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Hydrogen Sulfide Viscosity Modeling

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As regulations for emissions of carbon dioxide and hydrogen sulfide into the atmosphere are becoming stricter and the penalty for violation increases, new and economical ways of reducing these emissions are becoming increasingly important to everyday operations. One promising sequestering option is the injection of acid gas mixtures into formations for disposal/storage. During the design of these acid gas injection schemes a comprehensive knowledge of the thermo-physical properties is of utmost importance in determining the feasibility and size of these operations. Recently, the friction theory (f-theory) for viscosity modeling has been shown to accurately determine the viscosity behavior of a wide range of petroleum fluid systems ranging from natural gases to heavy crude oils. This technique has also been shown to accurately model mixtures containing various concentrations of CO₂. However, in the development of the f-theory hydrogen sulfide was not explicitly studied and therefore needs to be accounted for to ensure it is accurately modeled. The development/validation of any modeling approach requires a thorough knowledge of the available data. With this in mind, an exhaustive collection of the data available in the literature has been performed revealing a very limited number of experimental points available in the open literature for the viscosity of pure H₂S and H₂S mixtures. Although limited data for pure H₂S exists in the literature, a critical evaluation of the data was performed and a reference viscosity model based on the generalized friction theory (f-theory) was developed. The developed reference viscosity model gives reasonable modeling results over the *T*-*η*-*P* surface for H₂S. The one parameter f-theory was also extended to include H₂S, and the model was shown to accurately reproduce existing experimental viscosities of hydrogen sulfide and its mixtures in ranges relevant to the natural gas and petroleum industry.

1. Introduction

Acid gas injection (AGI) is a widely used process for the disposal of mixtures of hydrogen sulfide and carbon dioxide. The acid gas is the byproduct of the sweetening process, which is used to remove H₂S and CO₂ from raw natural gas. Typically these AGI schemes are small scale (less than 5 MMSCFD or 140 × 10³ Sm³/d) and are for the disposal of the gas mixture. However some have used the acid gas as a miscible flood fluid or for pressure maintenance. In addition larger producers are considering acid gas injection as an option to the production of elemental sulfur.

Although basically the same, when compared to traditional schemes these large injection schemes pose some new problems. In the small injection schemes the pressure drop due to fluid flow in both the acid gas pipeline and the injection well are negligibly small. Thus, it is not necessary to have an accurate prediction of the viscosity. However for the large injection schemes the selection of the optimum pipeline and well diameter requires a more accurate calculation of the viscosity.

Accurate viscosity data are also useful for the estimation of the injection pressure. The viscosity is a key parameter for

modeling the flow of the fluid through the reservoir. Fortunately there is a plethora of data for the viscosity of carbon dioxide, which are useful for model building and testing. On the other hand, there is a dearth of data for the viscosity of hydrogen sulfide. Even worse, some of the available data are not accurate enough even for engineering purposes.

2. Literature Review

As accurate modeling techniques are data driven, the development of these models requires a thorough knowledge of existing literature data and the acquisition of new experimental measurements to fill the void of the existing data sets. There are few data for the viscosity of hydrogen sulfide and these data are scattered throughout the open literature and a complete databank containing a critical analysis of the published results has not been fully developed yet. Such a compilation is necessary for model development and will certainly benefit scientists and engineers working in this field. It is important to identify where additional data are needed to fill voids, resolve discrepancies of existing data sets and to extend regions where the physical properties (e.g., viscosity) are insufficiently modeled with the current techniques.

A comprehensive literature review revealed relatively few investigations into viscosity of hydrogen sulfide. A complete list of the data sets used in this investigation is presented in Table 1 indicating a limited number of the corresponding existing data sets; the bulk of the data is for gaseous H₂S at 1.013 bar and the saturation liquid. The remainder of H₂S *T*-*η*-*P*

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Table 1. Experimental Investigations of the Viscosity of Hydrogen Sulfide

investigators	year	no. of points	temperature (K)	pressure (bar)	method	fluid state	stated accuracy	references
Graham	1846	2 ^a	288.2	1.01	capillary	vapor	5% ^c	1
Steele et al.	1904, 1906	6	191.0–209.8	saturation	capillary	liquid	5% ^c , 0.5% ^b	2–4
Rankine and Smith	1921	2	290.2–373.2	1.01	capillary	vapor	3%, 2% ^b	5
Jung and Schmick	1930	1	290.4	1.01	capillary	vapor	5% ^c	6
Hennel and Krynicki	1959	8	261.7–323.2	saturation	capillary	liquid	4%	7
Pal and Barua	1967	5	306.7–483.2	1.01	oscillating disc	vapor	1%	8
Monteil et al.	1969	33	388.2–413.2	100–500	capillary	supercritical	3%	9
Pal and Bhattacharya	1969	3	298–373	1.01	oscillating disc	vapor	1%	10
Bhattacharya et al.	1970	5, smoothed	220.9–308	1.01	oscillating disc	vapor	0.6%	11
Bhattacharya	1970	4	238.2–308.2	1.01	oscillating disc	vapor	0.6%	12
Runnovskaya et al.	1970	smoothed equation	190.1–211.8	saturation	capillary	liquid	5% ^c	13
Nieto-Draghi et al.	2005	6	217.2–333.2	saturation	MD simulation	liquid	10–15%	14
Nieto-Draghi et al.	2005	4	243–333.2	saturation	MD simulation	vapor	10–20%	14

^a Kaye and Laby¹⁵ and Andrussow et al.¹⁶ report Graham's data at two different temperatures (273.2 and 293.2 K). Joshi and Saxena¹⁷ report the two data points at 273.2 K. ^b Estimated. ^c Not given; estimated to be 5%.

surface is not well represented and no consistent effort has been made to fill the voids. Most of the experimental work was performed in the 1960s and 1970s after which no further measurements appear to have been carried out.

