	C	
160	631	60	600	3419.79	599.8	-0.2	HC	630.6(-0.4)
161	620.2	60	650	2718.90	651.8	1.8	C	
162	611	60	700	2247.79	705	5.0	HC	610.6(-0.4)

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Model Validation Data

The data for testing (validating) the model was randomly generated pairs of values for V100 and V210. Any pairs not on the chart were discarded. The H100 values were calculated and used with the V210 to estimate the MW from the chart.

Table 34 Data and Results for Testing Model Fit

		Raw Data	Raw Data	Raw Data		
Test		Input	Input	Input	Output	
Point	H100	V210	MW	V100	MWC	Residual
1	369.13	6.10	352	57.9	355.3	3.3
2	681.68	16.90	258	11000.0	260.3	2.3
3	395.38	6.68	345	77.8	343.3	-1.7
4	586.34	30.10	464	1380.0	460.3	-3.7
5	526.09	18.60	450	475.0	447.1	-2.9
6	343.95	4.92	309	44.4	312.4	3.4
7	216.21	4.52	512	14.5	514.9	2.9
8	553.37	31.70	616	754.0	615.8	-0.2
9	531.36	21.20	488	518.0	489	1.0
10	407.34	6.18	297	89.6	297	0.0
11	617.31	51.80	594	2560.0	589.7	-4.3
12	327.32	5.41	383	37.6	382.9	-0.1
13	480.67	13.00	420	236.0	422.7	2.7
14	150.67	4.59	660	9.2	658	-2.0
15	360.03	8.38	540	52.5	538.4	-1.6
16	430.96	6.71	289	120.0	290.1	1.1
17	584.01	16.40	320	1320.0	318.8	-1.2
18	303.22	6.85	569	29.9	571.8	2.8
19	648.76	21.20	308	5060.0	306.6	-1.4
20	424.07	7.90	351	110.0	353.2	2.2
21	545.44	8.59	240	657.0	238.7	-1.3
22	234.68	3.66	361	16.7	362.1	1.1
23	387.32	7.27	392	70.9	392.6	0.6
24	261.29	3.75	330	20.7	330.3	0.3
25	301.39	4.80	374	29.4	376.7	2.7
26	450.53	7.49	297	155.0	296.2	-0.8
27	460.71	13.40	493	178.0	493.5	0.5
28	593.34	50.00	697	1580.0	692.5	-4.5

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Test Point	H100	Raw Data Input V210	Raw Data Input MW	Raw Data Input V100	Output MWC	Residual
29	683.48	14.40	235	11500.0	237.2	2.2
30	434.77	13.10	568	126.0	567.8	-0.2
31	714.07	37.80	326	25300.0	325.4	-0.6
32	731.47	18.40	244	40800.0	244.6	0.6
33	401.52	6.86	340	83.6	342.3	2.3
34	461.53	16.00	590	180.0	590.8	0.8
35	616.74	28.00	381	2530.0	375.5	-5.5
36	405.45	6.77	332	87.6	330.9	-1.1
37	433.52	5.71	242	124.0	240.8	-1.2
38	110.86	3.19	479	7.2	480	1.0
39	466.95	6.99	262	194.1	259.6	-2.4
40	286.92	3.52	259	25.8	261.7	2.7

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Experimental Data

Table 35 is the experimental data used by Hirschler to generate the ASTM D2502 chart. The Chart Label column uses single characters for some figures to make them more readable.

Table 35 Experimental Data (Hirschler's Reference) and Model Fitting Results

		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
1	384.5	5.59	287	68.7			26	2	296.5	9.5
2	493.2	10.5	330	284			26	2	329.2	-0.8
3	536.9	14.5	351	568			26	2	347.1	-3.9
4	562.7	18.9	372	890			26	2	371.4	-0.6
5	623.1	35.3	429	2890			26	2	415.2	-13.8
6	648.2	54	491	5000			26	2	478.6	-12.4
7	529.2	9.4	269	500			26	2	268.6	-0.4
8	514.9	9.03	282	397			26	2	272.6	-9.4
9	505.6	9.46	298	343			26	2	290.9	-7.1
10	436.6	7.63	318	129			26	2	321.0	3.0
11	375.4	6.02	329	62			26	2	338.9	9.9
12	323.4	4.96	348	36.2			26	2	351.2	3.2
13	249.6	3.95	357	18.8			26	2	375.1	18.1
14	619.3	15.3	281	2670			26	2	284.3	3.3
15	601.9	14.6	288	1870			26	2	289.0	1.0
16	578.5	15.1	311	1190			26	2	310.6	-0.4
17	571.8	14.9	313	1050			26	2	314.1	1.1
18	545.5	13.4	326	658			26	2	320.3	-5.7
19	518.3	12.3	330	419			26	2	334.0	4.0
20	433.5	8.43	354	124			26	2	359.0	5.0
21	396.3	7.11	360	78.6			26	2	365.5	5.5
22	346.5	5.75	366	45.6			26	2	373.1	7.1
23	306.8	5.06	383	30.9			26	2	391.4	8.4
24	676.9	26.4	312	9780			26	2	313.3	1.3
25	653.4	24.6	321	5620			26	2	320.6	-0.4
26	629.2	23	329	3290			26	2	330.0	1.0
27	592.7	20.1	337	1560			26	2	343.7	6.7

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
28	553.9	16.6	354	761			26	2	354.2	0.2
29	536.4	15.3	362	563			26	2	361.0	-1.0
30	475.2	11.3	378	218			26	2	381.1	3.1
31	432.3	9.08	390	122			26	2	389.0	-1.0
32	375.7	7.14	395	62.2			26	2	409.7	14.7
33	408.4	8.45	412	90.7			26	2	411.7	-0.3
34	324.0	5.79	420	36.4			26	2	421.9	1.9
35	661.1	35.9	361	6720			26	2	362.8	1.8
36	614.2	27.9	379	2400			26	2	378.6	-0.4
37	480.7	12.9	414	236			26	2	418.0	4.0
38	436.6	10.1	430	129			26	2	423.2	-6.8
39	346.8	6.86	457	45.7			26	2	461.6	4.6
40	703.0	59.9	409	18900			26	2	390.3	-18.7
41	592.4	28.9	436	1550			26	2	428.9	-7.1
42	480.7	14.3	469	236			26	2	464.1	-4.9
43	380.8	8.65	496	65.9			26	2	497.5	1.5
44	441.2	7.4	314	137			27	3	305.1	-8.9
45	447.6	7.91	324	149			27	3	315.7	-8.3
46	443.9	8.09	329	142			27	3	327.9	-1.1
47	492.0	9.07	309	279			27	3	295.6	-13.4
48	510.0	10.7	329	367			27	3	312.8	-16.2
49	517.9	12.1	341	416			27	3	330.8	-10.2
50	489.8	11.2	353	270			27	3	351.6	-1.4
51	460.7	10.2	376	178			27	3	374.2	-1.8
52	437.2	9.12	384	130			27	3	380.5	-3.5
53	407.5	8.09	393	89.8			27	3	394.9	1.9
54	384.5	7.18	396	68.7			27	3	393.1	-2.9
55	370.2	6.91	402	58.6			27	3	406.6	4.6
56	324.3	5.71	417	36.5			27	3	414.5	-2.5
57	647.2	28.2	367	4880			27	3	342.2	-24.8
58	499.2	15.6	455	311			27	3	449.3	-5.7
59	369.0	6.56	380.6	57.85			24	4	386.0	5.4
60	353.2	6.06	385.8	48.87			24	4	383.1	-2.7

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
61	313.2	5.11	385.5	32.81			24	4	383.8	-1.7
62	274.1	4.38	385.2	23.06			24	4	382.9	-2.3
63	257.7	4.14	386.6	20.1			24	4	384.2	-2.4
64	244.7	3.98	392.4	18.08			24	4	387.2	-5.2
65	357.0	6.3	395.4	50.84			24	4	392.8	-2.6
66	348.3	6.12	398.2	46.41			24	4	397.6	-0.6
67	323.2	5.48	401	36.12			24	4	397.0	-4.0
68	273.6	4.52	406.4	22.98			24	4	399.1	-7.3
69	379.4	7.1	400.2	64.87			24	4	399.0	-1.2
70	370.2	7.12	412.9	58.57			24	4	420.6	7.7
71	324.5	5.65	417.2	36.57			24	4	409.0	-8.2
72	285.4	4.72	424	25.45			24	4	398.6	-25.4
73	424.6	9.35	421	110.7			24	4	418.3	-2.7
74	376.8	7.67	444	63			24	4	440.8	-3.2
75	334.7	6.34	451.5	40.45			24	4	444.0	-7.5
76	310.3	5.77	458.6	31.93			24	4	449.8	-8.8
77	441.8	10.97	431.3	138			24	4	450.2	18.9
78	406.7	9.39	452	88.93			24	4	469.5	17.5
79	386.7	8.53	477	70.37			24	4	474.1	-2.9
80	374.0	8.02	481.7	61.07			24	4	475.2	-6.5
81	361.0	7.82	495.3	53.03			24	4	496.0	0.7
82	451.2	12.8	511	156.4			24	4	499.6	-11.4
83	442.0	12.24	519	138.5			24	4	504.7	-14.3
84	414.4	10.53	523	97.65			24	4	508.2	-14.8
85	400.7	9.82	525	82.8			24	4	510.7	-14.3
86	390.3	9.48	537	73.32			24	4	521.9	-15.1
87	265.7	3.9	348	21.47			9	5	341.7	-6.3
88	318.3	5.2	390	34.44			9	5	382.2	-7.8
89	385.0	7.74	431	69.06			9	5	425.8	-5.2
90	418.0	9.7	474	102			9	5	455.3	-18.7
91	333.1	5.9	395	39.81			9	5	411.9	16.9
92	217.6	3.12	338	14.65			9	5	310.1	-27.9
93	288.6	4.53	363	26.2			9	5	372.7	9.7

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
94	327.2	5.7	388	37.56			9	5	407.6	19.6
95	360.8	7.05	414	52.93			9	5	437.3	23.3
96	384.6	8.36	440	68.75			9	5	469.1	29.1
97	403.2	9.63	482	85.32			9	5	492.5	10.5
98	450.2	14.19	521	154.3			9	5	561.1	40.1
99	332.9	5.84	397	39.73			9	5	407.4	10.4
100	251.6	3.59	329	19.12			9	5	325.2	-3.8
101	271.8	4.05	356	22.61			9	5	349.3	-6.7
102	305.3	4.96	384	30.48			9	5	384.8	0.8
103	332.7	5.82	400	39.63			9	5	406.3	6.3
104	346.1	6.33	412	45.41			9	5	417.9	5.9
105	373.2	7.61	442	60.54			9	5	450.4	8.4
106	426.6	9.64	400	113.6			9	5	426.8	26.8
107	202.1	2.67	263	13.07			9	5	256.8	-6.2
108	215.1	2.79	277	14.38			9	5	260.0	-17.0
109	293.4	4	306	27.34			9	5	307.5	1.5
110	369.7	6.28	363	58.29			9	5	366.1	3.1
111	465.8	12.38	422	191			9	5	440.5	18.5
112	518.8	21.36	497	422			9	5	539.0	42.0
113	545.4	29.57	571	656.6			9	5	611.4	40.4
114	376.5	7.1	377	62.81			9	5	405.2	28.2
115	222.7	2.99	265	15.23			9	5	282.0	17.0
116	258.6	3.54	292	20.24			9	5	307.6	15.6
117	314.0	4.78	338	33.07			9	5	351.7	13.7
118	370.8	6.7	381	58.96			9	5	391.7	10.7
119	406.1	8.5	403	88.28			9	5	419.5	16.5
120	439.6	11.29	417	134.1			9	5	470.2	53.2
121	514.0	21.9	494	391.1			9	5	571.8	77.8
122	400.5	7.03	330	82.59			9	5	353.3	23.3
123[2]	86.5[2]	1.78[2]	218	6.26			9	5	195.2	-22.8
124	134.6	2.05	239	8.31			9	5	213.3	-25.7
125	271.5	3.55	277	22.56			9	5	288.7	11.7
126	395.1	6.4	313	77.54			9	5	328.1	15.1

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
127	490.5	12.06	363	272.5			9	5	372.9	9.9
128	538.3	17.74	409	581.5			9	5	399.7	-9.3
129	578.8	29.57	456	1197			9	5	477.4	21.4
130	235.7	3.04	268	16.83			9	5	271.1	3.1
131	268.3	3.5	283	21.95			9	5	287.3	4.3
132	337.4	4.99	316	41.56			9	5	329.2	13.2
133	406.3	7.45	355	88.49			9	5	364.5	9.5
134	465.6	10.78	378	190.5			9	5	383.9	5.9
135	253.0	3.86	324	19.33	39.0	95.0	18	6	357.7	33.7
136	387.6	8.48	427	71.14	54	330.0	18	6	468.3	41.3
137	503.6	20.59	552	332.44	101	1540	18	6	577.9	25.9
138	164.1	2.82	280	10.05	35.6	59	18	6	336.0	56.0
139	245.0	3.73	324	18.13	38.6	90	18	6	355.0	31.0
140	402.0	9.50	443	84.12	57.5	390	18	6	488.8	45.8
141	487.0	17.01	513	259.04	86	1200.0	18	6	532.4	19.4
142	543.6	29.01	604	636.82	138	2950	18	6	608.2	4.2
143[3]	62.9	2.20[3]	221	5.51[3]	33.5	44	18	6	325.0	104.0
144	139.8	2.49	242	8.58	34.5	54	18	6	304.2	62.2
145	207.6	2.79	258	13.60	35.5	72	18	6	270.6	12.6
146	238.1	3.09	264	17.15	36.5	86	18	6	275.7	11.7
147	301.5	3.92	281	29.44	39.2	139	18	6	285.7	4.7
148	307.1	4.01	282	31.00	39.5	146	18	6	287.0	5.0
149	323.1	4.32	289	36.10	40.5	169	18	6	293.0	4.0
150	401.2	6.47	316	83.26	47.4	386	18	6	322.0	6.0
151	506.1	13.22	349	345.39	71	1600.0	18	6	372.2	23.2
152[3]	619.7	33.21	409	2689.75	157[4]	12460	18	6	406.5	-2.5
153	423.5	8.86	372	109.19	55.3	506	18	6	398.1	26.1
154	412.9	7.79	347	95.79	51.7	444	18	6	368.8	21.8
155	422.2	8.18	337	107.46	53	498.0	18	6	369.3	32.3
156	417.2	7.39	315	100.98	50.4	468	18	6	341.9	26.9
157	499.4	11.47	337	311.93	64.5	1445	18	6	343.3	6.3
158	439.4	8.48	341	133.81	54	620.0	18	6	350.3	9.3
159	418.7	7.39	316	102.93	50.4	477	18	6	339.3	23.3

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
160	424.6	7.27	312	110.70	50	513.0	18	6	324.2	12.2
161	469.7	9.07	322	201.83	56	935.0	18	6	323.0	1.0
162	424.4	8.62	365	110.49	54.5	512	18	6	385.2	20.2
163	441.7	9.73	377	137.92	58.3	639	18	6	396.0	19.0
164	467.6	9.65	329	196.00	58	908.0	18	6	343.9	14.9
165	507.9	12.02	344	355.10	66.5	1645	18	6	342.9	-1.1
166	467.4	18.41	585	195.35	91.8	905	18	6	650.3	65.3
167	478.5	19.37	594	228.81	95.8	1060	18	6	638.4	44.4
168	467.6	13.50	420	196.00	72.1	908	18	6	475.8	55.8
169	434.3	12.21	485	125.17	67.2	580	18	6	528.4	43.4
170	459.2	13.53	491	174.41	72.2	808	18	6	503.4	12.4
171	471.8	14.51	472	207.87	76	963.0	18	6	499.2	27.2
172	444.9	14.51	494	143.75	76	666	38	7	593.1	99.1
173	440.3	13.22	450	135.33	71	627	38	7	554.1	104.1
174	434.4	11.61	463	125.39	65	581	38	7	500.2	37.2
175	470.7	13.64	406	204.63	72.6	948	38	7	471.2	65.2
176	457.9	11.34	378	171.17	64	793.0	38	7	420.7	42.7
177	331.5	5.73	358	39.18	45	183.0	38	7	400.9	42.9
178	323.8	5.38	336	36.32	43.9	170	38	7	387.5	51.5
179	338.5	5.44	327	42.03	44.1	196	38	7	364.4	37.4
180	336.4	5.13	311	41.15	43.1	192	38	7	342.7	31.7
181	346.8	6.47	398	45.74	47.4	213	5	8	427.0	29.0
182	412.1	8.65	365	94.93	54.6	440	5	8	413.5	48.5
183	344.0	6.47	384	44.43	47.4	207	5	8	433.3	49.3
184	326.8	6.16	395	37.42	46.4	175	5	8	447.1	52.1
185	351.8	7.58	425	48.14	51	224.0	5	8	502.7	77.7
186	369.2	7.58	425	57.92	51	269.0	5	8	458.0	33.0
187	431.2	10.22	395	120.42	60	558.0	5	8	445.1	50.1
188	381.8	8.12	404	66.59	52.8	309	5	8	461.4	57.4
189	368.5	7.79	413	57.49	51.7	267	5	8	474.0	61.0
190	347.8	7.21	445	46.18	49.8	215	5	8	485.7	40.7
191	435.1	12.42	480	126.47	68	586.0	5	8	535.8	55.8
192	489.0	17.01	453	266.59	86	1235.0	5	8	525.3	72.3