After an extensive examination of all the data, the data sets of Steele et al.^{2–4} and Monteil et al.⁹ could not be considered as primary and were excluded in the development of the reference H₂S viscosity f-theory model and the subsequent development of the one parameter form of the f-theory. These data exhibited inconsistencies with the rest of the data set, with results from molecular dynamics (MD) simulations,¹⁴ with corresponding

states reasoning based on carbon dioxide and ethane.¹⁹ Another consideration for the rejection of these two data sets was based on previous critical reviews into the groups equipment, measurements and accuracy.^{20,21} Additionally, Monteil et al.⁹ stated that their results cannot be used for theoretical treatment. Molecular dynamics simulation¹⁴ supports the results from Runnovskaya et al.¹³ and confirms the rejection of the data from Steele et al.^{2–4}

3. Friction Theory

The friction theory or f-theory for viscosity modeling has been developed based on friction concepts of classical mechanics and the van der Waals theory of fluids. The theory was originally developed on the basis that the van der Waals repulsive and attractive pressure terms, which can be obtained from simple cubic equation of states, could be connected to the Amonton-Coulomb friction law. This connection results in a residual viscosity term that is added to the dilute gas viscosity term to estimate the viscosity of fluids over a wide range of temperature and pressure conditions. As a result, this model has been shown to be widely versatile and accurate in the correlation and prediction of the viscosity of well-defined pure, binary and multicomponent systems^{19,22–27} and even complex reservoir fluid systems ranging from natural gases to heavy crude oils.^{28–32}

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The f-theory was originally applied to several widely used cubic equations of state (EoS) of the van der Waals type, such as the Soave-Redlich-Kwong (SRK) EoS³³ or the Peng–Robinson (PR) EoS,³⁴ as well as to the PC-SAFT EoS,^{35–37} a noncubic EoS consisting of separate repulsion and attraction terms. However, in a recent work,¹⁹ the restriction of having to use an EoS constructed on an explicit separation between attractive and repulsive terms has been removed which allows for the application of the f-theory to practically all types of EoS. This has led to the possible use of highly accurate reference type EoS which would also result in highly accurate reference quality viscosity models. Consequently, the f-theory models presented in this work consist of two levels: level 1 relates to the development of a reference type f-theory model for H₂S as accurate as the available data and extended knowledge allows. Level 2 uses the developed reference model as a base for the derivation of the required scaling parameters inherent to the one-parameter f-theory model.²⁶ The one parameter f-theory is the basic model that has been extensively applied for the accurate description of reservoir fluids.

3.1. H₂S f-Theory Reference Model. Following the f-theory for viscosity modeling, the viscosity of a fluid can be separated into a dilute gas term, η_0 , and a residual friction term, η_f .

$$\eta = \eta_0 + \eta_f \quad (1)$$

According to the kinetic theory of Chapman and Engskog,³⁸ the dilute gas limit, η_0 , is due to particle kinematics, is only temperature dependent and it is most relevant for the gas phase. In previous f-theory related works the semiempirical predictive model of Chung et al.³⁹ which delivers a reasonable absolute

average deviation (AAPD) of around 1.5% for nonpolar compounds, has been extensively used for the calculation of η_0 . However, in the derivation of the H₂S viscosity reference model, a simple yet accurate empirical equation for η_0 ,¹⁹ was used in this work

$$\eta_0 = d_0 + d_1 T_r^{1/4} + d_2 T_r^{1/2} + d_3 T_r^{3/4} \quad (2)$$

where T is the reduced temperature ($T_r = T/T_c$). The values of the coefficients in eq 2 have been obtained by regressing all of the available low-pressure H₂S data in combination with a first order f-theory model. Unfortunately, the accuracy of the raw experimental data does not allow for high accuracy in the dilute gas model and therefore the best derived results corresponds to values for the coefficients of $d_0 = 4.36694 \times 10^{-2}$, $d_1 = -0.121530$, $d_2 = 9.35279 \times 10^{-2}$ and $d_3 = 0$, with units of mPa·s. The accuracy of the model is of only around 1.25% for the dilute gas limit.

For the derivation of the friction theory, a quadratic f-theory model,¹⁹

$$\eta = \eta_0 + \kappa_i P_{id} + \kappa_r \Delta P_r + \kappa_a P_a + \kappa_{ii} P_{id}^2 + \kappa_{rr} \Delta P_r^2 + \kappa_{aa} \Delta P_a^2 \quad (3)$$

was used in combination with the short Span-Wagner H₂S EoS recently published by Lemmon and Span.⁴⁰ Following the generalization f-theory work by Quiñones-Cisneros and Deiters,¹⁹ the pressure terms in eq 3 were related to the internal pressure (π_T) according to the following expressions:

$$P_r = T(\partial P / \partial T)_v \quad (4)$$

$$P_a = P - P_r = -\pi_T \quad (5)$$

and

$$P_r = P_{id} + \Delta P_r \quad (6)$$

where ΔP_r is a residual of the repulsive term after subtracting the ideal pressure term from P_r . Finally, the temperature dependencies of the friction constants in eq 3, were based on previously proposed equations:¹⁹