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
193	451.3	13.87	455	156.70	73.5	726	5	8	543.8	88.8
194	412.1	11.34	500	94.93	64	440.0	5	8	558.0	58.0
195	402.7	10.78	505	84.77	62	393.0	5	8	558.7	53.7
196	473.3	17.74	551	212.41	89	984.0	5	8	607.5	56.5
197[3]	550.1	29.59	452	712.37	140.6	3300	5	8	591.6	139.6
198	463.3	16.86	536	184.56	85.4	855	5	8	614.8	78.8
199	441.1	14.72	612	136.84	76.8	634	5	8	614.4	2.4
200	443.0	15.65	597	140.29	80.5	650	5	8	643.4	46.4
201	220.9	3.2	310	15.02			10	9	317.5	7.5
202	277.5	4.2	338	23.75			10	9	356.7	18.7
203	302.8	4.84	350	29.77			10	9	378.0	28.0
204	322.4	5.51	362	35.85			10	9	401.2	39.2
205	339.8	6.13	374	42.59			10	9	416.0	42.0
206	264.0	3.42	305	21.18			10	9	283.3	-21.7
207	335.5	4.77	328	40.76			10	9	313.8	-14.2
208	383.9	6.19	356	68.22			10	9	334.7	-21.3
209	434.6	8.29	369	125.8			10	9	351.1	-17.9
210	477.2	11.87	404	224.5			10	9	394.2	-9.8
211	240.0	3.27	304	17.42			10	9	298.9	-5.1
212	311.2	4.77	349	32.22			10	9	355.8	6.8
213	366.5	6.54	374	56.25			10	9	390.0	16.0
214	394.1	7.7	390	76.62			10	9	403.0	13.0
215	-717.2	0.402	114.9	0.658			12	a	-150.4	-265.3
216[3]	-550.3	0.481[3]	131.2	0.829			12	a	-109.6	-240.8
217[3]	-440.4	0.459[3]	142.5	1.012			12	a	-132.0	-274.5
218	-349.0	0.647	153	1.237			12	a	-36.7	-189.7
219[3]	-230.2	0.803	172.5	1.700[5]			12	a	18	-154.6[+*]
220	-570.3	0.467	127.3	0.803			12	a	-116.8	-244.1
221	-232.2	0.779	165.1	1.69			12	a	6.9	-158.2
222	-174.6	0.897	178.8	2.025			12	a	45.1	-133.7
223	-122.2	1.054	188.3	2.43			12	a	92.8	-95.5
224	-61.2	1.199	203.3	3.08			12	a	120.0	-83.3
225	35.5	1.581	232.2	4.78			12	a	183.4	-48.8

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		Raw Data[1]	Raw Data	Raw Data[1]	Raw Data	Raw Data	Reference	Chart Label		
Model		Input	Input	Input					Output	
Point	H100	V210	MWE	V100	SUS210	SUS100			MWC	Residual
226	148.6	2.352	257.2	9.08			12	A	263.9	6.7
227	417.8	8.58	330.9	101.7			12	A	397.3	66.4
228	67.7	1.728	266	5.65			12	a	198.4	-67.6
229	-202.6	0.856	186.6	1.85			12	a	35.2	-151.4
230	277.2	4.26	370.1	23.7			12	A	363.8	-6.3
231	35.5	1.523	241.2	4.78			12	a	165.8	-75.4
232	5.9	1.371	221.6	4.14			12	a	139.2	-82.4
233	-16.1	1.276	205.3	3.74			12	a	121.5	-83.8
1 V100 and V210 calculated from SUS100 and SUS210										
2 Point H100 is off chart, V210 is low making and likely off the chart										
3 Point suspect see erratum										
4 Point suspect and changed from 15.7 to 157										
5 Point suspect and changed from 17.00 to 1.700										

Table 36 contains tracking data for referencing back to the original sources and the types of oils used to generate the data.

Table 36 Experimental Data: Reference Source Tables, Sample Codes and Oil Source

Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
1	26	6	F	MidConUSA1
2	26	6	F	MidConUSA1
3	26	6	F	MidConUSA1
4	26	6	F	MidConUSA1
5	26	6	F	MidConUSA1
6	26	6	F	MidConUSA1
7	26	9 & 10	A1	MidConUSA1
8	26	9 & 10	A5	MidConUSA1
9	26	9 & 10	A10	MidConUSA1
10	26	9 & 10	A17	MidConUSA1

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
11	26	9 & 10	A22	MidConUSA1
12	26	9 & 10	A27	MidConUSA1
13	26	9 & 10	Ares	MidConUSA1
14	26	9 & 10	B2	MidConUSA1
15	26	9 & 10	B6	MidConUSA1
16	26	9 & 10	B13	MidConUSA1
17	26	9 & 10	B14	MidConUSA1
18	26	9 & 10	B18	MidConUSA1
19	26	9 & 10	B21	MidConUSA1
20	26	9 & 10	B28	MidConUSA1
21	26	9 & 10	B31	MidConUSA1
22	26	9 & 10	B35	MidConUSA1
23	26	9 & 10	Bres	MidConUSA1
24	26	9 & 10	C5	MidConUSA1
25	26	9 & 10	C8	MidConUSA1
26	26	9 & 10	C12	MidConUSA1
27	26	9 & 10	C17	MidConUSA1
28	26	9 & 10	C22	MidConUSA1
29	26	9 & 10	C24	MidConUSA1
30	26	9 & 10	C28	MidConUSA1
31	26	9 & 10	C32	MidConUSA1
32	26	9 & 10	C36	MidConUSA1
33	26	9 & 10	C3940	MidConUSA1
34	26	9 & 10	Cres	MidConUSA1
35	26	9 & 10	D11	MidConUSA1
36	26	9 & 10	D16	MidConUSA1
37	26	9 & 10	D25	MidConUSA1
38	26	9 & 10	D2829	MidConUSA1
39	26	9 & 10	Dres	MidConUSA1
40	26	9 & 10	E13	MidConUSA1
41	26	9 & 10	E21	MidConUSA1
42	26	9 & 10	E27	MidConUSA1
43	26	9 & 10	Eres	MidConUSA1
44	27	2	B12H	MidConUSA1

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
45	27	2	B16H	MidConUSA1
46	27	2	B19H	MidConUSA1
47	27	2	C1H	MidConUSA1
48	27	2	C7H	MidConUSA1
49	27	2	C13H	MidConUSA1
50	27	2	C20H	MidConUSA1
51	27	2	C26K27H	MidConUSA1
52	27	2	C30H	MidConUSA1
53	27	2	C33H	MidConUSA1
54	27	2	C35H	MidConUSA1
55	27	2	C37H	MidConUSA1
56	27	2	CresH	MidConUSA1
57	27	2	E1H	MidConUSA1
58	27	2	E25H	MidConUSA1
59	24	3	a1	MidConUSA1
60	24	3	a1	MidConUSA1
61	24	3	a2	MidConUSA1
62	24	3	a2	MidConUSA1
63	24	3	a3	MidConUSA1
64	24	3	a3	MidConUSA1
65	24	3	b	MidConUSA1
66	24	3	b	MidConUSA1
67	24	3	b	MidConUSA1
68	24	3	b	MidConUSA1
69	24	3	c	MidConUSA1
70	24	3	c	MidConUSA1
71	24	3	c	MidConUSA1
72	24	3	c	MidConUSA1
73	24	3	d	MidConUSA1
74	24	3	d	MidConUSA1
75	24	3	d	MidConUSA1
76	24	3	d	MidConUSA1
77	24	3	e	MidConUSA1
78	24	3	e	MidConUSA1

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
79	24	3	e	MidConUSA1
80	24	3	e	MidConUSA1
81	24	3	e	MidConUSA1
82	24	3	f	MidConUSA1
83	24	3	f	MidConUSA1
84	24	3	f	MidConUSA1
85	24	3	f	MidConUSA1
86	24	3	f	MidConUSA1
87	9	1	14	MidConUSA2
88	9	1	17	MidConUSA2
89	9	1	21	MidConUSA2
90	9	1	23	MidConUSA2
91	9	III	PaO	PaUSA1
92	9	III	Pa1	PaUSA1
93	9	III	Pa6	PaUSA1
94	9	III	Pa11	PaUSA1
95	9	III	Pa16	PaUSA1
96	9	III	Pa19	PaUSA1
97	9	III	Pa21	PaUSA1
98	9	III	Pares	PaUSA1
99	9	III	RO	LaUSA1
100	9	III	R1	LaUSA1
101	9	III	R2	LaUSA1
102	9	III	R5	LaUSA1
103	9	III	R9	LaUSA1
104	9	III	R11	LaUSA1
105	9	III	R15	LaUSA1
106	9	III	MCIO	MidConUSA1A
107	9	III	MCI1	MidConUSA1A
108	9	III	MCI2	MidConUSA1A
109	9	III	MCI4	MidConUSA1A
110	9	III	MCI8	MidConUSA1A
111	9	III	MCI12	MidConUSA1A
112	9	III	MCI17	MidConUSA1A

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
113	9	III	MCIres	MidConUSA1A
114	9	III	MCIIO	MidConUSA2A
115	9	III	MCII1	MidConUSA2A
116	9	III	MCII2	MidConUSA2A
117	9	III	MCII5	MidConUSA2A
118	9	III	MCII10	MidConUSA2A
119	9	III	MCII14	MidConUSA2A
120	9	III	MCII18	MidConUSA2A
121	9	III	MCIIres	MidConUSA2A
122	9	III	CaO	CaUSA1
123	9	III	Ca1	CaUSA1
124	9	III	Ca2	CaUSA1
125	9	III	Ca5	CaUSA1
126	9	III	Ca10	CaUSA1
127	9	III	Ca15	CaUSA1
128	9	III	Ca18	CaUSA1
129	9	III	Cares	CaUSA1
130	9	III	CG1	GCUSA1
131	9	III	CG2	GCUSA1
132	9	III	CG5	GCUSA1
133	9	III	CG10	GCUSA1
134	9	III	CG14	GCUSA1
135	18	I	725	MidConUSA3
136	18	I	726	MidConUSA3
137	18	I	727	MidConUSA3
138	18	I	4697	MidConUSA3
139	18	I	4698	MidConUSA3
140	18	I	4699	MidConUSA3
141	18	I	4700	MidConUSA3
142	18	I	4701	MidConUSA3
143	18	I	2655	TxCoast
144	18	I	2654	TxCoast
145	18	I	2657	TxCoast
146	18	I	3002	TxCoast

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
147	18	I	2656	TxCoast
148	18	I	3001	TxCoast
149	18	I	2659	TxCoast
150	18	I	2658	TxCoast
151	18	I	2660	TxCoast
152	18	I	2661	TxCoast
153	18	II	HAFF	HumbleATx
154	18	II	HAFC	HumbleATx
155	18	II	HAOD	HumbleATx
156	18	II	HAAE	HumbleATx
157	18	II	HAFE	HumbleATx
158	18	II	MARac	MirandoTx
159	18	II	MAAc	MirandoTx
160	18	II	MAE	MirandoTx
161	18	II	MFE	MirandoTx
162	18	II	CFR	Columbia
163	18	II	CARc	Columbia
164	18	II	CAE	Columbia
165	18	II	CFE	Columbia
166	18	II	PAFR	PaUSA2
167	18	II	PAFRdc	PaUSA2
168	18	II	PAAE	PaUSA2
169	18	II	MCFR	MidConUSA3
170	18	II	MCFRdac	MidConUSA3
171	18	II	MCO	MidConUSA3
172	38	I	1P40	SAE40
173	38	I	2MC40	SAE40
174	38	I	3WT40	SAE40
175	38	I	4C40	SAE40
176	38	I	5CG40	SAE40
177	38	I	2MC20	SAE20
178	38	I	3WT20	SAE20
179	38	I	4C20	SAE20
180	38	I	5CG20	SAE20

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
181	5	III	C30	PaUSA2
182	5	III	C31	PaUSA2
183	5	III	C32	PaUSA2
184	5	III	C33	PaUSA2
185	5	III	C34	PaUSA2
186	5	III	C40	PaUSA2
187	5	III	C41	PaUSA2
188	5	III	C42	PaUSA2
189	5	III	C43	PaUSA2
190	5	III	C44	PaUSA2
191	5	III	C50	PaUSA2
192	5	III	C51	PaUSA2
193	5	III	C52	PaUSA2
194	5	III	C53	PaUSA2
195	5	III	C54	PaUSA2
196	5	III	C60	PaUSA2
197	5	III	C61	PaUSA2
198	5	III	C62	PaUSA2
199	5	III	C63	PaUSA2
200	5	III	C64	PaUSA2
201	10	III & VI	SC1	Unknown
202	10	III & VI	SC2	Unknown
203	10	III & VI	SC3	Unknown
204	10	III & VI	SC4	Unknown
205	10	III & VI	SC5	Unknown
206	10	III & VI	SC6	Unknown
207	10	III & VI	SC7	Unknown
208	10	III & VI	SC8	Unknown
209	10	III & VI	SC9	Unknown
210	10	III & VI	SC10	Unknown
211	10	III & VI	SC11	Unknown
212	10	III & VI	SC12	Unknown
213	10	III & VI	SC13	Unknown
214	10	III & VI	SC14	Unknown

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Point	Reference	Table(s) In References	Code to Sample in Reference	Oil Type Table 37
215	12	II	218	Unknown
216	12	II	221	Unknown
217	12	II	223	Unknown
218	12	II	225	Unknown
219	12	II	228	Unknown
220	12	II	232	Unknown
221	12	II	235	Unknown
222	12	II	238	Unknown
223	12	II	242	Unknown
224	12	II	246	Unknown
225	12	II	249	Unknown
226	12	II	250	Unknown
227	12	II	251	Unknown
228	12	II	300	Unknown
229	12	II	307	Unknown
230	12	II	A308	Unknown
231	12	II	310	Unknown
232	12	II	330	Unknown
233	12	II	350	Unknown

Table 37 Oil Type Codes Used in Table 36

Code	Description
CaUSA1	California, USA, Crude 1
Columbia	Unknown, Columbia, SA?
GCUSA1	Gulf Coast, USA, Crude 1
GCUSA2	Gulf Coast, Bosca, La, USA, Crude 2
HumbleATx	Likely Gulf coast as Humble was Gulf Refining in Humble, Texas
LaUSA1	Ridessam, La, USA, Crude 1
MidConUSA1	Kay County, Oklahoma, USA Crude 1
MidConUSA1A	Midcontinent, Undefined, USA, Crude 2A
MidConUSA2	Oklahoma County, Oklahoma, USA Crude 2
MidConUSA2A	Midcontinent, Undefined, USA, Crude 1A
MidConUSA3	Midcontinent, Undefined, USA, Crude 3

Code	Description
MirandoTx	Mirando Refining, Zapata County, Texas
PaUSA1	Pennsylvania, USA, Crude 1
PaUSA2	Pennsylvania, USA, Crude 2
PaUSA2	Pennsylvania, USA, Crude 2
SAE20	Unknown source
SAE40	Unknown source
TxCoast	Texas Coastal, USA
Unknown	Source not given

CALCULATION CODES

GW-BASIC

The code listing has inputs of the 2 viscosities and outputs the calculated molecular weight. There were some issues with using various forms of BASIC. Some require line numbers and a termination line at the end of the listing; others do not. In hexadecimal, the line termination line was 1A 20 0D 0A and in decimal 26 32 13 10. These represent ASCII characters for SUB SPACE CR LF (substitute[28], space, carriage return, line feed). CR and LF are commonly used to terminal ASCII text files.

GW-BASIC Code listing:

```
10 Rem for V1 and V2 of 145 and 10
20 Rem the MWC is 398.3604
30 DEFINT K
40 DIM C(32)
50 C(1) = 4.11
60 C(2) = 1.358
70 C(3) = 1.5414
80 C(4) = -0.4106
90 C(5) = 197.6
100 C(6) = -592.944
110 C(7) = -96.08
120 C(8) = 0.8759
130 C(9) = 154.29
140 C(10) = -1.513
150 C(11) = 4.126
160 C(12) = 2.356
170 C(13) = 1.07
180 C(14) = 1.446
190 C(15) = -31.5
200 C(16) = -0.64
210 C(17) = 0.069
220 C(18) = 0.31
230 C(19) = -0.032
```

```
240 C(20) = 0.002
250 C(21) = -1.267
260 C(22) = 8.05
270 C(23) = -4.326
280 C(24) = 6.223
290 C(25) = 300
300 C(26) = -0.00326
310 C(27) = 19.54
320 C(28) = -30.387
330 C(29) = -12.02
340 C(30) = 7.276
350 C(31) = 6.498
360 C(32) = 52.3
370 INPUT "Enter Viscosity at 100F in cSt: ",V1
380 INPUT "Enter Viscosity at 210F in cSt: ",V2
390 F1=LOG(LOG(V1+C(1)))
400 F2=LOG(LOG(V2+C(2)))
410 F12=LOG(F1-C(3)*F2-C(4))
420 MW0=C(5)+C(6)*F12+C(7)*F12*F2^2+C(8)*F1^4+C(9)*F1*F2*F12
430 MWS=MW0*.01
440 FOR K=0 TO 1
450 K11=K*11
460 SI=SIN(C(10+K11))
470 CO=COS(C(10+K11))
480 X=(MWS*CO+F2*SI-C(11+K11)*CO-C(12+K11)*SI)/C(13+K11)
490 X2=X*X
500 Y=(F2*CO-C(12+K11)*CO-MWS*SI+C(11+K11)*SI)/C(14+K11)
510 Y2=Y*Y
520 EL=X2+Y2
530 SG=TAN(C(10+K11))*(-C(11+K11)+MWS)+C(12+K11)-F2
540 IF SC<0 THEN SG=-1 ELSE SG=1
550 EX=SG*EL
560 EX1=EX*(C(19+K11)+EX*C(20+K11))
570 EX2=EX*(C(17+K11)+EX*(C(18+K11)+EX1))
580 MW2=C(15+K11)*EXP(-(C(16+K11)+EX2))
590 IF K=0 THEN MW1=MW2
600 NEXT K
610 MWC=MW0+MW1+MW2+C(32)
620 PRINT USING "MWC= ####.####"; MWC
```

Excel VBA Functions

Molecular Weight Calculation Functions

There are 4 functions used to calculate the molecular weight from viscosities at temperatures more common today than when the chart was developed. The code for the functions is at the end of this section.

1. MW40_100 is the top level function. Viscosities in cSt at 40°C, 100°C and the type of viscosity boundary error checking are the inputs. The function is hard coded to convert

viscosities from 40°C and 100°C to 37.778°C and 98.889°C (100°F and 210°F). It uses the viscosity-temperature conversion function VisAtTC (Viscosity at Temperature C) and passes the converted viscosities to the MW function.

2. VisAtTC converts the viscosities from two temperatures to the viscosity at a 3rd temperature. It is usable as a standalone function as long as the required Log10 function in VBA is available.
3. The Log10 function converts the native VBA *Log* (base ***e***) function to base 10[29]. As a standalone function, it is usable as needed in VBA. It is not for use in spreadsheet cells as the spreadsheet has both the Log and Ln as native functions.
4. The MW function calculates the molecular weight using viscosities at 100°F and 210°F, checks the viscosities for chart boundary violations and returns the MW or boundary violation code. It is usable as a standalone function if V100 and V210 are the inputs.

MW Calculation from Viscosities at 40°C and 100°C
The function is MW40_100(V40C,V100C, optional Error Report Code).

The molecular weight data used to check the viscosity boundary violations was used to check the conversion of the viscosities from 100°F and 210°F to 40°C and 100°C and their use in this function. For all values that are on the chart, the difference between the originally calculated MWC and that from the viscosity converted MW40_100 version had a difference of <0.15. Any values that showed larger differences had viscosities that would not be on the chart, a V210 that was difficult to interpolate below 2.6 cSt (lower left corner highlighted in yellow) or above 60 cSt. All the viscosity boundary violations had the same error code except the point in the lower left corner of the chart.

Table 38 Viscosities Converted to 40°C and 100°C, Checked Against Previous Calculations

V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
Extreme Data										
6	1	5.41	1.00	#OoB	#OoB	V1(low) V2(low)	V1(low) V2(low)	-26	-12	-14.3
29.03	10	27.64	9.85	#OoB	#OoB	RB	RB	859	859	0
314.6	5	240.8	4.81	#OoB	#OoB	LB	LB	154	154	0
12.69	2.6	11.68	2.55	250	250	250	250	250	250	-0.1
Systematic Extreme Data										
5.15	1	4.69	1.00	#OoB	#OoB	V1(low) V2(low)	V1(low) V2(low)	-12	3	-15
6.76	1	6.04	1.00	#OoB	#OoB	V2(low)	V1(low) V2(low)	-37	-23	-14

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
111.29	1	75.29	0.99	#OoB	#OoB	V2(low) LB	V2(low) LB	-245	-230	-15
69560	1	19734	0.98	#OoB	#OoB	V2(low) LB	V2(low) LB	-450	-432	-18
336898	1	75381	0.98	#OoB	#OoB	V1(high) V2(low)	V1(high) V2(low)	-474	-455	-19
5.15	1.92	4.91	1.90	#OoB	#OoB	V1(low) V2(low)	V1(low) V2(low)	267	268	-1
6.76	1.92	6.34	1.89	#OoB	#OoB	V2(low)	V1(low) V2(low)	218	219	-1
111.29	1.92	83.24	1.86	#OoB	#OoB	V2(low) LB	V2(low) LB	-44	-43	-1
69560	1.92	24773	1.82	#OoB	#OoB	V2(low) LB	V2(low) LB	-220	-219	-1
336898	1.92	97591	1.82	#OoB	#OoB	V1(high) V2(low)	V1(high) V2(low)	-236	-235	-1
5.15	10	5.27	10.13	#OoB	#OoB	V1(low)	V1(low)	#VALUE!	#VALUE!	#VALUE!
6.76	10	6.86	10.07	#OoB	#OoB	RB	RB	#VALUE!	#VALUE!	#VALUE!
111.29	10	97.91	9.72	451	451	451	451	451	451	0.0
69560	10	35787	9.37	#OoB	#OoB	LB	LB	152	152	0.0
336898	10	148184	9.32	#OoB	#OoB	V1(high)	V1(high)	138	138	0.0
5.15	60	5.51	63.62	#OoB	#OoB	V1(low)	V1(low)	#VALUE!	#VALUE!	#VALUE!
6.76	60	7.20	63.05	#OoB	#OoB	RB	RB	#VALUE!	#VALUE!	#VALUE!
111.29	60	108.42	59.43	#OoB	#OoB	RB	RB	#VALUE!	#VALUE!	#VALUE!
69560	60	45094	56.03	343	343	343	343	343	343	0.0
336898	60	192662	55.53	#OoB	#OoB	V1(high)	V1(high)	311	311	0.0
5.15	70	5.53	74.58	#OoB	#OoB	V1(low) V2(high)	V1(low) V2(high)	#VALUE!	#VALUE!	#VALUE!
6.76	70	7.23	73.88	#OoB	#OoB	V2(high) RB	V2(high) RB	#VALUE!	#VALUE!	#VALUE!
111.29	70	109.16	69.49	#OoB	#OoB	V2(high) RB	V2(high) RB	#VALUE!	#VALUE!	#VALUE!
69560	70	45800	65.38	#OoB	#OoB	V2(high)	V2(high)	359	359	0.0
336898	70	196088	64.77	#OoB	#OoB	V1(high) V2(high)	V1(high) V2(high)	321	321	0.0
From ASTM Chart										
6.76	1.93	6.34	1.90	#OoB	#OoB	V2(low)	V1(low) V2(low)	221	222	-1.00
12.69	2.6	11.68	2.55	250	250	250	250	250	250	-0.13
9.71	2.6	9.09	2.56	301	301	301	301	301	301	-0.13

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
7.56	2.6	7.18	2.56	352	352	352	352	352	352	-0.14
20.45	3	18.42	2.93	231	231	231	231	231	231	-0.04
18.41	3	16.70	2.94	249	249	249	249	249	249	-0.04
15.99	3	14.64	2.94	274	274	274	274	274	274	-0.04
14.05	3	12.97	2.94	299	299	299	299	299	299	-0.04
12.30	3	11.45	2.95	326	326	326	326	326	326	-0.04
10.95	3	10.27	2.95	350	350	350	350	350	350	-0.04
9.65	3	9.12	2.95	376	376	376	376	376	376	-0.04
8.65	3	8.22	2.96	400	400	400	400	400	400	-0.04
7.71	3	7.38	2.96	425	425	425	425	425	425	-0.04
6.93	3	6.67	2.96	449	449	449	449	449	449	-0.05
29.56	3.6	26.33	3.51	249	249	249	249	249	249	-0.006
22.09	3.6	20.06	3.52	299	299	299	299	299	299	-0.006
17.01	3.6	15.71	3.53	350	350	350	350	350	350	-0.007
13.45	3.6	12.60	3.54	400	400	400	400	400	400	-0.007
45.20	4	39.41	3.89	231	231	231	231	231	231	-0.0015
38.98	4	34.34	3.90	250	250	250	250	250	250	-0.0017
28.76	4	25.87	3.91	299	299	299	299	299	299	-0.0019
22.09	4	20.21	3.92	348	348	348	348	348	348	-0.0020
17.41	4	16.17	3.93	398	398	398	398	398	398	-0.0022
13.92	4	13.10	3.93	449	449	449	449	449	449	-0.0023
11.50	4	10.93	3.94	501	501	501	501	501	501	-0.0024
9.62	4	9.23	3.95	549	549	549	549	549	549	-0.0026
8.12	4	7.87	3.96	596	596	596	596	596	596	-0.0028
6.94	4	6.77	3.97	643	643	643	643	643	643	-0.0029
89.77	5	75.87	4.85	231	231	231	231	231	231	-0.0001
74.81	5	64.07	4.85	249	249	249	249	249	249	-0.0001
49.78	5	43.88	4.87	301	301	301	301	301	301	-0.0002
36.76	5	33.06	4.88	352	352	352	352	352	352	-0.0001
28.76	5	26.28	4.89	401	401	401	401	401	401	-0.0001
23.09	5	21.38	4.90	450	450	450	450	450	450	-0.0001
19.02	5	17.82	4.91	504	504	504	504	504	504	-0.0002
15.83	5	14.98	4.92	554	554	554	554	554	554	-0.0002
13.45	5	12.84	4.93	601	601	601	601	601	601	-0.0002
11.38	5	10.96	4.94	653	653	653	653	653	653	-0.0002
9.72	5	9.44	4.95	706	706	706	706	706	706	-0.0002

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
136.61	6	113.73	5.80	247	247	247	247	247	247	0.0000
81.16	6	70.15	5.83	299	299	299	299	299	299	0.0000
56.58	6	50.12	5.84	353	353	353	353	353	353	0.0000
43.97	6	39.60	5.86	399	399	399	399	399	399	0.0000
28.76	6	26.59	5.88	502	502	502	502	502	502	0.0000
19.98	6	18.86	5.90	604	604	604	604	604	604	0.0000
339.21	7	267.29	6.73	227	227	227	227	227	227	0.0000
233.72	7	189.53	6.75	248	248	248	248	248	248	0.0000
123.17	7	104.69	6.78	300	300	300	300	300	300	0.0000
82.12	7	71.79	6.80	353	353	353	353	353	353	0.0000
63.13	7	56.16	6.82	398	398	398	398	398	398	0.0000
49.94	7	45.10	6.83	452	452	452	452	452	452	0.0000
40.97	7	37.46	6.84	499	499	499	499	499	499	0.0000
33.96	7	31.40	6.86	549	549	549	549	549	549	0.0000
28.24	7	26.39	6.87	602	602	602	602	602	602	0.0000
23.90	7	22.54	6.88	652	652	652	652	652	652	0.0000
20.43	7	19.43	6.90	704	704	704	704	704	704	0.0000
378.94	8	299.93	7.69	250	250	250	250	250	250	0.0000
183.71	8	153.46	7.73	298	298	298	298	298	298	0.0000
114.12	8	98.57	7.76	352	352	352	352	352	352	0.0000
85.08	8	74.95	7.78	400	400	400	400	400	400	0.0000
54.78	8	49.63	7.81	501	501	501	501	501	501	0.0000
37.85	8	35.06	7.84	601	601	601	601	601	601	0.0000
27.74	8	26.15	7.86	697	697	697	697	697	697	0.0000
1651	10	1190	9.53	232	232	232	232	232	232	0.0000
961.92	10	723.86	9.56	252	252	252	252	252	252	0.0000
367.22	10	297.44	9.62	298	298	298	298	298	298	0.0000
202.59	10	171.22	9.67	351	351	351	351	351	351	0.0000
143.99	10	124.56	9.69	400	400	400	400	400	400	0.0000
112.41	10	98.84	9.71	449	449	449	449	449	449	0.0000
91.41	10	81.44	9.73	496	496	496	496	496	496	0.0000
73.87	10	66.69	9.75	551	551	551	551	551	551	0.0000
61.75	10	56.36	9.77	600	600	600	600	600	600	0.0000
52.43	10	48.31	9.79	647	647	647	647	647	647	0.0000
44.88	10	41.73	9.80	694	694	694	694	694	694	0.0000
2294	12	1642	11.42	253	253	253	253	253	253	0.0000

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
674.85	12	531.27	11.51	299	299	299	299	299	299	0.0000
324.40	12	269.30	11.57	351	351	351	351	351	351	0.0000
220.63	12	188.08	11.60	401	401	401	401	401	401	0.0000
136.61	12	120.18	11.65	497	497	497	497	497	497	0.0000
91.41	12	82.45	11.70	602	602	602	602	602	602	0.0000
65.28	12	60.07	11.74	698	698	698	698	698	698	0.0000
5203	14	3543	13.27	253	253	253	253	253	253	0.0000
1157	14	887	13.38	300	300	300	300	300	300	0.0000
498.23	14	406.49	13.46	350	350	350	350	350	350	0.0000
324.40	14	272.68	13.51	399	399	399	399	399	399	0.0000
194.23	14	168.91	13.57	496	496	496	496	496	496	0.0000
129.68	14	115.69	13.62	599	599	599	599	599	599	0.0000
91.41	14	83.27	13.66	696	696	696	696	696	696	0.0000
20100	15	12302	14.12	231	231	231	231	231	231	0.0000
1483.6	15	1124.2	14.32	301	301	301	301	301	301	0.0000
618.35	15	499.75	14.41	348	348	348	348	348	348	0.0000
381.33	15	318.76	14.46	400	400	400	400	400	400	0.0000
282.19	15	240.71	14.50	451	451	451	451	451	451	0.0000
225.11	15	194.88	14.52	498	498	498	498	498	498	0.0000
184.99	15	162.17	14.55	546	546	546	546	546	546	0.0000
152.06	15	134.95	14.58	598	598	598	598	598	598	0.0000
125.89	15	113.02	14.60	648	648	648	648	648	648	0.0000
105.47	15	95.69	14.63	697	697	697	697	697	697	0.0000
17019	17	10735	16.01	251	251	251	251	251	251	0.0000
2440	17	1802	16.18	301	301	301	301	301	301	0.0000
863.19	17	688.60	16.30	350	350	350	350	350	350	0.0000
514.95	17	425.94	16.36	402	402	402	402	402	402	0.0000
296.10	17	254.14	16.43	500	500	500	500	500	500	0.0000
196.97	17	173.50	16.49	603	603	603	603	603	603	0.0000
136.61	17	123.05	16.55	701	701	701	701	701	701	0.0000
69560	20	39658	18.70	246	246	246	246	246	246	0.0000
51985	20	30404	18.72	250	250	250	250	250	250	0.0000
4755	20	3390	18.96	302	302	302	302	302	302	0.0000
1371	20	1073	19.12	351	351	351	351	351	351	0.0000
762.37	20	621.94	19.20	403	403	403	403	403	403	0.0000
554.08	20	461.94	19.25	450	450	450	450	450	450	0.0000

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
430.37	20	364.86	19.29	500	500	500	500	500	500	0.0000
352.62	20	302.83	19.33	547	547	547	547	547	547	0.0000
283.04	20	246.49	19.36	602	602	602	602	602	602	0.0000
233.04	20	205.42	19.40	652	652	652	652	652	652	0.0000
191.53	20	170.85	19.44	705	705	705	705	705	705	0.0000
13531	25	9094	23.56	300	300	300	300	300	300	0.0000
2765	25	2098	23.80	350	350	350	350	350	350	0.0000
1371	25	1094	23.92	400	400	400	400	400	400	0.0000
710.86	25	592.99	24.05	503	503	503	503	503	503	0.0000
459.11	25	393.97	24.14	606	606	606	606	606	606	0.0000
314.63	25	276.41	24.22	704	704	704	704	704	704	0.0000
69560	30	41755	28.02	286	286	286	286	286	286	0.0000
31368	30	20104	28.14	300	300	300	300	300	300	0.0000
4974	30	3676	28.46	350	350	350	350	350	350	0.0000
2202	30	1726	28.63	400	400	400	400	400	400	0.0000
1450	30	1169	28.72	451	451	451	451	451	451	0.0000
1094	30	899	28.78	501	501	501	501	501	501	0.0000
886.73	30	739.15	28.83	547	547	547	547	547	547	0.0000
698.62	30	591.38	28.89	604	604	604	604	604	604	0.0000
590.66	30	505.35	28.94	645	645	645	645	645	645	0.0000
474.32	30	411.39	28.99	702	702	702	702	702	702	0.0000
69560	40	43176	37.35	309	309	309	309	309	309	0.0000
13195	40	9322	37.73	350	350	350	350	350	350	0.0000
4755	40	3618	37.99	400	400	400	400	400	400	0.0000
2920	40	2299	38.13	451	451	451	451	451	451	0.0000
2158	40	1734	38.23	500	500	500	500	500	500	0.0000
1801	40	1465	38.28	536	536	536	536	536	536	0.0000
1674	40	1368	38.30	552	552	552	552	552	552	0.0000
1371	40	1135	38.37	598	598	598	598	598	598	0.0000
1131	40	948	38.43	644	644	644	644	644	644	0.0000
944.6	40	800.8	38.50	694	694	694	694	694	694	0.0000
69560	50	44243	46.69	327	327	327	327	327	327	0.0000
28901	50	19672	46.94	350	350	350	350	350	350	0.0000
8903	50	6607	47.31	400	400	400	400	400	400	0.0000
6322	50	4806	47.43	427	427	427	427	427	427	0.0000
5007	50	3869	47.52	453	453	453	453	453	453	0.0000

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V100F	V210F	V40C	V100C	MW	MW40_100	MW Verbose	MW40_100 Verbose	MW NC	MW40_100 NC	MW NC Diff
3649	50	2881	47.63	500	500	500	500	500	500	0.0000
2782	50	2237	47.74	553	553	553	553	553	553	0.0000
2248	50	1832	47.82	601	601	601	601	601	601	0.0000
1823	50	1506	47.91	650	650	650	650	650	650	0.0000
1539	50	1286	47.98	698	698	698	698	698	698	0.0000
69560	60	45094	56.03	343	343	343	343	343	343	0.0000
53503	60	35389	56.12	351	351	351	351	351	351	0.0000
17464	60	12551	56.54	395	395	395	395	395	395	0.0000
15359	60	11141	56.59	398	398	398	398	398	398	0.0000
8286	60	6277	56.85	447	447	447	447	447	447	0.0000
5700	60	4430	57.01	497	497	497	497	497	497	0.0000
5203	60	4069	57.05	513	513	513	513	513	513	0.0000
4292	60	3400	57.14	550	550	550	550	550	550	0.0000
3420	60	2750	57.25	600	600	600	600	600	600	0.0000
2719	60	2219	57.36	652	652	652	652	652	652	0.0000
2248	60	1857	57.45	705	705	705	705	705	705	0.0000

Conversion of Viscosity from 40°C and 100°C to 100°F and 210°F
The function is VisAtTC(p1, p2, p3, p4, p5). The parameter p1 represents the viscosity in cSt at the lower temperature p2 in Celsius. Parameters p3 is the viscosity at the higher temperature p4. The parameter p5 is the temperature in Celsius at which the viscosity is wanted.