$$\kappa_a = (a_0 + a_1 \psi_1 + a_2 \psi_2) \Gamma \quad (7)$$

$$\kappa_{aa} = (A_0 + A_1 \psi_1 + A_2 \psi_2) \Gamma^3 \quad (8)$$

$$\kappa_r = (b_0 + b_1 \psi_1 + b_2 \psi_2) \Gamma \quad (9)$$

$$\kappa_{rr} = (B_0 + B_1 \psi_1 + B_2 \psi_2) \Gamma^3 \quad (10)$$

$$\kappa_i = (c_0 + c_1 \psi_1 + c_2 f(\Gamma)) \Gamma \quad (11)$$

$$\kappa_{ii} = (C_0 + C_1 \psi_1 + C_2 \psi_2) \Gamma^3 \quad (12)$$

where

$$\psi_1 = \exp(\Gamma) - 1 \quad (13)$$

$$\psi_2 = \exp(\Gamma^2) - 1 \quad (14)$$

$$\Gamma = \frac{T_c}{T} \quad (15)$$

The model given by eq 3 along with the proposed temperature parametrization is highly accurate but also sensitive and requires a good data set to be regressed against for optimal performance. Based on this, the proposed f-theory model can be used for the derivation of reference quality models with very low uncertainties.¹⁹ However, the lack of reliable H₂S data is a major

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limitation in this case since, as discussed in the previous section, outside of the coexistence liquid and the low-pressure vapor regions there are no reliable H₂S viscosity measurements.

Nevertheless, the situation is not as grim as it may at first glance appear. Quiñones-Cisneros and Deiters¹⁹ have pointed out that the proposed approach strongly relies on the physics already built into the EoS which is at the core of the f-theory model. In fact, it has been shown that the f-theory models can reveal remarkable and different viscosity behavior as a sole direct consequence of the physics already included in the EoS. Therefore, the underlying claim of the general friction theory for H₂S is that the basic physics of this compound should be delivered by the Lemmon and Span EoS.⁴⁰ With this assumption, it is reasonable to presuppose that the available liquid and low-density data should suffice for the development of at least a reasonable first order f-theory model. It is also important to remark that even with the limited amount of experimental data, the existing liquid and vapor/gas data cover a wide range of temperature and this information is sufficient to anchor, in a reasonable way, the basic temperature performance of the model. As such, the generalized f-theory model should be capable of delivering a reasonable performance up to moderate pressures, i.e., up to around 100 bar.

In the range of temperatures from close to the triple point to 600 K and pressures up to 100 bar, a first order f-theory model should perform with an uncertainty consistent with that of the available data. For such a model, the major weak point should not be the extrapolated compressed region, where the EoS is expected to provide the correct trend, but rather the low density region where the actual contribution from the friction model becomes negligible. The low-pressure data is basically limited to measurements at 1.013 bar and the available data at these conditions are not of enough accuracy to derive a reference quality model (with uncertainties of the order of 0.2%) for either the dilute gas limit or for the initial viscosity density dependency (i.e., the second virial viscosity coefficient) of the model. Nevertheless, in the low-density region the viscosity is not expected to have large variations and the actual uncertainty in this region should be consistent with that of the available data and, therefore, could be expected to be around 1–3%. The exception will be a small region corresponding to the low-density critical region where the deviations could be as large as 10–15%. Naturally, this excludes the actual critical point where the viscosity is expected to weakly diverge.

In spite of the absence of experimental low-pressure viscosity data, it could be argued that the overall quantitative contribution of the low-density region to the uncertainty of the model is not significant. However, its theoretical and, therefore, qualitative performance should be addressed. The dilute gas limit model, eq 2, was derived by a direct regression of the available low-density region data. In this region, polarity becomes quite relevant as it may induce a flat, or even decreasing initial density dependency of the fluid's viscosity. The region which is most of a concern corresponds to temperatures above 300 K; below this temperature the vapor branch of the phase envelope will occur before any potentially large deviation, due to an incorrect initial density dependency, may become relevant. However, the largest region of modeling uncertainty, due to the initial density dependency, occurs around the critical temperature, where the fluid goes (continuously) from a low-density state to a compressed state with a steep slope. In this region the viscosity of the fluid strongly depends on the initial slope of the density dependency and this is even more the case due to the fact that H₂S has a particularly high critical pressure. The initial density

dependency is related to the polarity as phenomena such as association has a direct influence on the effective collision area which is considered in the kinematics theory.³⁸ H₂S is slightly polar and therefore it is likely to have an initial density viscosity behavior qualitatively similar to other slightly polar molecules.

For the dense region, even though a first order model regressed against the available data should result in a reasonable performance up to moderate pressures, the final objective of this work is a model relevant to reservoir applications (high temperatures and pressures). Reservoir conditions can be as high as 1000 bar, or even higher, and for such conditions a second order model is required. Unfortunately, the available data are definitely insufficient for stable regression of the second order terms in eq 3. Nevertheless, the high-pressure viscosity performance is most sensitive to molecular structure and therefore, for substances having simple molecular structures, the high-pressure viscosity performance may qualitatively resemble that of other substances with similar acentric factors (this would definitely not apply to molecules with structures containing branching, aromatic rings, etc.).