The viscosity conversion uses the Wright equation[30], which is the basis[31] for ASTM D341[32]. Four sets of data were used to check VisAtTC (Viscosity at Temperature C) function code against online calculations and gave comparable results. Five other data sets were used to check its viscosity range (Table 39). The differences seen on the low viscosities are irrelevant as they would not be on the ASTM chart.

Table 39 Preliminary Testing of Viscosity-Temperature Conversion Code

Test Data	1	2	3	4	5	6	7	8	9
Viscosity (cSt)	500	2000	100	22.8	2	2	2	2	2
Temperature (°C)	40	40	40	40	40	40	40	40	40
Viscosity (cSt)	450	10	20	3.8	0.412	0.402	0.30001	0.2062	Fails at
Temperature (°C)	100	100	100	100	100	100	100	100	100
Temperature (°C)	60	60	60	50	50	50	50	50	50
VisAtTC VBA Excel	481.639	153.263	52.615	15.163	1.397	1.387	1.266	0.538	<0.206

Anton Paar[33]	481.639	153.263	52.615	15.163	0.913	0.7	blank	blank	<.402
Paragon[34]	481.6	153.3	52.61	15.16	1.245	1.224	0.4345	NaN[#]	<=0.30001
#Not a Number									

This function requires the use of the log (base 10) function, which is not native to VBA. Included in the code list is the function Log10, which converts the VBA natural *Log* (base ***e***) to the log base 10.

MW Calculation from Viscosities at 100°F and 210°F with Boundary Violation Discussion
The code is a VBA function MW(number1, number2, optional text) that calculates the molecular weight using the method described in this paper. It includes validating that both viscosities are within the chart area. The inputs number1 and number2 are numbers or cell references to the viscosities with number1 as the viscosity in cSt at 100°F and number2 as the viscosity in cSt at 210°F. The optional text is either a text string in quotes or a cell reference to text content. The optional text controls the type of error message reported by the function.

The output is the calculated molecular weight or an error code. The error codes will help determine which viscosities or which chart boundaries are violated. The code terminology relates to the ASTM chart, as that is more familiar than the modified charts (Figure 51 and Figure 52) based on viscosity axes.

Table 40 Output Controlled by the Optional Text

Optional text	**Error Reported**
Omitted or “”	MWC if there is no error. Reports “#OoB” (Out of Bounds) if a viscosity is not in the chart area and no MWC is calculated.
“V” verbose	Gives a viscosity and/or a boundary violation code instead of “#OoB”.
“NC” no check	It does not check for viscosities or boundary violations It returns an MWC or Excel calculation error code like #VALUE!

Table 41 Boundary Violation Codes

Code	**Explanation**
V1(low)	Viscosity at 100°F is below 6.76 cSt for an H100 of <100.
V1(high)	Viscosity at 100°F is above 69560 cSt for an H100 of >750.
V2(low)	Viscosity at 210°F is below 2.6 cSt.
V2(high)	Viscosity at 210°F is above 60 cSt.
LB	Left Boundary, the viscosities at 100°F and 210°F do not intersect on the chart but might intersect off the chart on the left or top left.
RB	Right Boundary, the viscosities at 100°F and 210°F do not intersect on the chart but might intersect off the chart on the right or right bottom.

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Boundary Violation Details

The ASTM D2502 chart has a distinct form (Figure 50). Figure 50 shows the vertex points and boundary lines. The legend refers to those boundaries on the chart. Table 42 has the color-coding for the boundaries with descriptions and limits.

Table 42 Boundary Descriptions

Color	Boundary	Type	Value cSt	MW	Violation Code
Red	V210	Minimum to Maximum	4.25 to 60 Depends on V1	700	RB
Orange	V210	Maximum	60	344 to 700	V2(high)
Yellow	V100	Maximum H100 of 750	69560.2	220 to 344	V1(high)
Green	V210	Minimum to Maximum	2.6 to 16.17 Depends on V1	220	LB
Blue	V210	Minimum	2.6	220 to 372	V2(low)
Purple	V100	Minimum H100 of 100	6.759	372 to 700	V1(low)

The chart area below a V210 of 2.6 was not considered for determining boundary limits because of the difficulty in determining the V210 at the point MW=220 and H100=100. The MWC estimates a viscosity of 1.927 cSt, while estimating the point from the chart was between 1.725 (linear) and 1.95 (non-linear). Using the MWC value to fit the left boundary limit equation gave a very high residual. If the higher residual for the corner point is used, the left boundary constraint equation values would not flag V210 values that are well off the chart and would be ineffective as a warning for invalid V210s.

A modified version of the chart (Figure 51) used the viscosities for the axes. The legend and color-coding of the boundary lines is consistent between the 2 charts. Some of the bottom boundaries are difficult to discern and are visually clearer in Figure 52, which is the same as Figure 51 but with both scales logarithmic. This helps with deciding how to set up the boundary conditions.

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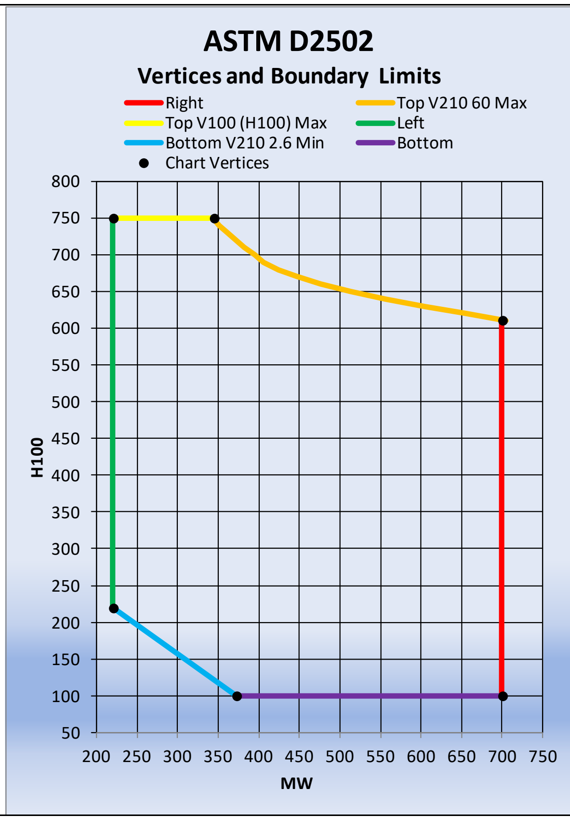

Figure 50 Vertices and Boundary Lines on the ASTM D2502 Chart

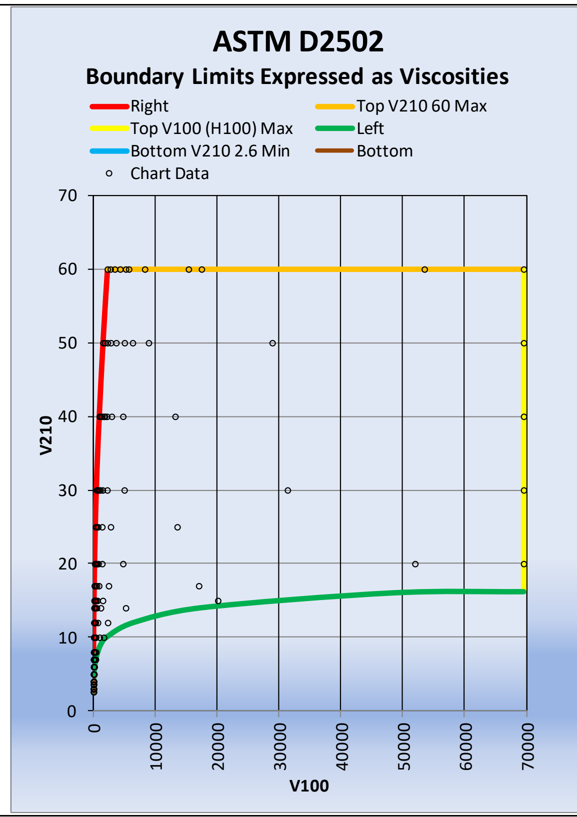

Figure 51 Fitting Data and Boundary Lines with Viscosities as Axis

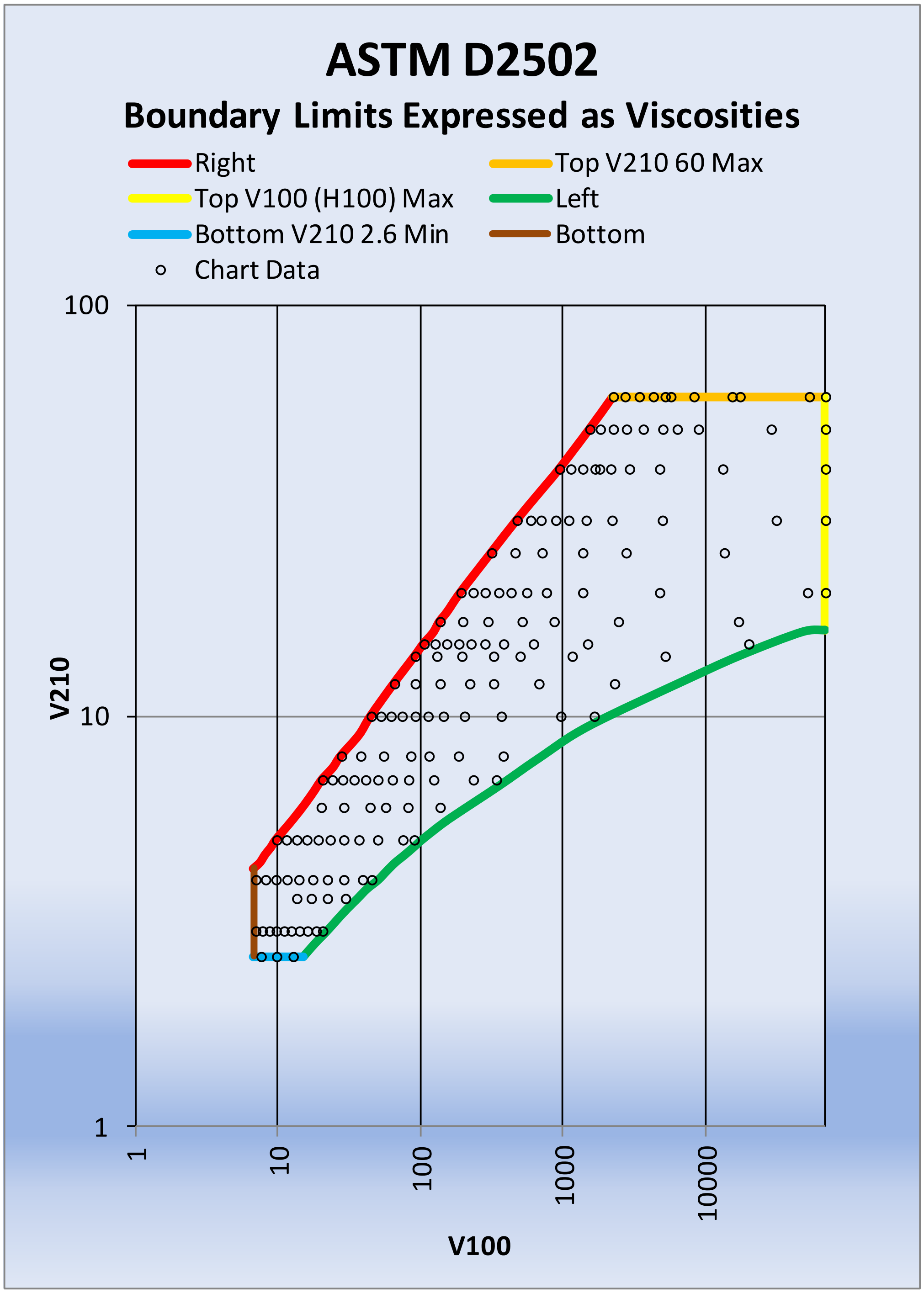

Figure 52 Logarithmic Axis Scaling of Viscosities Axes in Figure 51

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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Equations were determined for both the right and left edges (boundaries) of the ASTM chart. Table Curve 2D[35] fitted V2 as a function of V1. The criterion for the function was the smallest standard error that was consistent with a function that was rational, smoothly increasing over the V1 range and computational straightforward to implement. Consideration was not given to whether single or double precision was required.

There is no data for the left boundary of the chart from previous work. An expanded digital picture was used to estimate the values for the fit. Table 43 has the raw data values read or estimated from the ASTM chart, the input and output for TC2D and a comparison of the chart MW with the MWC. The MWC compares favorably to the chart MW with a standard deviation of 2.4 for the difference between the chart MW and MWC. This is consistent with the standard deviation for the chart fit in Table 4.

Table 43 Chart Points for Fitting Left Edge Boundary Equation TC2D

Chart LB		Raw Data			Raw Data			Raw Data
TC2D	Input	Input	Output	Output				
Point	V100	V210	V210	V210 Residual	MW	MWC	MWC Residual	H100
1	14.86	2.6	2.601	-0.001	220	221.7	-1.7	219.5
2	17.94	2.8	2.794	0.006	220	222.9	-2.9	243.7
3	21.77	3	3.008	-0.008	220	221.3	-1.3	267.3
4	25.73	3.2	3.204	-0.004	220	222.4	-2.4	286.6
5	30.27	3.4	3.396	0.004	220	223.0	-3	304.6
6	35.76	3.6	3.595	0.005	220	222.1	-2.1	322.2
7	41.69	3.8	3.784	0.016	220	222.3	-2.3	337.7
8	50.16	4	4.022	-0.022	220	218.4	1.6	355.7
9	57.43	4.2	4.203	-0.003	220	219.9	0.1	368.4
10	65.78	4.4	4.390	0.010	220	220.9	-0.9	380.7
11	77.06	4.6	4.610	-0.010	220	219.4	0.6	394.6
12	88.93	4.8	4.810	-0.010	220	219.2	0.8	406.7
13	101.5	5	4.994	0.006	220	219.9	0.1	417.6
14	144.5	5.5	5.480	0.020	220	219.2	0.8	445.3
15	209.6	6	5.995	0.005	220	217.2	2.8	472.4
16	298.6	6.5	6.512	-0.012	220	216.4	3.6	496.6
17	409.8	7	7.016	-0.016	220	217.3	2.7	516.9
18	543.7	7.5	7.501	-0.001	220	219.2	0.8	534.3
19	715.1	8	8.001	-0.001	220	220.9	-0.9	550.3

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Chart LB		Raw Data			Raw Data			Raw Data
TC2D	Input	Input	Output	Output				
Point	V100	V210	V210	V210 Residual	MW	MWC	MWC Residual	H100
20	1183	9	8.957	0.043	220	224.6	-4.6	578.2
21	2105	10	10.036	-0.036	220	224.4	-4.4	607.8
22	6505	12	11.989	0.011	220	223.1	-3.1	659.7
23	17464	14	14.003	-0.003	220	224.1	-4.1	700.0
24	48341	16	16.000	0.000	220	224.1	-4.1	737.5

Figure 52 is the left boundary calculation for V2 in terms of V1 from Table Curve 2D. The function begins to become bimodal after the maximum V1. In Excel, the VBA MW calculation function will never check for a V1> than the maximum for the boundary, so the second value for V2 will not be encountered and cause the V2 value to be misreported as being on the chart when it is not.

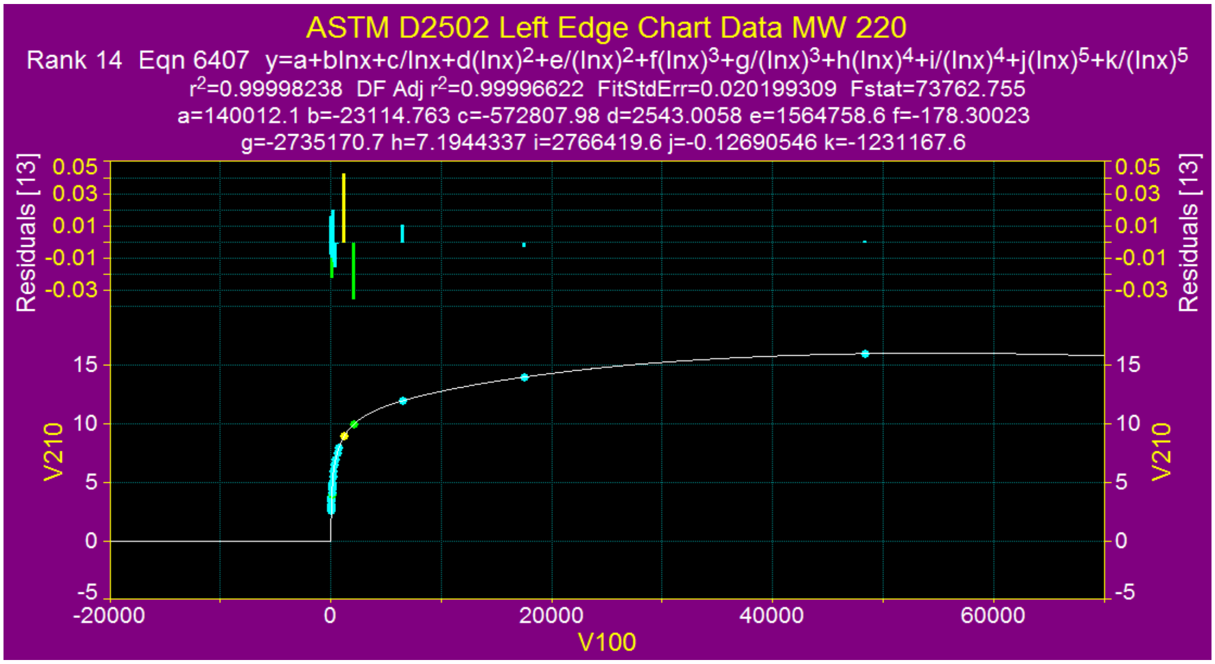

Figure 53 Table Curve 2D Equation Fitted to Left Edge of Chart

The boundary limit function and coefficients for the left boundary are in Table 44. The coefficients were initially single precision but it introduced some minor differences in the calculated boundary values. Using double precision eliminated the differences.

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Table 44 Equation and Coefficient for Left Boundary Limit of V210

V2=a+bLnV1+c/lnV1+d(LnV1)^2+e/(LnV1)^2+f(LnV1)^3 +g/(LnV1)^3+h(LnV1)^4+i/(LnV1)^4+j(LnV1)^5+k/(LnV1)^5					
a	140012.095739587	e	1564758.63486259	I	2766419.62786965
b	-23114.7634370257	f	-178.300226912808	J	-0.126905455696835
c	-572807.982232585	g	-2735170.67925539	k	-1231167.60935815
d	2543.00575316951	h	7.19443368988872		

The residuals in the calculated V210 were similar in scale so an absolute value was used to adjust the boundary limit calculation. The boundary limit calculated was adjusted by adding a value (-0.040) slightly less than the largest negative fit residual for the data (-0.036 Table 43 point 21) and testing if V210 was < the adjusted limit. This assures that none of the chart limit points would be incorrectly reported as out of bounds due to residual fit errors. Figure 54 is a stylized graph with example values showing the methodology. At first glance, the stylized graph may seem peculiar but it has to be referenced back to Figure 51 with viscosity data, where the lower V100 boundary represents the left ASTM chart boundary and the V210 data above the green line is V210 values on the ASTM chart.

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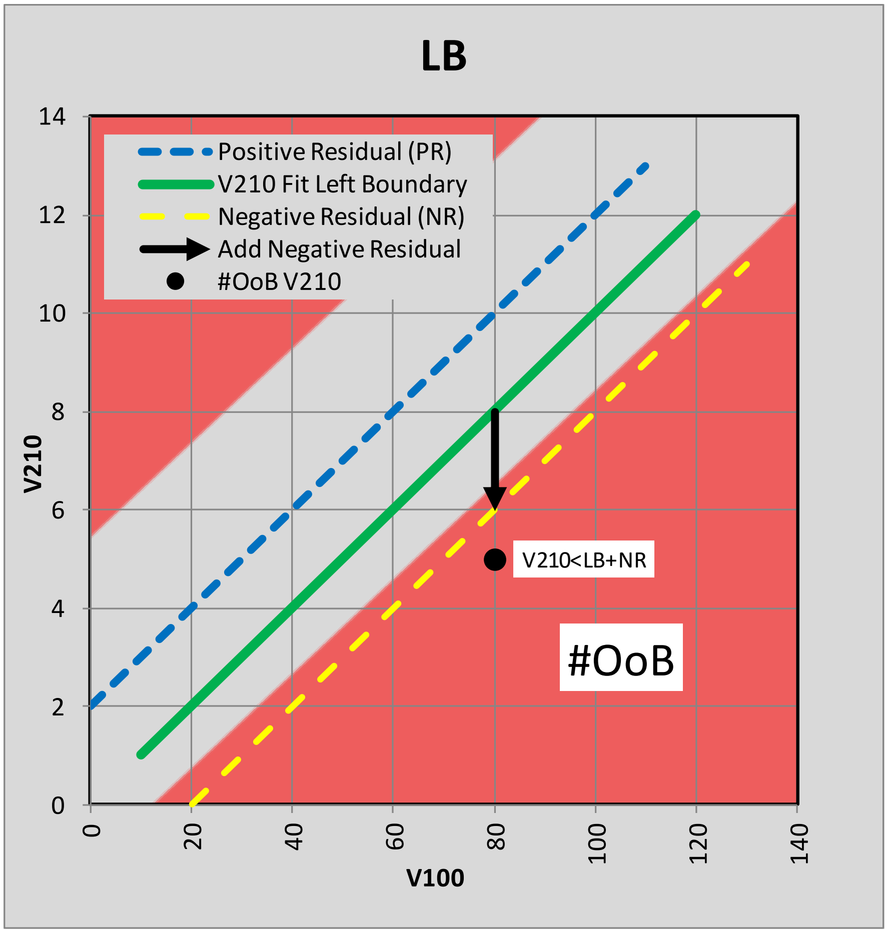

Figure 54 Stylized Chart Showing Adjustment to the Left Boundary Limit

A similar procedure was done for the RB. The data is in Table 45. There was some previous data on the RB and this was augmented with additional points highlighted in yellow.

Table 45 Chart Points for Fitting Right Edge Boundary Equation TC2D

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		Raw Data			Raw Data			Raw Data
RB	Input	Input	Output	Output				
Point	V100	V210	V210	V210 Residual	MW	MWC	MWC Residual	H100
1	7.54	4	4.96	0.038	700	691.1	8.9	118.6
2	8.19	5	6.92	0.077	700	698.7	1.3	132.3
3	9.02	5	7.97	0.032	700	699.6	0.4	147.6
4	9.72	5	9.98	0.025	700	706.3	-6.3	159.2
5	12.28	6	11.91	0.090	700	699.1	0.9	193.4
6	14.99	6	13.98	0.015	700	696.2	3.8	220.6
7	17.70	7	14.97	0.025	700	698.6	1.4	242.1
8	20.43	7	16.95	0.054	700	704.2	-4.2	259.7
9	24.50	8	19.89	0.107	700	691.9	8.1	281.1
10	27.74	8	25.03	-0.030	700	696.7	3.3	295.0
11	37.34	9	29.99	0.009	700	680.8	19.2	326.6
12	44.88	10	39.99	0.008	700	694.0	6.0	345.0
13	65.28	12	50.00	-0.002	700	697.9	2.1	380.0
14	91.41	14	60.00	0.000	700	695.9	4.1	409.0
15	105.47	15	4.44	-0.040	700	697.5	2.5	420.7
16	123.87	16	4.60	-0.003	700	691.7	8.3	433.4
17	136.61	17	4.80	-0.001	700	700.7	-0.7	441.0
18	155.78	18	5.50	-0.003	700	698.9	1.1	450.9
19	191.53	20	6.02	-0.016	700	704.9	-4.9	466.0
20	314.63	25	6.49	0.014	700	703.6	-3.6	500.0
21	474.32	30	7.53	-0.026	700	702.5	-2.5	526.0
22	685.86	35	9.15	-0.150	700	697.5	2.5	547.9
23	944.60	40	16.17	-0.172	700	693.7	6.3	566.0
24	1539.28	50	18.04	-0.039	700	697.7	2.3	592.0
25	2247.79	60	35.01	-0.011	700	705.0	-5.0	611.0
Data supplemental to original fit data from chart								

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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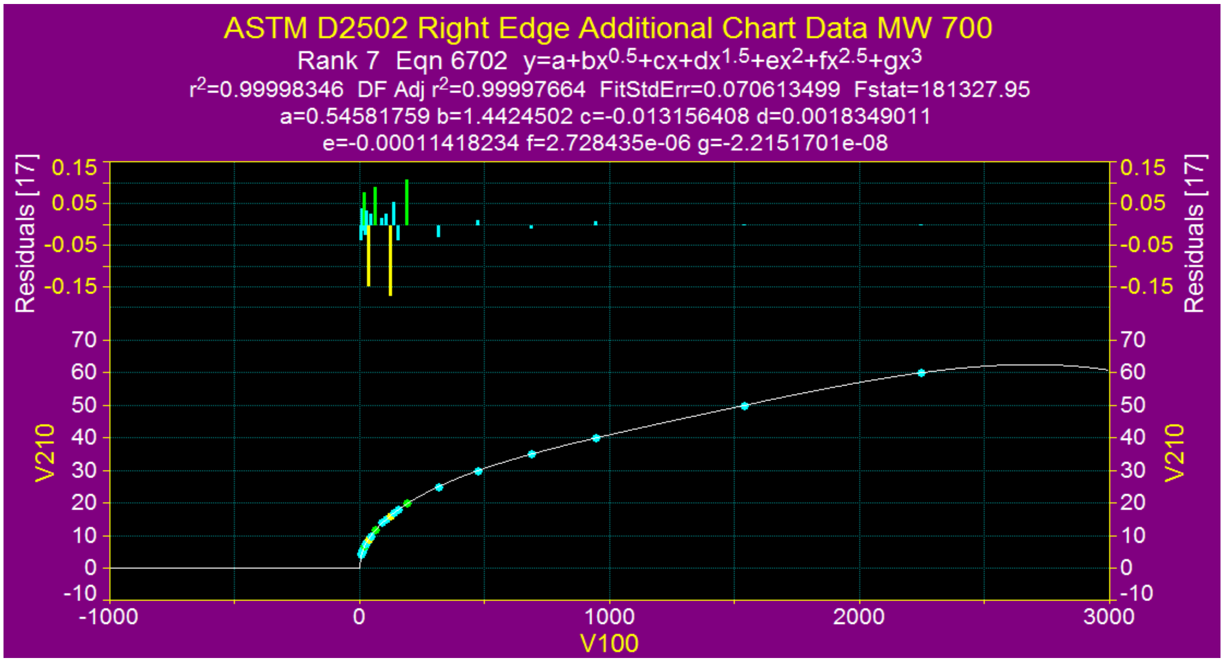

Figure 55 Table Curve 2D Equation Fitted to Right Edge of Chart

The boundary limit function and coefficients for the right boundary are in Table 46.

Table 46 Equation and Coefficient for Right Boundary Limit of V210

V2=a+bV1^(0.5)+cV1+dV1^(1.5)+eV1^2+fV1^(2.5)+gV1^3			
a	0.545817589635799	e	-0.000114182344081125
b	1.44245021850922	f	2.72843501043909E-06
c	-0.0131564083827617	g	-2.21517012538976E-08
d	0.00183490105482591		

For the right boundary limit the methodology was similar but the maximum residual was added and the test for OoB was V210 > the adjusted limit. Again, the fit residuals were similar in scale so an absolute value was used. The adjustment value added was slightly greater (0.110) than the largest positive fit residual for the data (0.107 Table 46 point 9). This assures none of the chart boundary limit points would be incorrectly reported as out of bounds due to residual fit errors. Figure 56 is a stylized graph with example values showing the methodology.

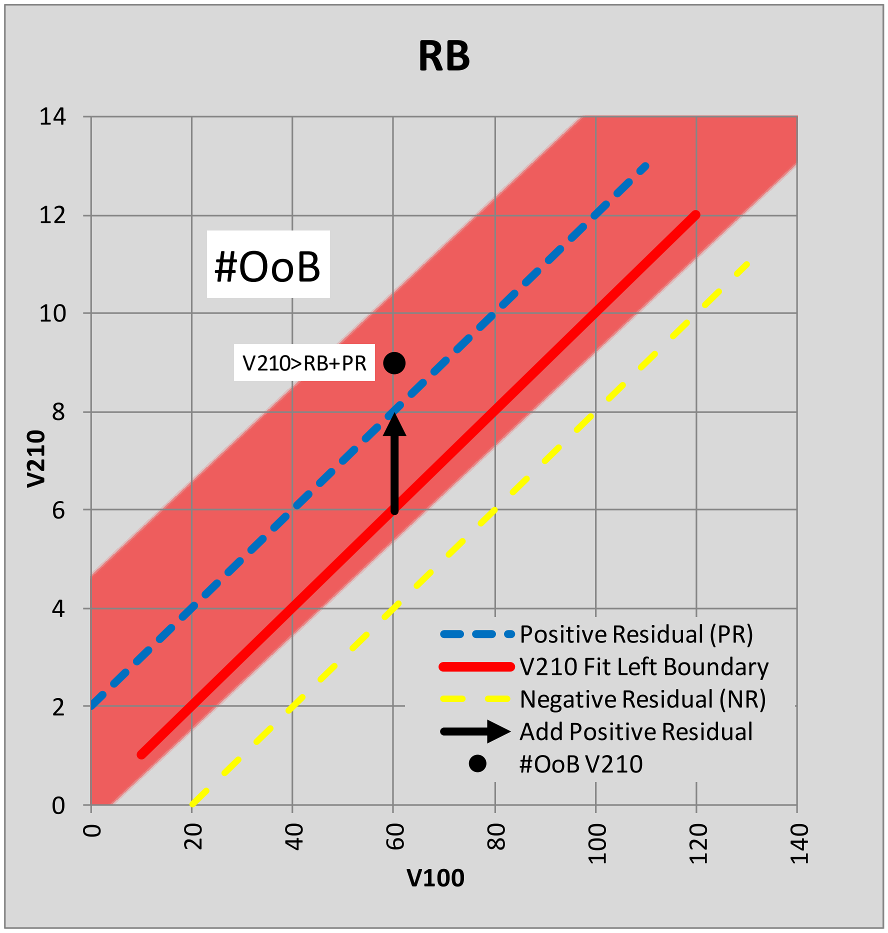

Figure 56 Stylized Chart Showing Adjustment to the Right Boundary Limit

Testing the calculation against the experimental data from the references gave 16 out of bounds points for the 19 experimental points in reference 12. This agreed with previous evaluations of the data from that reference. One additional point of the 37 points in reference 18 was out of bounds. The V210 was 2.2 cSt. The boundary was set at 2.6 because the non-linearity in the V210 isostokes made estimating viscosities in this area difficult. The lower left corner was estimated to be H100=100 and V210=1.98 but in setting up the boundary values, this viscosity gave an extremely high residual for the fit and it was elected to make the lower boundary 2.6.

The augmented left and right boundary data could be added to the fit data if the coefficients for the MW calculation model were to be refined. Figure 57 shows the data point locations and is Figure 1 with the augmented boundary points. Figure 58 shows the residuals and is Figure 9 with the augmented boundary points. The points with white circles are those that have residual >±4.5. These charts do not have the 3 corners of the chart (bottom left, top left, bottom right) as boundary points (Table 47). The V210 viscosities for these points were estimated using the

MWC calculation to give the MW expected so the residuals are artificial and exactly 0. The left boundary corners gave high residual when fit to the boundary equation than the lower right corner so it more realistically models that corner but still had a residual high enough that it was not included in the fit.