In summary, in order to “guide” the regression of a second order model into a stable performance for the initial density dependency region and into the high pressure region, two well-known and well-characterized reference fluids, one slightly polar and another of similar acentric factor, were chosen. For the initial density dependency region the chosen fluid was carbon dioxide and for the high-pressure region ethane was chosen. As such, the H₂S reference model was fundamentally developed based upon the reliable experimental H₂S data and, for stability purposes, the combination of low pressure scaled CO₂ data and elevated pressure scaled C₂H₆ data. In this case, the CO₂ and C₂H₆ viscosity data were calculated from reference models¹⁹ at relevant conditions.

The cited models CO₂ and C₂H₆ as well as the EoS (Lemmon et al.⁴⁰) used here are all classical models, i.e., of an analytical nature showing any kind of critical anomalies, and therefore a convenient scaling parameter is the estimated residual viscosity, η_f , evaluated at the critical point. The scaling procedure was performed as follows: (1) low-density CO₂ and dense C₂H₆ data were reduced by using their estimated η_f critical values and (2) the data was then scaled up using the η_f critical value predicted from the model. Necessarily, step 2 was iteratively carried out until a smooth blending of the scaled data with the available primary data was achieved. Then just enough of the additional data was supplemented in order for the final model to reproduce the H₂S primary data reasonably well as well as being able to extrapolate to the high pressure region in a stable manner and deliver a critical isotherm with a reasonable shape (i.e., with flatten initial density dependency). Although it is not possible to make any quantitative assertions about the model performance in the extended region, the model reproduces the extended database (H₂S database and supplemental scaled CO₂ and C₂H₆ data) with an absolute average percentage deviation (AAPD) of only 1.06% with a negligible bias of 0.03%. The very low bias indicates a well-balanced performance between the low-density and the dense phases. In addition, the statistics also reveals that the scaling process resulted in a smooth blending of the CO₂ and C₂H₆ data with the primary data. The derived second order f-theory H₂S reference model can therefore be considered a hybrid corresponding states model.

The resulting f-theory parameters for the H₂S f-theory reference model coupled with the H₂S Lemmon-Span⁴⁰ short form of the Span-Wagner EoS are reported in Table 2. Included in this table are the critical temperature, pressure and density

Table 2. Hydrogen Sulfide Reference Friction Theory Model Parameters

parameter	(mPa·s/bar)
a_0	5.46919×10^{-5}
a_1	-7.32295×10^{-6}
a_2	-7.35622×10^{-6}
b_0	4.56159×10^{-5}
b_1	-1.82572×10^{-5}
b_2	-6.59654×10^{-6}
c_0	-4.33882×10^{-6}
c_1	6.13716×10^{-6}
c_2	0
parameter	(mPa·s/bar ²)
A_0	6.67324×10^{-9}
A_1	-2.16365×10^{-9}
A_2	0
B_0	-1.53973×10^{-9}
B_1	2.17652×10^{-9}
B_2	0
C_0	3.54228×10^{-7}
C_1	-4.76258×10^{-8}
C_2	0
T_c	373.1 K
P_c	90.0 bar
ω	0.1005
ρ_c	347.3 kg/m ³
	(10.19 mol/dm ³)
MW	34.08088 kg/kmol
ΔT (K)	190–600
Max. P (bar)	1000
AAPD	1.06%
bias	0.03%

of hydrogen sulfide, required in the Lemmon and Span EoS, that were taken from the original reference.⁴⁰ The overall model performance is depicted in Figure 1 where the coexisting phase viscosity and some selected isobars are shown along with all of the available experimental and simulation data. In addition to the information depicted in Figure 1, Figure 2 compares the results delivered by the H₂S model with the NIST package of thermo-physical properties REFPROP 7,^{41,42} which can be considered a reference viscosity model in the field.

Figure 3 shows a performance comparison between the reference model derived in this work and a linear f-theory model regressed against only the primary data (i.e., no scaled data was used). For the regression of the depicted linear model only four constants were used (a_0 , a_1 , a_2 and b_0) in the mathematical form proposed in eqs (32) and (33) of the original f-theory work.²⁷ In spite of the intrinsic limitation that this linear model may have, Figure 3, clearly shows that up to 200 bar both models deliver a very similar compressed region performance. However, at low pressures and temperatures around the critical temperature it is evident the performance difference due to the initial density dependency, which in the case of the reference model follows from the scaled CO₂ data while for the linear model the regression is all prediction since there is no data to guide its performance in that region. It should also be pointed out that CO₂ has a high critical pressure and therefore its low-density physics is expected to be more consistent with H₂S than that of a substance such as ethane which has a relatively low critical

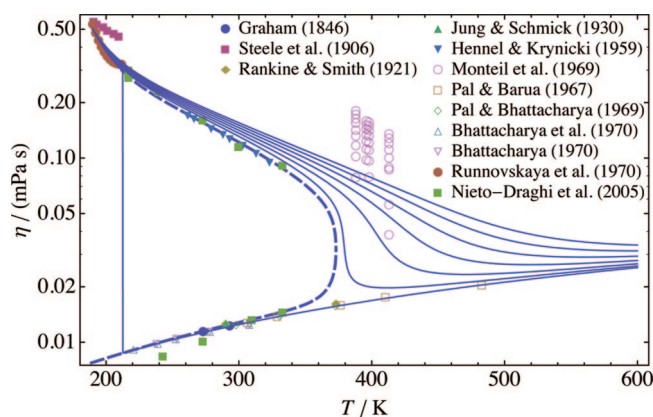


Figure 1. Reference H₂S viscosity model performance. Solid line: isobaric curves (1, 100, 150, 200, 250, 300, and 350 bar). Dashed line: equilibrium phase curves. The data shown corresponds to the following references: Hennel and Krynicki,⁷ Runnovskaya et al.,¹³ Steele et al.,^{2–4} Pal and Bhattacharya,¹⁰ Bhattacharya et al.,¹¹ Bhattacharya,¹² Pal and Barua,⁸ Rankine and Smith,⁵ Graham,¹ and Monteil et al.⁹ Molecular Dynamics Simulation: Nieto-Draghi.¹⁴