Table 47 Boundary Points Not Used

Corner	V100	V210	MW	H100	MWC	Residual
Bottom Left	6.76	1.927	200	100	220.0	0
Top Left	69560	16.17	220	750	220.0	0
Bottom Right	6.76	4.25	700	100	700.0	0

Calculation to Estimate the Molecular Weight of a Petroleum Oil from Two Viscosity Measurements That Models ASTM D2502 Chart

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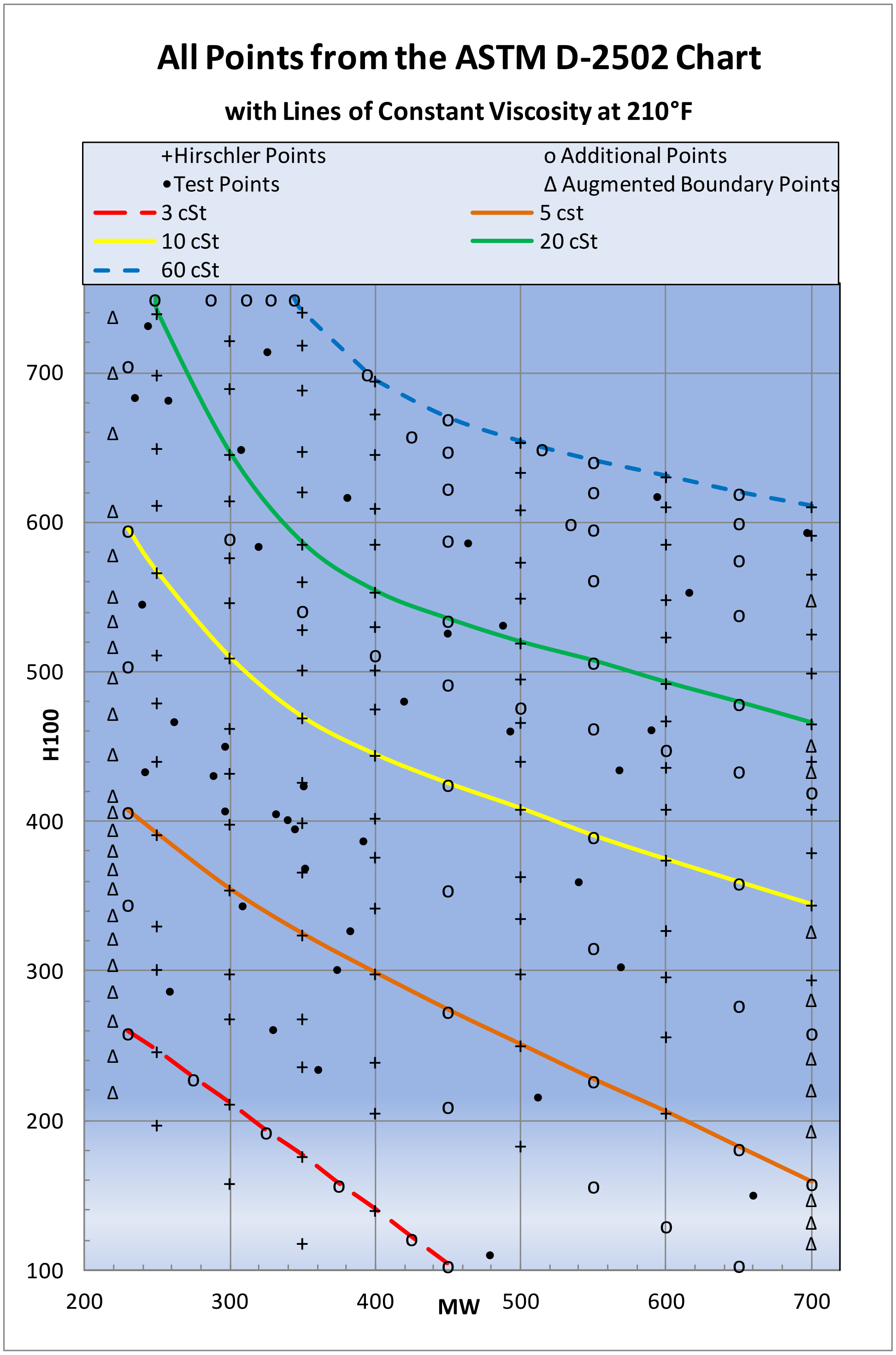

Figure 57 All Data Points from the ASTM D2502 Chart

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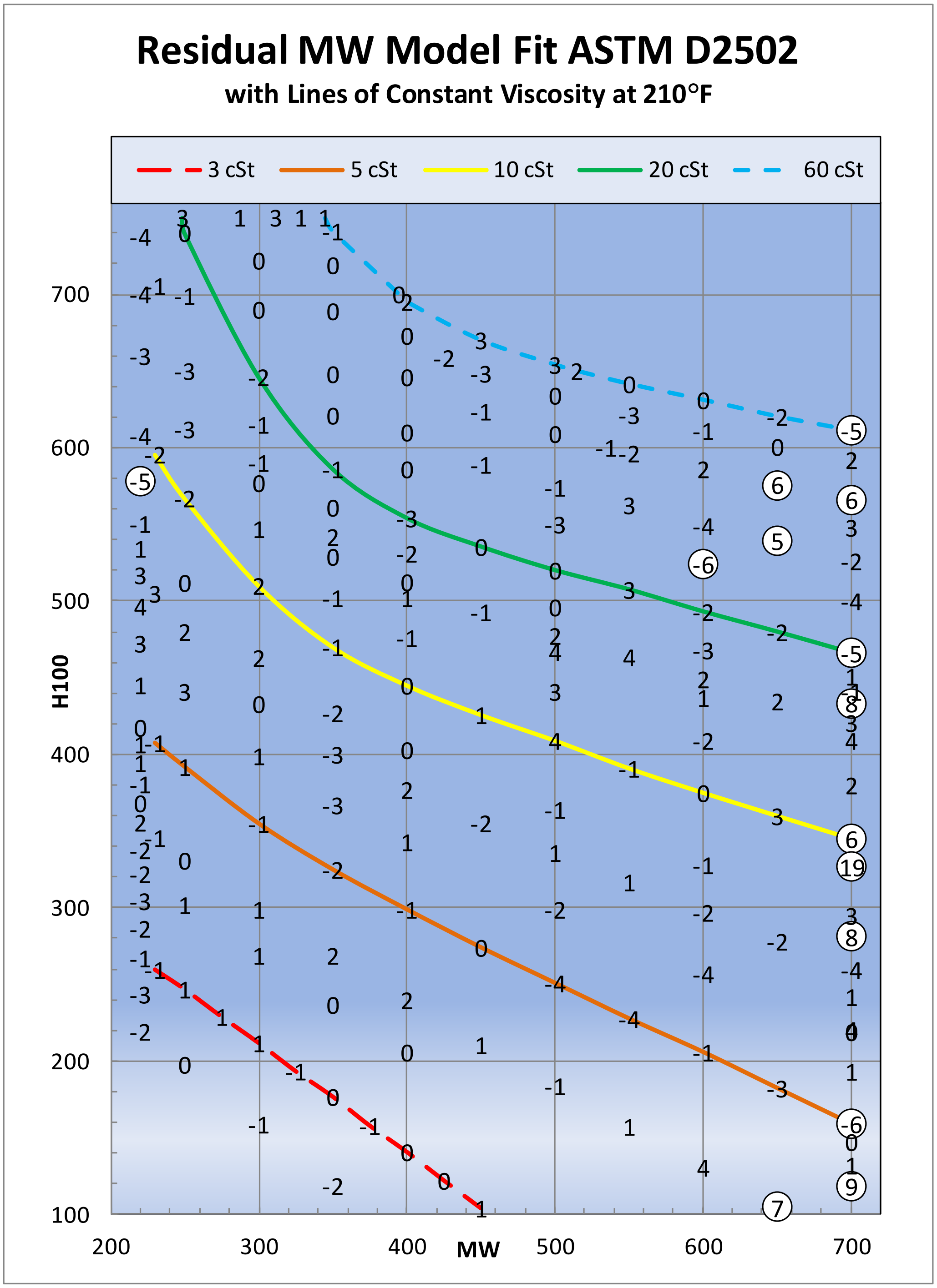

Figure 58 Residual for All Chart Points from ASTM D2502

VBA Code

Molecular Weight Calculation Using Viscosities at 40°C and 100°C

```
Option Explicit
Function MW40_100(V40 As Double, V100 As Double, Optional ReportErr As String) As Variant
'Joseph A. Weaver, Jr. 08/19/20
'Calculates the molecular weight (MW) of a petroleum oil from 2 viscosities
'   modeling ASTM D2502 chart but uses 40C and 100C cSt viscosities
'Input is V40 is viscosity at 40C in cSt, V100 is viscosity at 100C in cSt
'   and optional ReportErr parameter for checking and reporting viscosity validity.
'   Default: "ReportErr" is missing or "" then reports viscosities are
'       "#OoB" Out of Bounds and not on the chart
'   "V" or "v" verbose: The function will report violations codes
'       related to ASTM D2502 chart.
'   "NC", "nc", "Nc", or "nC": Function does not check viscosities and
'       report a molecular weight if there are no Excel calculation errors.
'       Excel calculation errors with return #VALUE.
'Boundary Violation Codes
'   "V1(low)"  Viscosity at 100F is below 6.76 cSt = H100 of 100
'   "V1(high)" Viscosity at 100F is above than 69560 cSt = H100 of 750
'   "V2(low)"  Viscosity at 210F is below 1.93 cSt (estimated low left corner of the chart)
'   "V2(high)" Viscosity at 210F is above 60 cSt
'   "LB" left boundary, The viscosity at 100F and 210 do not intersect on the chart
'       but might intersect outside the left boundary or top left.
'   "RB" right boundary, The viscosity at 100F and 210 do not intersect on the chart
'       but might intersect outside the right boundary or right bottom.
'   It can report a combination of these.
'It uses the VisAtTC to convert the viscosities from 40C and 100C in cSt to
'   the viscosities in cSt at 37.777...F and 98.888...F
'The converted viscosities are input along with the ReportErr into the
'   MW (molecular weight) calculation developed from 1980 to April 1985
'   to model ASTM D2502
`
Dim V100F As Double, V210F As Double, TCof100F As Double, TCof210F As Double
TCof100F = (100 - 32) * 5 / 9
TCof210F = (210 - 32) * 5 / 9
V100F = VisAtTC(V40, V100, 40, 100, TCof100F)
V210F = VisAtTC(V40, V100, 40, 100, TCof210F)
MW40_100 = MW(V100F, V210F, ReportErr)
End Function
```

Viscosity-Temperature Conversion Code

```
Function VisAtTC(V1c As Double, V2c As Double, T1C As Double, T2C As Double, T3C As Double) As
Double
'Viscosity at Temperature C
'Joseph A. Weaver, Jr. 8/19/20
'Based on the Wortley Andrew Wright equation Journal of Materials, JMLSA (1969), vol. 4.11 pp.
1927
'Converts a petroleum oil viscosity to a viscosity at another temperature
'Requires the viscosity of the oil at 2 temperatures
'V1c and V2c are the viscosity in cSt at temperatures in Celsius T1C and T2C
'T3C is the temperature in Celsius of the converted viscosity
'It REQUIRES the LOG10 function below to calculate the base 10 log
'     as VBA does not have this as a native function
`
Dim V(2) As Double, C(2) As Double, Co(6, 6) As Double
Dim K0 As Double, K1 As Double, TK(3) As Double
Dim A As Double, B As Double
Dim I As Integer, J As Integer, K As Integer
K0 = 273.15
K1 = 0.7
V(1) = V1c
```

```
V(2) = V2c
TK(1) = T1C + K0
TK(2) = T2C + K0
TK(3) = T3C + K0
Co(1, 1) = -1.14883
Co(1, 2) = -2.65868
Co(2, 1) = -0.0038138
Co(2, 2) = -12.5645
Co(3, 1) = 5.46491
Co(3, 2) = -37.6289
Co(4, 1) = 13.0458
Co(4, 2) = -74.6851
Co(5, 1) = 37.4619
Co(5, 2) = -192.643
Co(6, 1) = 80.4945
Co(6, 2) = -400.468
I = 1
For J = 1 To 2
    C(J) = 0
    For K = 1 To 6
            C(J) = (-1) ^ (K + 1) * (Exp(Co(K, I) + Co(K, I + 1) * V(J))) + C(J)
    Next K
    V(J) = V(J) + 0.7 + C(J)
Next J
A = (Log10(Log10(V(2))) - Log10(Log10(V(1))) * Log10(TK(2)) / Log10(TK(1))) / (1 - Log10(TK(2)) / 
Log10(TK(1)))
B = (A - Log10(Log10(V(1)))) / Log10(TK(1))
VisAtTC = 10 ^ (10 ^ (A - B * Log10(TK(3)))) - 0.7
End Function
```

Conversion Code for Log to base *e* to Base 10

```
Function Log10(Arg1 As Double) As Double
'Converts the VBA Log (base e) function to base 10 as
'VBA does not have a native Log base 10 function
Log10 = Log(Arg1) / Log(10#)
End Function
```

Molecular Weight Calculation Using Viscosities at 100°F and 210°F

```
Function MW(V1 As Single, V2 As Single, Optional ReportErr As String) As Variant
'Joseph A. Weaver, Jr. 08/19/20
'Calculates the molecular weight (MW) of a petroleum oil from the 2 viscosities
'   used to make the ASTM D2502 chart
'Input is V1 is viscosity at 100F in cSt, V2 is viscosity at 100F in cSt
'   and optional ReportErr parameter for checking and reporting viscosity validity.
'   Default: "ReportErr" is missing or "" then reports viscosities are
'       "#OoB" Out of Bounds and not on the chart
'   "V" or "v" verbose: The function will report violations codes
'       related to ASTM D2502 chart.
'   "NC", "nc", "Nc", or "nC": Function does not check viscosities and
'       report a molecular weight if there are no Excel calculation errors.
'       Excel calculation errors with return #VALUE.
'Boundary Violation Codes
'   "V1(low)"  Viscosity at 100F is below 6.76 cSt = H100 of 100
'   "V1(high)" Viscosity at 100F is above than 69560 cSt = H100 of 750
'   "V2(low)"  Viscosity at 210F is below 1.93 cSt (estimated low left corner of the chart)
'   "V2(high)" Viscosity at 210F is above 60 cSt
'   "LB" left boundary, The viscosity at 100F and 210 do not intersect on the chart
'       but might intersect outside the left boundary or top left.
'   "RB" right boundary, The viscosity at 100F and 210 do not intersect on the chart
'       but might intersect outside the right boundary or right bottom.
'   It can report a combination of these.
```

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```
'It uses the VisAtTC to convert the viscosities from 40C and 100C in cSt to
'   the viscosities in cSt at 37.777...F and 98.888...F
'The converted viscosities are input along with the ReportErr into the
'   MW (molecular weight) calculation developed from 1980 to April 1985
'   to model ASTM D2502
'It has been augmented 08/15/20 to check that the viscosities will be
'   in the range of the chart
`
    MW = ""
    ReportErr = UCase(ReportErr)

'Initialize Viscosities Min Max and constrained
    Dim V1Min As Single, V1MaxRB As Single, V1Max As Single
    Dim V2Min As Single, V2MinRB As Single, V2Max As Single
    Dim NumVisOutOfRange As Integer
    V1Min = 6.7590916903038
    V1MaxRB = 2247.7890693438
    V1Max = 69560.1787709072
    'V2Min = 1.92659741640091
    V2Min = 2.6
    V2MinRB = 4.25037789344788
    V2Max = 60
    NumVisOutOfRange = 0

'Left Boundary Parameters and Calculation
    'The calculation in VBA and the worksheet gave different result
    'unless the LB coefficients were defined as double
    Dim LB(11) As Double, LBVal As Single, LBTol As Single
    LB(1) = 140012.095739587
    LB(2) = -23114.7634370257
    LB(3) = -572807.982232585
    LB(4) = 2543.00575316951
    LB(5) = 1564758.63486259
    LB(6) = -178.300226912808
    LB(7) = -2735170.67925539
    LB(8) = 7.19443368988872
    LB(9) = 2766419.62786965
    LB(10) = -0.126905455696835
    LB(11) = -1231167.60935815
    'y=a+blnx+c/lnx+d(lnx)^2+e/(lnx)^2+f(lnx)^3+g/(lnx)^3+h(lnx)^4+i/(lnx)^4+j(lnx)^5+k/(lnx)^5
    LBVal = LB(1) + LB(2) * Log(V1) + LB(3) / Log(V1) + LB(4) * Log(V1) ^ 2 _
    + LB(5) / Log(V1) ^ 2 + LB(6) * Log(V1) ^ 3 + LB(7) / Log(V1) ^ 3 _
    + LB(8) * Log(V1) ^ 4 + LB(9) / Log(V1) ^ 4 + LB(10) * Log(V1) ^ 5 _
    + LB(11) / Log(V1) ^ 5
    'Maximum residual added to boundary calculation to make sure V2 <= boundary across all values
    'Residual from fit -0.036 to 0.043
    LBTol = -0.04
    LBVal = LBVal + LBTol

'Right Boundary Parameters and Calculations
    Dim RB(7) As Single, RBVal As Single, RBMinV2 As Single, RBTol As Single
    RB(1) = 0.545817589635799
    RB(2) = 1.44245021850922
    RB(3) = -1.31564083827617E-02
    RB(4) = 1.83490105482591E-03
    RB(5) = -1.14182344081125E-04
    RB(6) = 2.72843501043909E-06
    RB(7) = -2.21517012538976E-08
    'y=a+bx^(0.5)+cx+dx^(1.5)+ex^2+fx^(2.5)+gx^3
    RBVal = RB(1) + RB(2) * V1 ^ 0.5 + RB(3) * V1 + RB(4) * V1 ^ 1.5 + RB(5) _
    * V1 ^ 2 + RB(6) * V1 ^ 2.5 + RB(7) * V1 ^ 3
    'Minimum residual added to boundary calculation to make sure V2 >= boundary
    '     across all values
```

```
    'Residual from fit -0.172 to 0.107
    RBTol = 0.11
    RBVal = RBVal + RBTol

If ReportErr = "NC" Then GoTo SkipInputCheck
'Check if V1 is too high or low
    If V1 < V1Min Then
        MW = "V1(low) "
        NumVisOutOfRange = NumVisOutOfRange + 1
    End If
    If V1 > V1Max Then
        MW = "V1(high) "
        NumVisOutOfRange = NumVisOutOfRange + 1
    End If
    If V2 < V2Min Then
        MW = MW + "V2(low) "
        NumVisOutOfRange = NumVisOutOfRange + 1
    End If
    If V2 > V2Max Then
        MW = MW + "V2(high) "
        NumVisOutOfRange = NumVisOutOfRange + 1
    End If
    If NumVisOutOfRange = 2 Then GoTo SkipEdgeCheck

'Check left boundary for valid V1&V2
    If V1 >= V1Min And V1 <= V1Max Then
        If V2 < LBVal Then MW = MW + "LB"
    End If

'Check Right boundary for valid V1&V2
    If V1 >= V1Min And V1 <= V1MaxRB Then
        If V2 > RBVal Then MW = MW + "RB"
    End If

SkipEdgeCheck:
    If MW <> "" And ReportErr = "V" Then
        'Assures that only "V" input will report codes in MW
    Else
        If MW <> "" Then MW = "#OoB"
    End If
    If MW <> "" Then Exit Function
SkipInputCheck:

'Coefficients
Dim C(32) As Single
C(1) = 4.11
C(2) = 1.358
C(3) = 1.5414
C(4) = -0.4106
C(5) = 197.6
C(6) = -592.944
C(7) = -96.08
C(8) = 0.8759
C(9) = 154.29
C(10) = -1.513
C(11) = 4.126
C(12) = 2.356
C(13) = 1.07
C(14) = 1.446
C(15) = -31.5
C(16) = -0.64
C(17) = 0.069
C(18) = 0.31
```