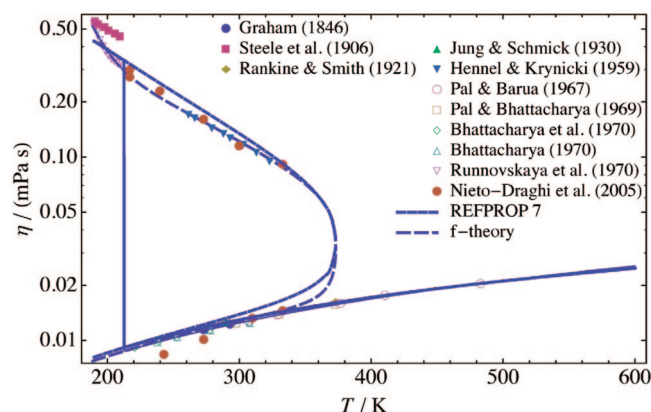


Figure 2. Reference H₂S viscosity model performance together with the model implemented in the NIST REFPROP 7 package for the coexistence viscosity curves and the 1.013 bar isobar. Closed circles: coexisting liquid and low pressure data (corresponding to pressures at or close to 1.013 bar).

pressure. In addition, it is relevant to remark that in the case of the linear model, the initial density performance follows from the ideal gas term in the EoS, this would normally result in a good performance for simple nonpolar molecules as has been shown in the original f-theory work.²⁷ However, in the case of polar molecules a corrective model for the initial density dependency, taking into account the association effects, must be included. Therefore, given the current lack of experimental or theoretical information, this correction has followed from using CO₂ as a reference fluid which is an assumption that will have to be reviewed in the future.

Figure 4 depicts the high-pressure performance of the reference model compared with the database (scaled and primary data) that was used for the regression. Although the accuracy of the model can certainly be argued, the derived model can also be categorized as a carefully guided regression with a clearly stable and rational performance. Furthermore, based on previous experience with the f-theory,¹⁹ it is assumed that the performance of the model is enhanced by the physics in the Lemmon and Span EoS.⁴⁰ Therefore, optimal performance is expected as a result of not only the regression but also by some degree of physics that may be revealed by the EoS found at the core model of the f-theory viscosity model. Consequently, it is underlined that the use of the model is recommended and not

(41) Lemmon, E. W.; McLinden, M. O.; Huber, M. L. *NIST Reference Fluid Thermodynamic and Transport Properties*, REFPROP 7, NIST Standard Reference Database 23; National Institute of Standards and Technology: Gaithersburg, MD, 2005.

(42) Lemmon, E. W.; McLinden, M. O.; Friend, D. G. *Thermophysical Properties of Fluid Systems. NIST Chemistry WebBook, NIST Standard Reference Database 69*; Linstrom, P. J., Mallard, W. G., Eds.; National Institute of Standards and Technology: Gaithersburg, MD, 2005.

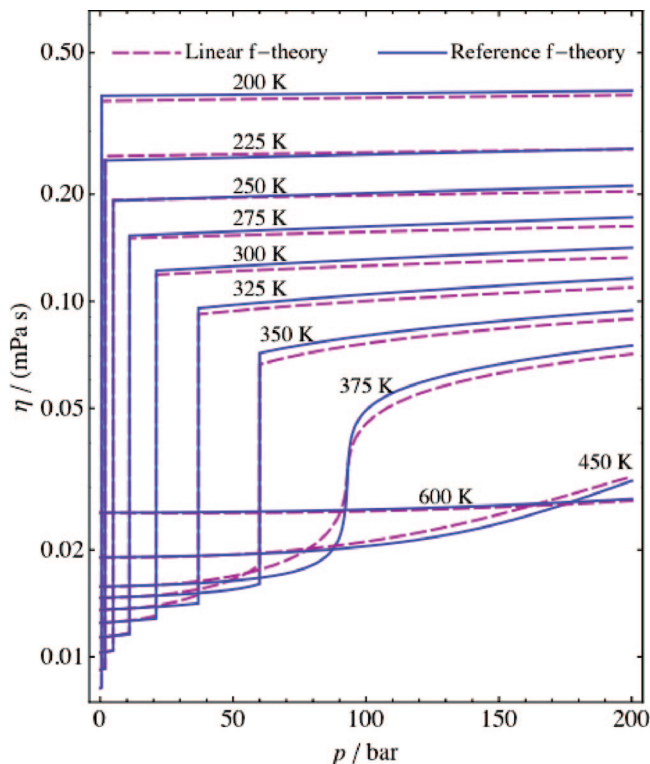


Figure 3. Comparison between a linear f-theory model regressed against solely the available primary data and the reference model regressed against the extended database.