```
C(19) = -0.032
C(20) = 0.002
C(21) = -1.267
C(22) = 8.05
C(23) = -4.326
C(24) = 6.223
C(25) = 300
C(26) = -0.00326
C(27) = 19.54
C(28) = -30.387
C(29) = -12.02
C(30) = 7.276
C(31) = 6.498
C(32) = 52.3

Dim K As Integer, K11 As Integer
Dim F1 As Single, F2 As Single, F12 As Single
Dim MW0 As Single, MW1 As Single, MW2 As Single, MWS As Single, MWC As Single
Dim X As Single, X2 As Single, Y As Single, Y2 As Single, EL As Single
Dim SI As Single, CO As Single
Dim SG As Single, EX As Single, EX1 As Single, EX2 As Single

'MW Calculation
F1 = Log(Log(V1 + C(1)))
F2 = Log(Log(V2 + C(2)))
F12 = Log(F1 - C(3) * F2 - C(4))
MW0 = C(5) + C(6) * F12 + C(7) * F12 * F2 ^ 2 + C(8) * F1 ^ 4 + C(9) * F1 * F2 * F12
MWS = MW0 * 0.01
For K = 0 To 1
K11 = K * 11
SI = Sin(C(10 + K11))
CO = Cos(C(10 + K11))
X = (MWS * CO + F2 * SI - C(11 + K11) * CO - C(12 + K11) * SI) / C(13 + K11)
X2 = X * X
Y = (F2 * CO - C(12 + K11) * CO - MWS * SI + C(11 + K11) * SI) / C(14 + K11)
Y2 = Y * Y
EL = X2 + Y2
SG = Tan(C(10 + K11)) * (-C(11 + K11) + MWS) + C(12 + K11) - F2
If SG < 0 Then SG = -1 Else SG = 1
EX = SG * EL
EX1 = EX * (C(19 + K11) + EX * C(20 + K11))
EX2 = EX * (C(17 + K11) + EX * (C(18 + K11) + EX1))
MW2 = C(15 + K11) * Exp(-(C(16 + K11) + EX2))
If K = 0 Then MW1 = MW2
Next
MWC = MW0 + MW1 + MW2 + C(32)
MW = MWC
End Function
```

Conversion of SUS and cSt, VBA Code and Cell Formula:

It is difficult to algebraically manipulate the ASTM calculation to convert cSt to SUS in equation {1} to give a reverse calculation (InvSUS).

An-in cell calculation was developed that used a reiterative calculation with successive approximations. This became the basis for a VBA function.

The VBA code for conversion of cSt to SUS is;

```
Function cSt40From(SUSAt100 As Single, Optional Temp As Single = 104) As Single
```

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```
'Calculates SUS from cSt at 40C (104F) based on ASTM D 2161
'Temp is the temperature of the cSt in F (40C =104F exactly)other cSt temperatures can be used
'The calculation from cSt to SUS is done iteratively and takes about 6 loops.
'Joseph A. Weaver, Jr. 2010
Dim SUS1 As Double
Dim SUS2 As Double
Dim SUSd As Double
Dim cSt1 As Double
SUS1 = SUSAt100
cSt1 = SUS1 / 4.6324
SUS2 = (1 + 0.000061 * (Temp - 100)) * (4.6324 * cSt1 + (1 + 0.03264 * cSt1) / ((3930.2 + 262.7 *
cSt1 + 23.97 * cSt1 ^ 2 + 1.646 * cSt1 ^ 3) * 0.00001))
SUSd = SUS1 - SUS2
Do Until Abs(SUSd) < 0.000001
    cSt1 = cSt1 + SUSd / 4.6324
    SUS2 = (1 + 0.000061 * (Temp - 100)) * (4.6324 * cSt1 + (1 + 0.03264 * cSt1) / ((3930.2 +
262.7 * cSt1 + 23.97 * cSt1 ^ 2 + 1.646 * cSt1 ^ 3) * 0.00001))
    SUSd = SUSAt100 - SUS2
    SUS1 = SUSAt100 + SUSd
Loop
cSt40From = cSt1
End Function
```

The circular 1-cell calculation based on the iteration calculation feature of Excel refines the cSt (InvSUS) by successively reducing the difference between a calculated SUS value and the SUS entered for conversion. Further below is the procedure to set up Excel and use the calculation.

The InvSUS calculation used reiteratively in Excel is

```
cSt =
A2+(B2-                                                                            {2}
(1+0.000061*(C2-100))*                                                             {3}
(4.6324*A2+(1+0.03264*A2)/((3930.2+262.7*A2+23.97*A2^2+1.646*A2^3)*0.00001))       {4}
)*0.1                                                                              {5}
```

where

Excel cell	Content
A2	contains the formula {6} InvSUS to calculate SUS from cSt
B2	SUS viscosity
C2	temperature °F

Lines {3} and {4}, which uses the ASTM D2161 calculation for converting cSt to SUS, calculates an new estimate of temperature corrected SUS from the cSt previously calculated in A2 (circular self referencing). The newly estimated SUS ({3} and {4}) is subtracted from the SUS being converted (B2 in line {2}) to give the error. Ten percent (0.1, line {5}) of the error is added to the value previously in A2 and Excel places the new value in A2. This is repeated until the limit of the Maximum Iterations or the Maximum Change options iterations is reached.

Typically, it takes about 23 iterations to reach a precision of 0.001. For a precision of 0.0000000000001, it takes about 75 iterations. Calculating SUS to a cSt and that value back to SUS showed no difference between the initial SUS and final SUS.

For copy and pasting into Excel the one line version of InvSUS (cSt) is

```
= A2+(B2-(1+0.000061*(C2-100))*(4.6324*A2+(1+0.03264*A2)/((3930.2+262.7*A2+23.97*A2^2+1.646*A2^3)*0.00001)))*0.1
```
{6}

To use {6} the calculation options must have iterative calculation enabled. Any changes will affect all open workbooks[36].

To access and set up the iterative calculation in Excel 2007:

1. click on the Application button ,
2. select Excel Options at the bottom,
3. select Formulas on the left side bar,
4. in the Calculation Options panel on the right click on the Automatic circular radio button,
5. click on Enable iterative calculation box to check it,
6. set Maximum Iterations: box to 100,
7. set the Maximum Change: box to 0.001,
8. click on the OK button at the bottom.

To use equation {6}:

1. copy and paste the green highlighted of {6} into cell A2
   Calculation {6} is on two lines but has no return or paragraph mark so it pastes as a formula in the cell.
   If the iterative calculation is not enabled, a “Circular Reference Warning” will appear and the iterative calculation will have to be enabled. The iterative calculation may or may not be permanently stored with the workbook[37].
2. enter the SUS to be converted into cell B2,
3. enter the °F temperature in C2 , which is usually 100 or 210.
4. cell A2 will have the result.
5. If equation {6} is used in other cells, it will have to be edited to refer to them

For completeness, the VBA calculation function to convert cSt to SUS is:

```
Function SUS100From(cStAtTemp As Single, Optional Temp As Single = 104) As Single
'Calculates SUS at 100F from cSt at 40C based on ASTM D 2161
'Temp is the temperature of the cSt in F (40C =104F exactly) - other cSt temperatures can be used
SUS100From = (1 + 0.000061 * (Temp - 100)) * (4.6324 * cStAtTemp + (1 + 0.03264 * cStAtTemp) /
((3930.2 + 262.7 * cStAtTemp + 23.97 * cStAtTemp ^ 2 + 1.646 * cStAtTemp ^ 3) * 0.00001))
End Function
```

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Chebyshev Bivariate 10th Order Polynomial C++ Code

NOTE: The x and y input is H100 and H210 NOT V100 and V210 so the viscosities would have to be preprocessed to use the code.

There is no check if H100 or H210 are in the valid range of the ASTM D2502 chart.

In C++ log is to the base ***e***. The C++ code was not edited to show it as ***Log***.

C++ Code listing:

```
/*--------------------------------------------------------------*
               TableCurve 3D CPP Code Output
            To modify generated output, edit CPP.TCL

Joseph A. Weaver, Jr. 07/18/2020 Notes added
   CPP is C++, NOTE x and y are the H100 and H210 functions
calculated from the viscosity at 100F in cSt (V100) and
210F (V210) using the calculations H100=870*Log(Log(V100
+ 0.6))+154 and H210=870*Log(Log(V210 + 0.6))+154
*--------------------------------------------------------------*/

#include <math.h>
#include <stdio.h>

class eqn409
{
public:
  eqn409(){ XLo=104.3; XHi=750; YLo=-104.0243053; YHi=372.3898956; }
  ~eqn409(){}
  double Eval(double x, double y);
  int RootsX(double y, double z, double *roots, int maxcnt=10, double
xlo=0.0, double xhi=0.0);
  int RootsY(double x, double z, double *roots, int maxcnt=10, double
ylo=0.0, double yhi=0.0);
protected:
  int Roots(double fixed, double z, double *roots, int maxcnt, double varlo,
double varhi, int isvarx);
private:
  double XLo,XHi,YLo,YHi;
};

void main(void)
{
  int i,ix,iy;
  double x,y,z,xr[10],yr[10];
  char str[80];
  eqn409 *e = new eqn409();
  while(1){
    printf("Enter x: ");
    gets(str);
```

```
    if(!*str) break;
    sscanf(str,"%lg",&x);
    printf("Enter y: ");
    gets(str);
    if(!*str) break;
    sscanf(str,"%lg",&y);
    z = e->Eval(x,y);
    ix = e->RootsX(y,z,xr);
    iy = e->RootsY(x,z,yr);
    printf("      z=%.15lg\n",z);
    for(i=0; i<ix; i++)
      printf("      x root at [y,z]=%.15lg\n",xr[i]);
    for(i=0; i<iy; i++)
      printf("      y root at [x,z]=%.15lg\n",yr[i]);
    }
  delete e;
}

class CEvalChebPoly
{
public:
  CEvalChebPoly(int Order, int LogX, int LogY, double *Parms, double Scale0,
double Scale1,
   double Scale2, double Scale3, double Scale4, double Scale5, double Scale6,
double Scale7){
    order=Order; logx=LogX; logy=LogY; p=Parms;
    s0=Scale0; s1=Scale1; s2=Scale2; s3=Scale3; s4=Scale4; s5=Scale5;
s6=Scale6; s7=Scale7;
    }
  ~CEvalChebPoly(){}
  double Eval(double x, double y);
private:
  int order, logx, logy;
  double *p, s0, s1, s2, s3, s4, s5, s6, s7;
};

double CEvalChebPoly::Eval(double x, double y)
{
  int tcnt,j,m,iv;
  double tx[12],ty[12],v[70],ans;
  if(!logx) x=(x-s0)/s1;
  else x=(log(x)-s2)/s3;
  if(!logy) y=(y-s4)/s5;
  else y=(log(y)-s6)/s7;
  switch(order){
    case 5:  tcnt=3; break;
    case 9:  tcnt=4; break;
    case 14: tcnt=5; break;
    case 20: tcnt=6; break;
    case 27: tcnt=7; break;
```

```
    case 35: tcnt=8; break;
    case 44: tcnt=9; break;
    case 54: tcnt=10; break;
    case 65: tcnt=11; break;
    default: return 0.0;
    }
  if(tcnt>6){
    if(x<-1.0) x=-1.0;
    if(x>1.0)  x= 1.0;
    if(y<-1.0) y=-1.0;
    if(y>1.0)  y= 1.0;
    }
  tx[0]=ty[0]=1.0;
  tx[1]=x; ty[1]=y;
  for(j=2;j<tcnt;j++){
    tx[j]=2*x*tx[j-1]-tx[j-2];
    ty[j]=2*y*ty[j-1]-ty[j-2];
    }
  iv=0;
  for(j=0;j<tcnt;j++){
    for(m=j; m>=0; m--)
      v[iv++]=tx[m]*ty[j-m];
    }
  ans=0.0;
  for(j=0;j<=order;j++)
    ans += p[j]*v[j];
  return ans;
}


double eqn409::Eval(double x, double y)
/*--------------------------------------------------------------*
   TableCurve 3D
   File Source= z:\hhmwfit.txt
   Date= Jul 18, 2020
   Time= 0:14:49 AM
   Data Set= hhmwfit.txt, X , Y , Z
   X=
   Y=
   Z=
   Eqn#= 409
   Eqn= Chebyshev X,Y Bivariate Polynomial Order 10
   r2=0.999913899675761
   r2adj=0.9998540826083949
   StdErr=1.735624555169359
   Fstat=17152.03660867905
   a= 68764722.53589136
   b= 28756470.71514429
   c= -28979595.67667712
   d= 95177034.75920626
```

```
e= -229982373.5206862
f= 97092667.93893693
g= 12569683.13775275
h= -38351570.13231931
i= 39252125.19130948
j= -13476720.83923102
k= 30709893.98453927
l= -108737098.5923456
m= 132747209.3528934
n= -113137642.8373347
o= 33227767.91511252
p= 2210622.296494415
q= -10660333.93822856
r= 16572348.0760467
s= -17227243.48209736
t= 11974585.28015124
u= -2683099.775541091
v= 4218182.280174093
aa= -22905905.57409191
ab= 41034779.01510019
ac= -50626098.48131823
ad= 43529710.5471436
ae= -25742538.44318724
af= 5008018.216648622
ag= 126060.7178656597
ah= -1072545.105023687
ai= 2653713.014563096
aj= -4211585.987928544
ak= 4446945.663222158
al= -3123361.193343093
am= 1406400.919557086
an= -184036.4261667721
ao= 201554.839972609
ap= -1854263.583254318
aq= 5096769.362522405
ar= -9240567.062948906
as= 11520713.29494397
at= -9987286.810286814
au= 5937407.288753645
av= -2314246.129918459
ba= 266729.2466010882
bb= 1297.672695887418
bc= -26214.83213007698
bd= 115893.3501681627
be= -295493.5573140769
bf= 479746.6641668526
bg= -514563.3816430145
bh= 364433.9830717448
bi= -164155.3575705012
bj= 42597.36066984419
```

```
   bk= -2420.107626222836
   bl= 1973.035134363025
   bm= -39945.61001880958
   bn= 185159.4332253456
   bo= -514410.5164602132
   bp= 943363.2102345941
   bq= -1188169.123533947
   br= 1037703.359409076
   bs= -619120.0327639152
   bt= 241003.9999587515
   bu= -55146.10647030385
   bv= 2808.54446405081
 *--------------------------------------------------------------*/
{
  double z;
  static double c[]= {
    68764722.53589136,
    28756470.71514429,
    -28979595.67667712,
    95177034.75920626,
    -229982373.5206862,
    97092667.93893693,
    12569683.13775275,
    -38351570.13231931,
    39252125.19130948,
    -13476720.83923102,
    30709893.98453927,
    -108737098.5923456,
    132747209.3528934,
    -113137642.8373347,
    33227767.91511252,
    2210622.296494415,
    -10660333.93822856,
    16572348.07604670,
    -17227243.48209736,
    11974585.28015124,
    -2683099.775541091,
    4218182.280174093,
    -22905905.57409191,
    41034779.01510019,
    -50626098.48131823,
    43529710.54714360,
    -25742538.44318724,
    5008018.216648622,
    126060.7178656597,
    -1072545.105023687,
    2653713.014563096,
    -4211585.987928544,
    4446945.663222158,
    -3123361.193343093,
```

```
    1406400.919557086,
    -184036.4261667721,
    201554.8399726090,
    -1854263.583254318,
    5096769.362522405,
    -9240567.062948906,
    11520713.29494397,
    -9987286.810286814,
    5937407.288753645,
    -2314246.129918459,
    266729.2466010882,
    1297.672695887418,
    -26214.83213007698,
    115893.3501681627,
    -295493.5573140769,
    479746.6641668526,
    -514563.3816430145,
    364433.9830717448,
    -164155.3575705012,
    42597.36066984419,
    -2420.107626222836,
    1973.035134363025,
    -39945.61001880958,
    185159.4332253456,
    -514410.5164602132,
    943363.2102345941,
    -1188169.123533947,
    1037703.359409076,
    -619120.0327639152,
    241003.9999587515,
    -55146.10647030385,
    2808.544464050810,
    };
  CEvalChebPoly *e = new CEvalChebPoly(65,0,0,c,
   427.1500000000000,322.8500000000000,
   5.633672284268541,0.9864009222618147,
   134.1827951500000,238.2071004500000,
   0.000000000000000,0.000000000000000);
  z = e->Eval(x,y);
  delete e;
  return z;
}

int eqn409::Roots(double fixed, double z, double *roots, int maxcnt, double
varlo, double varhi, int isvarx)
{
  int i,j,k=0;
  double v1,v2,vl,vh,vctr,dv,f,fmid,vmid,rt,vacc,delta;
  if(varlo==0.0 && varhi==0.0){
    vl=(isvarx)? XLo : YLo;
```

```
    vh=(isvarx)? XHi : YHi;
    }
  else{ vl=varlo; vh=varhi; }
  delta=(vh-vl)*0.01;
  for(i=0; i<100; i++){
    v1=vl+((double)i+1e-8)*delta;
    v2=vl+((double)(i+1)+1e-8)*delta;
    vctr=(v1+v2)*0.5;
    vacc=(vctr==0)?1e-8:fabs(1e-8*vctr);
    f=z-((isvarx)? Eval(v1,fixed) : Eval(fixed,v1));
    fmid=z-((isvarx)? Eval(v2,fixed) : Eval(fixed,v2));
    if(f*fmid >=0.0)
      continue;
    if(f<0.0){
      dv=v2-v1;
      rt=v1;
      }
    else{
      dv=v1-v2;
      rt=v2;
      }
    for(j=1; j<=100; j++){
      dv *= 0.5;
      vmid=rt+dv;
       fmid=z-((isvarx)? Eval(vmid,fixed) : Eval(fixed,vmid));
      if(fmid<=0)
        rt=vmid;
      if(fabsl(dv)<vacc || fmid==0.0){
        if(k<maxcnt)
          roots[k++]=rt;
        if(k==maxcnt) return k;
        break;
        }
      }
    }
  return k;
}

int eqn409::RootsX(double y, double z, double *xr, int maxcnt, double xlo,
double xhi)
{
  return Roots(y,z,xr,maxcnt,xlo,xhi,1);
}

int eqn409::RootsY(double x, double z, double *yr, int maxcnt, double ylo,
double yhi)
{
  return Roots(x,z,yr,maxcnt,ylo,yhi,0);
}
```

ERRATUM

Table 48 Incorrect or Suspect Experimental Data Values

		Raw Data	Raw Data	Raw Data	Raw Data	Raw Data	Reference	Chart Label
Model		Input	Input	Input				
Point	H100	V210	MWE	V100	SUS210	SUS100		
143	62.9	2.20	221	5.51	33.5	44	18	6
152	619.7	33.21	409	2689.75	157	12460	18	6
197	550.1	29.59	452	712.37	140.60	3300	5	8
216	-550.3	0.481	131.2	0.829			12	a
217	-440.4	0.459	142.5	1.012			12	a
219	-230.2	0.803	172.5	1.700			12	a

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Table 49 Reason Why Experimental Data is Incorrect or Suspect

Point[a]	Point[b]	Status	Reason	Description
143	2655	Suspect	Outlier	In plots of the H and F functions, the values for this point seemed to be an outlier. A review of the data did not show anything suspect and the data was not altered but used as given. It appeared as an outlier in the TC3D Simple 4 fit plot in Figure 38 and in Figure 39, it had a high residual.
152	2261	Incorrect	Typo	The SUS210 for the sample was reported as 15.7. The sample is part of a distillate series. The value is inconsistent with the data trend and the reported H210 value. It was changed to 157, which was consistent with the H210 value.
197	C61	Suspect	Outlier	A review of the data did not show anything suspect and the data was not altered. It appeared as an outlier in the TC3D Simple 4 fit plot in Figure 39 (point hidden) and in Figure 38 had a high residual.
216	221	Suspect	Outlier Transcription	The plot of an F function seemed to indicate this might be an outlier. The sample was part of a distillate cut series. The V210 data was not consistent with the data trend. The V210 values for this sample and sample 221 in the may have been switched and transcribed incorrectly. The data was not altered. This data is not encompassed by the ASTM chart.
217	223	Suspect	Transcription	See point number 216.
219	228	Incorrect	Typographical Error	The value of V100 was reported as 17.00. This sample is part of a distillate series. The value is inconsistent with the other values of the series and with V210 viscosity reported for the sample. It was changed to 1.700.
a Point numbers in this paper				
b Sample number in referenced paper				

GLOSSARY

Item	Description
*	In equations indicate multiplication

Item	Description
#	A number
#OoB	Out of bounds, error code returned by Excel VBA molecular weight calculation function MW(V1,V2)
(a)	Parenthesis surrounding lower case English alphabetic glyph(s) refer to a calculation or programming line with a as an example.
[#'s]	A number in a bracket references an equation
{#'s}	A number in a brace references an equation in the viscosity conversion calculation for cSt to SUS
°C	Temperature in degrees Celsius
°F	Temperature in degrees Fahrenheit
ASCII	American Standard Code for Information Interchange character encoding
ASTM	American Society for Testing and Materials
BMD	Biomedical Computer Programs were statistical programs from the UCLA Health Sciences Computer Facility
C#'s	A model coefficient, where # is an integer number
C(#'s)	A model coefficient, where # is an integer number
C++	C Plus Plus programming language
Calc.	Calculation
C-H	The difference between Hirschler data used to make the ASTM chart and that read from the chart
COS	Trigonometric cosine function
CPP	C Plus Plus programming language
CR	Carriage return ASCII computer character to go the beginning of a line
Cryo.	Cryoscopic is a method to determine MW by freezing point depression of a solvent.
cSt	Centistokes, unit cm/s, centimeter/second
DEFINT	GW-BASIC type code to define numeric variable as an integer
DEFSNG	GW-BASIC type code to define numeric variable as single precision
DF	Degrees of freedom
Diff.	Difference
DIM	GW-BASIC reserved word used to dimension and array
DOE	Design of experiments is a branch of statistics to plan and analysis experimental data
e	Euler's constant 2.71828
Ebul.	Ebullioscopic is a method to determine MW by boiling point elevation of a solvent.
Eqn.	Equation
Exp.	Experimental
F1	=(Ln(Ln(V100+#)), where # is a number

Item	Description
F12	=Ln(F1-#*F2-#), where # is a number and each # may be different
F2	=(Ln(Ln(V100+#)), where # is a number
F-ratio	It is a statistical measure of how much of the variation in data can be explained by a model.
g/mole	Molecular weight
GND	Generalized Normal Distribution
GW-BASIC	Beginners All-purpose Symbolic Instruction Code language by Microsoft
H	H function without a temperature reference like H100
H100	=870*(Log(Log(V100+0.6))+154
H12	H function that is a combination of the H100 and H210 functions.
H210	=870*(Log(Log(V210+0.6))+154
H_t	H function at temperature t.
invH_t	Inverse H_t function that calculates the viscosity in cSt at temperature t from H_t
InvSUS	Calculation to convert cSt to SUS
Isostoke	Line of constant viscosity
LB	Left boundary of ASTM D2502 chart
LF	Line Feed ASCII computer character to go the next line
Ln	Logarithmic function to the base ***e***, use in Excel worksheets
Log	Logarithmic function to the base 10, used in Excel worksheets
LOG	Logarithmic function to the base ***e***, used in GW-Basic and Excel VBA
Max	Maximum
MGND	Modified General Normal Distribution
Mid.	Middle, values in the middle between the high and low values
Min.	Minimum
MLR	Multiple linear regression
MW	Molecular weight on ASTM D2502 chart
MW0	Molecular weight from polynomial fit of F1, F2 and F12
MW1	Molecular weight correction calculated from the first elliptic fit
MW2	Molecular weight correction calculated from the second elliptic fit
MWC	Molecular weight calculated from a model
MWE	Molecular weight determined experimentally
MWS	MW0 scaled by dividing by 100
NaN	Not at number
NC	No check, A switch used by Excel VBA molecular weight calculation function MW(V1,V2) to bypass checking the validity of the input viscosities
NLLSQ	Non-Linear Least Squares GW-Basic program
No.	Number
O	Origin point on a figure
OT	Origin translated to a new point on the graph

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Item	Description
p.	Page
p1	Viscosity in cSt at the lower temperature used in function VisAtTC
p2	Lower temperature in °C used in function VisAtTC
p3	Viscosity in cSt at the higher temperature used in function VisAtTC
p4	Higher temperature in °C used in function VisAtTC
p5	Temperature in °C at which the viscosity in cSt is wanted from function VisAtTC
P1	Point 1 on a figure
PC	Personal Computer
PCA	Principle Component Analysis, a statistical procedure for modeling data by reducing the dimensionality
pp.	Pages
r	Pearson's r is a statistic that measures the linear correlation between 2 variables. It is called the coefficient of correlation and is the square root of R^2.
R^2	Coefficient of determination, A statistic that represents the proportion of the variance of the independent variable that is predictable from the independent variable(s).
RB	Right boundary of ASTM D2502 chart
Ref.	Reference
Refit	It is the process of fitting the model coefficients again after a change in data.
SAE20	Designation of a petroleum oil with a viscosity of 5.6 to <9.3 cSt at 100°C by the Society of Automotive Engineers
SAE40	Designation of a petroleum oil with a viscosity of12.5 to <16.3cSt at 100°C by the Society of Automotive Engineers
SD	Standard deviation
SG	Sign of a number
SG1	Sign of the first of two elliptic contours
SG2	Sign of the second of two elliptic contours
SIN	Trigonometric sin function
Sqrt	Square root
S_r	Repeatability standard deviation inferred from repeatability in ASTM D2502
S_R	Reproducibility standard deviation inferred from reproducibility in ASTM D2502
SS	Sum of squares, the summation of square of the residuals
SUS	Saybolt Universal Seconds, unit seconds
SUS100	Saybolt Universal Seconds at 100°F, unit seconds
SUS210	Saybolt Universal Seconds at 210°F
T, t	Temperature
TAN	Trigonometric tangent function

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Item	Description
TC2D	Table Curve 2D line regression program by Systat Software
TC3D	Table Curve 3D surface regression program Systat Software
V1	Kinematic viscosity in cSt at 100°F
V100	Kinematic viscosity in cSt at 100°F
V100C	Kinematic viscosity in cSt at 100°C
V2	Kinematic viscosity in cSt at 210°F
V210	Kinematic viscosity in cSt at 210°F
V40C	Kinematic viscosity in cSt at 40°C
VBA	Visual Basic for Application, Microsoft Office programming language
Ver.	Version
VisAtTC	Viscosity at Temperature C
Vol.	Volume
vs.	Versus
VSF	Viscosity Slope Function equation [5]
V_t	Viscosity at temperature t

REFERENCES - EXTERNAL LINKS AND CITATIONS

[1] https://www.astm.org/Standards/D2502.htm , *ASTM D2502. Standard Test Method for Estimation of Molecular Weight (Relative Molecular Mass) of Petroleum Oils From Viscosity Measurements* (ASTM Committee on Standards, Philadelphia, 1980), Annual Book of ASTM Standards, Vol. 05.03

[2] https://www.astm.org/Standards/D445.htm *ASTM D445-19a, Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (and Calculation of Dynamic Viscosity)*, Annual Book of ASTM Standards, Vol. 05.01

[3] The algorithm calculation syntax is GW-BASIC (https://hwiegman.home.xs4all.nl/gw-man/index.html) syntax for variables https://hwiegman.home.xs4all.nl/gw-man/index.html (a letter followed with up to a mix of 39 letters and/or #(s)) and reserved word function (SIN, COS, TAN, IF, THEN ELSE). The coefficient use the array syntax C(#). GW-BASIC's LOG function is base *e*. "#" is a numerical integer digit.

[4] Hirschler, A. E., "Molecular weights of viscous hydrocarbon oils: correlation of density with viscosity," J. Inst. Petrol. Tech., Vol. 32 pp.133-161, 1949

[5] T. G. Bell and L. H. Sharp, Oil Gas J. 32, 13 (1933).

[6] It is based on a simplex optimization. Validation used several functions described by Himmelblau, D. M., Applied Nonlinear Programming, McGraw-Hill, Inc., 1972 p. 195 run on an IBM PC. See endnote **Error! Bookmark not defined.** for more information on the method. It is not Dantzig's simplex for linear optimization of resource allocation.

[7] http://www.scholarpedia.org/article/Nelder-Mead_algorithm
https://en.wikipedia.org/wiki/Nelder%E2%80%93Mead_method
Walters F. H., Parker, Jr. L. R., Morgan S. L., and Deming S. N., (1991) *Sequential Simplex Optimization*, CRC Press, Chapter 4 pages 76-95
Nelder, J. A., and Mead, R. "A simplex method for function minimization," The Computer Journal, vol. 7, pp. 308-313, 1965
Other names for it are Nelder-Mead, modified sequential simplex, downhill simple, amoeba, polytope or variable size simplex method. Super modified simplex methods are extensions of the Nelder-Mead method.

---

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[9] GE Mark III Information Service regression program Stat II
[10] BMD Biomedical Computer Programs forward stepwise regression program BMD-07R
[11] https://systatsoftware.com/products/tablecurve-3d/ Table Curve 3D fits a selective subset of 36,000 surface equations out of 453,697,387 built in and user defined equations.
[12] https://en.wikipedia.org/wiki/Saybolt_universal_viscosity; https://www.astm.org/Standards/D2161.htm
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https://nvlpubs.nist.gov/nistpubs/jres/14/jresv14n3p345_A1b.pdf Mair, B. J., National Bureau of Standards, Vol 14, Research Paper RP772,"An Accurate Ebullioscopic Method for Determining the Molecular Weights of Nonvolatile Petroleum Fractions", March 1935
https://en.wikipedia.org/wiki/Cryoscopic_constant
Findlay, A., "Practical Physical Chemistry", Longmans, 1925
https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Book%3A_Physical_Methods_in_Chemistry_and_Nano_Science_(Barron)/02%3A_Physical_and_Thermal_Analysis/2.02%3A_Molecular_Weight_Determination
[14] J. A. Maroto, and F. J. de las Nieves, Computational Aids for the Estimation of the Molecular Weight of Petroleum Oils from Kinematic Viscosity Measurements, Petroleum Chemistry, 2007, Vol. 47, No. 2, pp. 87–91.
[15] J. Wei, "Least Square Fitting of an Elephant," *CHEMTECH*, **5**(2), 1975 pp. 128–129
[16] Runge's phenomenon https://en.wikipedia.org/wiki/Runge%27s_phenomenon
[17] https://asq.org/quality-resources/design-of-experiments, https://en.wikipedia.org/wiki/Design_of_experiments
[18] Hendrix C., "Through the response surface with test tube and pipe wrench", Chemtech August 1980 pages 488-497. Sequential simplex is for continuous variables. When used for formulations, it causes the total amount to change and therefore the percentages. This violates the mixture constraint for the DOE for mixtures. A modified version will work. In the modification, mixture constrained vertices are calculated, a number vertex trials equal to simplex dimensions (number of components is chosen (researcher option, D-optimal or other method) and these are used in the sequential simplex. Any trial that has a component <0 or >100 to the formulation boundaries is infeasible. The level can be set at the boundary for that component. If more constrained vertices are used than the simplex dimension, the reflection of the worst point through the centroid can actually be inside the constrained simplex vertices and the procedure will fail. If edge, face or centroid trails are selected, they could give set of collinear trials and fail.
[19] http://www.pearsoned.ca/highered/divisions/text/trim/data/additional/trim_4e_sec9.7.pdf equation 9.38
[20] https://pdfs.semanticscholar.org/71a0/64185e081401a137e0c2a9d08fe923bbd9ce.pdf Maters Thesis Dept. of Mathematics, "Multivariate Skew-Normal Distributions and their Extremal Properties", Rolf Waeber, Feb. 8.2008 Swiss Federal Institute of technology Zurich, Supervisor: Prof. Dr. Paul Embrechts,. Univariate distribution discussed in section 2.2.2 page12 and multivariate in section 3.11 page 45 with contour plots on pages 46 and 47. Y. Ma and M. G. Genton (2004): Flexible class of skew-symmetric distributions. Scandinavian Journal of Statistics 31:459–468
[21] http://www3.stat.sinica.edu.tw/statistica/oldpdf/A14n416.pdf J. Wang, J. Boyer and M. G. Genton (2004): A skew-symmetric representation of multivariate distributions. Statistica Sinica 14:1259–1270
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[24] https://en.wikipedia.org/wiki/Horner%27s_method Note: what was used was not the Horner method of finding polynomial roots but Horner's method of nesting the polynomial for calculation.
[25] Walther, C. 1931. The Evaluation of Viscosity Data. *Erdol Teer* **7:** 382–384
[26] https://en.wikipedia.org/wiki/Chebyshev_polynomials This polynomial is used to smooth the data and is continuous. The bivariate form makes a surface.

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[27] Ibid. 4, 158, TableXI, Data Necessary for Construction of Viscosity-Molecular Weight Correlation of Figures 1 and 6.

[28] https://en.wikipedia.org/wiki/Substitute_character "It is also used as an escape sequence in some programming languages."

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[30] Wright, Wortley Andrew, Journal of Materials, JMLSA (1969), vol. 4.11 pp. 1927

[31] https://www.imkt.uni-hannover.de/uploads/tx_tkpublikationen/Bader_diss.pdf, Norbert Fritz Bader, "Traction in EHL – Contacts – the influence of Local Fluid Rheology and Temperatures", Dissertation, Gottfried Wilhelm Leibniz University of Hanover, Mechanical Engineering, May, 2018, p. 34, equation 2.46

[32] https://www.astm.org/Standards/D341.htm, ASTM D341 "Standard Practice for Viscosity-Temperature Equations and Chars for Liquid Petroleum or Hydrocarbon Products", (ASTM Committee on Standards, Philadelphia), Annual Book of ASTM Standards, Vol. 05.01

[33] https://wiki.anton-paar.com/us-en/astm-d341-viscosity-temperature-extrapolation/

[34] https://www.paragon-sci.com/D341

[35] https://systatsoftware.com/products/tablecurve-2d/ Table Curve 2D fits 3,665 line and user defined equations.

[36] https://support.microsoft.com/en-us/office/change-formula-recalculation-iteration-or-precision-in-excel-73fc7dac-91cf-4d36-86e8-67124f6bcce4#:~:text=iterates%20a%20formula-,Click%20the%20File%20tab%2C%20click%20Options%2C%20and%20then%20click%20the,Enable%20iterative%20calculation%20check%20box.

[37] https://excelribbon.tips.net/T009748_Iterating_Circular_References.html

"It appears that the setting of the Enable Iterative Calculation check box is stored as part of a workbook, but it is not always paid attention to when the workbook is later loaded into Excel. In fact, the setting is ignored completely if any of the following occur before you open the workbook:

- You open any other workbook besides the default workbook created when you first start Excel.
- You change the Iteration check box while the default workbook is displayed."

Code to turn it on every time a workbook is opened

```
Private Sub Workbook_Open()
    Application.Iteration = True
End Sub
```