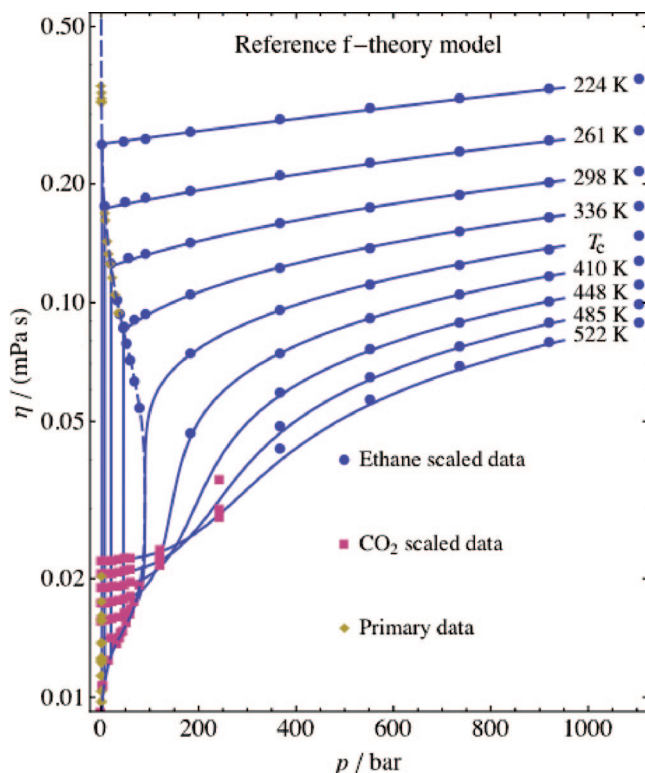


Figure 4. High-pressure performance of the reference f-theory H₂S model and comparison with the extended database used in the model's regression.

the supplementary regression database, which was only used to obtain a stable regression.

Clearly, the results obtained with the approach described above appear to be of good accuracy compared to the primary H₂S data (i.e., excluding the data of Steele et al. and Monteil et

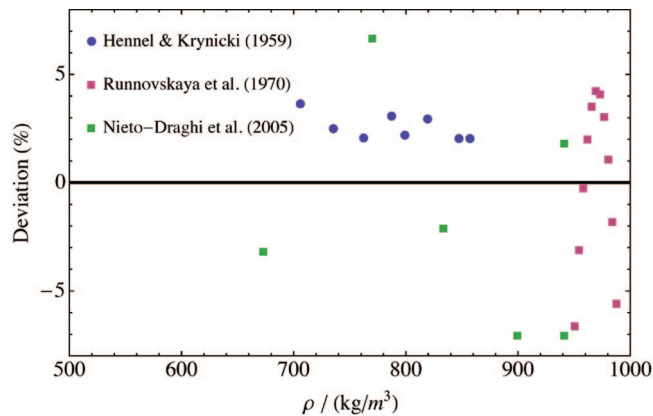


Figure 5. Deviations delivered by the f-theory reference model in relation to the dense primary data.

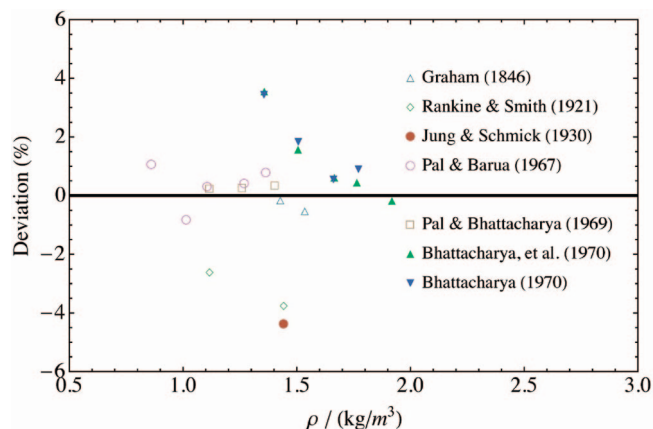


Figure 6. Deviations delivered by the f-theory reference model in relation to the low density primary data.

al.). The estimated deviations along the equilibrium curves and the low-pressure gas region (1.013 bar) are expected to be within $\pm 3\%$. The model also delivers a reasonably well-balanced extrapolation performance and a smooth performance in the critical region. Yet, as extrapolation is unavoidable, this must be taken with caution as at high pressures, such as 1000 bar, the isotherms may deviate up to $\pm 10\text{--}20\%$ in relation to what we consider the baseline. The model baseline corresponds to the agreement with the available liquid and gas phase data in the temperature range from close to the triple point to about 600 K. Figures 5 and 6 show, respectively, the achieved liquid and vapor/gas deviations with respect to the primary data.

Before closing this section it would be important to make some ending remarks regarding possible future improvements and limitations of the current model. A major shortcoming of the model is clearly the initial density dependency. Even though this may not have a great quantitative effect, it is a theoretical limitation that cannot be overlooked. Therefore, a major improvement for the reference model would unquestionable follow by the incorporation of a model for the second virial viscosity coefficient which could even follow from a theoretical approach.

The deviations from the experimental and molecular dynamics simulations for pure hydrogen sulfide obtained from the generalized f-theory model are presented in Table 3. Although excluded from the data set used to regress the parameters, the data from Steele et al. and Monteil et al. are presented in this table for comparison purposes. As previously discussed, these results indicate that the Steele et al. and Monteil et. al data are not consistent with the rest of the data set. The results from Nieto-Draghi et. al are also presented in Table 3. These data

Table 3. Comparison of the Predicted Viscosity with the Experimental and Molecular Dynamics Simulation Data

investigators	fluid state	BIAS %	AAPD %
Graham	vapor	−0.36	0.36
Rankine and Smith	vapor	−3.20	3.20
Jung and Schmick	vapor	−0.04	4.37
Pal and Barua	vapor	0.33	0.67
Pal and Bhattacharya	vapor	0.27	0.27
Bhattacharya et al.	vapor	1.19	1.26
Bhattacharya	vapor	1.67	1.67
Nieto-Draghi et al.	vapor ($P > 1$ bar)	9.60	9.60
Steele et al.	liquid	−22.3	22.3
Hennel and Krynicki	liquid	2.53	2.53
Runnovskaya et al.	liquid	0.03	3.21
Nieto-Draghi et al.	liquid	−1.85	4.66
Monteil et al.	supercritical	−41.6	41.6

Table 4. Comparison of the Predicted Viscosity with the Vapour Phase Molecular Dynamics Simulation Data

T (K)	P (bar)	η (mPa·s) ^{exp}	η (mPa·s) ^{calc}	AAPD %
243	3.75	8.33×10^{-3}	1.009×10^{-2}	21.1
273.15	10.26	1.004×10^{-2}	1.115×10^{-2}	14.5
310	26.7	1.312×10^{-2}	1.331×10^{-2}	1.5
333.15	42.7	1.443×10^{-2}	1.461×10^{-2}	1.3

were not included in the regression data set but rather used in a posteriori comparison with the reference friction theory model. As can be seen, the MD simulation data are in quite good agreement considering the estimated accuracy¹⁴ of the results. This is especially true in the liquid phase and for the vapor data greater than 300 K. The differences between the predictions and the vapor phase data below 300 K are still within Nieto-Draghi et al.'s estimated accuracy.

Although, this model has had no data to aid in the development of the initial viscosity density dependence, the MD simulation vapor data, at pressures greater than 1.013 bar were predicted with a surprisingly good agreement. This in spite of the fact that the data were expected to be in the region of poor performance concerning the initial density dependence. These results are compared with the MD simulations in Table 4 and are within their estimated accuracy (10–20%) when compared to other correlations. Unfortunately, no discussion or estimate of the statistical standard deviation or standard error arising from the MD simulations were presented by Nieto-Draghi et al.

A less severe limitation of the model is the high-pressure extrapolation. Although, some of the largest deviations may occur at the highest pressures, the model's high-pressure performance can be easily corrected when new reliable high-pressure data become available. This could even be inferred from sour gas mixture data and, therefore, a revision of the model may also be necessary a few years from now.

3.2. H₂S One Parameter f-theory Model. The development of the necessary H₂S scaling parameters inherent in the one-parameter f-theory models²⁶ is of relevance as such models have been shown to be capable of being able to accurately describe and even predict the viscosity of a wide variety of reservoir fluids under broad conditions³¹ in a very pragmatic manner. For that purpose, the general f-theory model described above has been used as a reference equation for the tuning of the one-parameter model. A detailed description of the f-theory one parameter viscosity modeling procedure is readily available²⁶ and only a brief summary will be given here.

For reservoir fluids applications the model of Chung et al.³⁹ provides sufficient accuracy and is recommended for the viscosity prediction of the dilute gas.

$$\eta_0 = 40.785 \frac{\sqrt{MWT}}{v_c^{2/3} \Omega^*} F_c \quad (16)$$

where the following empirical equation is used to estimate the reduced collision integral

$$\Omega^* = \frac{1.16145}{T^{*0.14874}} + \frac{0.52487}{\exp(0.77320T^*)} + \frac{2.16178}{\exp(2.43787T^*)} - 6.435 \times 10^{-4} T^{*0.14874} \sin(18.0323T^{*-0.76830} - 7.27371) \quad (17)$$

with

$$T^* = \frac{1.2593T}{T_c} \quad (18)$$

The F_c factor was empirically found to be

$$F_c = 1 - 0.2756\omega + 0.059035\mu_r^4 + \kappa \quad (19)$$

Here μ_r is a dimensionless dipole moment and κ is a hydrogen bonding correction factor. When nonpolar compounds are considered eq 19 reduces to

$$F_c = 1 - 0.2756\omega \quad (20)$$

For components without tabulated values of the critical volume, v_c , it can be obtained from the expression in Quiñones-Cisneros et al.,²⁸ which gives reasonable results for reservoir fluids applications.

The expression for the residual friction term in the one-parameter model is

$$\eta_f = \hat{\eta}_f \eta_c \quad (21)$$

where η_c represents the “one” characteristic viscosity scaling parameter.

The reduced friction term is made up of a contribution of a reduced repulsive and attractive contribution.

$$\hat{\eta}_f = \hat{\eta}_{f,r} + \hat{\eta}_{f,a} \quad (22)$$

where the attractive term is given by

$$\hat{\eta}_{f,a} = \kappa_a \left(\frac{P}{P_c} \right)^a \quad (23)$$

and the reduced term is given by

$$\hat{\eta}_{f,r} = \kappa_r \left(\frac{P_r}{P_c} \right) + \kappa_{rr} \left(\frac{P_r}{P_c} \right)^2 \quad (24)$$

The κ_a , κ_r and κ_{rr} parameters are only dependent on the reduced temperature and have been parametrized into 16 universal constants, which are scaled by the one η_c parameter, that are related to a specific EoS.²⁶ In this study, when the one parameter model was used, the original Peng–Robinson EoS, with the classical van der Waals mixing rules was used to model the PvT behavior of hydrogen sulfide and the sour gas fluids. The critical temperature, 373.53 K, critical pressure, 89.26 bar, and acentric factor, 0.0942, of hydrogen sulfide needed in the one parameter model were taken from the compilation of Rowley et al. (DIPPR).⁴³

For the sake of comparison, four other viscosity software packages were also used to model the viscosity of pure H₂S. These models were SUPERTRAPP, REFPROP 7, AQUAlibrium, and the correlations found in the DIPPR database.

SUPERTRAPP. SUPERTRAPP is a software package developed by NIST for the prediction of thermodynamic and transport properties of fluid mixtures. The software has been developed

for hydrocarbon mixtures, but nonhydrocarbon components found in natural gases are also included.⁴⁴

The SUPERTRAPP package, although based on the extended corresponding states principle uses a combination of pure component correlations for the calculation of the saturated liquid viscosity. The extended corresponding states principle for is used for the viscosity of mixtures.

NIST Chemistry Webbook - REFPROP 7. NIST has also developed a highly accurate software package for fluid thermodynamic and transport properties called REFPROP 7. This package uses the most accurate reference equations for the thermodynamic properties of pure fluid.^{41,42} Each substance has its own reference viscosity equation which has been evaluated by NIST.

AQUALibrium. AQUALibrium is a software package designed for predicting the phase equilibrium in acid gas mixtures, but is also applicable to sour and sweet gas systems. Recent versions of the software include predictions of the transport properties of the fluids using proprietary models.⁴⁵

DIPPR. The DIPPR database contains a number of empirical equations that can be used to determine the physical properties of pure component systems. The parameters for the DIPPR's equations are determined from the screened data found in the component's databank. The database contains a large number of components and equations for the viscosity of vapor phase (1.013 bar) and the saturation liquid phase both as functions of temperature.⁴³

The additional models tested here were ones that were available to the authors at the time and not selected, other than REFPROP 7, for a comprehensive review or test of all the potential modeling strategies for pure H₂S.

4. H₂S Viscosity Results

4.1. One Parameter f-Theory. In addition to the characteristic viscosity scaling parameter, the H₂S dilute gas term polarity and hydrogen bonding terms, of the Chung et al.³⁹ model requires estimation. Thus, the hydrogen bonding term in the Chung et al. model was optimally fit to dilute gas data calculated by the reference equation of state (eq 2). As can be seen in Figure 7, the one parameter f-theory reproduced the experimental data very well with the addition of the dipole moment term and the regressed hydrogen bonding correction factor term into the Chung et al. dilute gas viscosity model. The dipole moment of pure H₂S, 0.96835 Debye, was taken from the compilation of Rowley et al. (DIPPR).⁴³ The hydrogen bonding correction factor, κ , in eq 19 was determined to be 0.0539 with an AAPD of 2.1% and a bias of 0.06% for the experimental data set over a 410 K (186.6–596.6 K) temperature range.

Once the dilute limit was determined, the residual $T\eta$ - P surface was used to determine the critical scaling viscosity coefficient for hydrogen sulfide. For the sake of stability and consistency, the regression of the H₂S scaling parameter (η_c) was performed with a database constructed over a uniform mesh derived with the use of the reference viscosity equation over

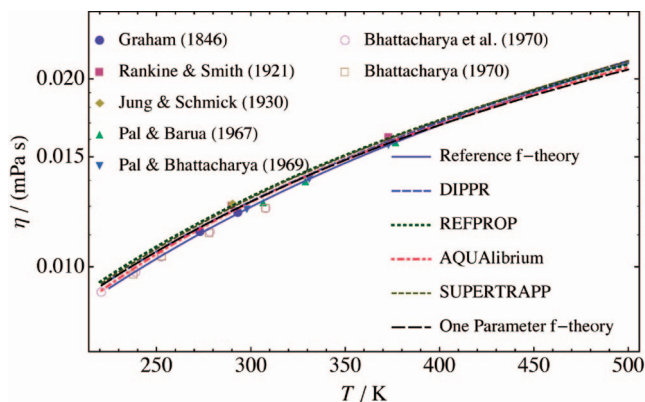


Figure 7. Comparison of the low-density H₂S viscosity calculated with several relevant models with the corresponding primary experimental data.

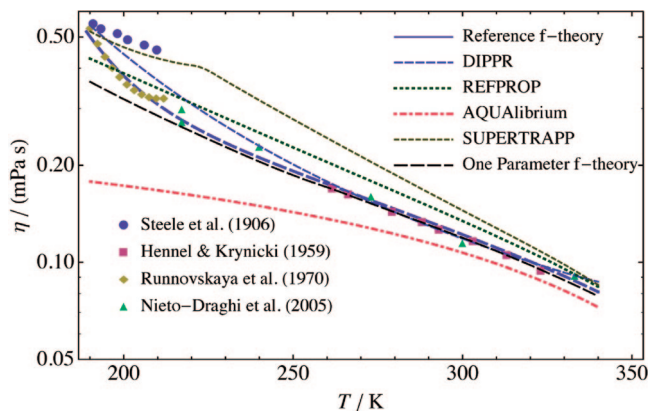


Figure 8. Comparison of the saturated liquid H₂S viscosity calculated with several relevant models with the corresponding primary experimental data.

reduced pressure intervals of 0.003–11.2 and reduced temperature intervals of 0.54 (200 K) to 1.6 (597 K). Again, this was done based on the assumption that the physics in the f-theory H₂S reference model not only follows from regression but also from the physics in the EoS (i.e., the physics originally considered by Lemmon and Span⁴⁰ in the development of the EoS). Therefore, by following this path we assume that the performance of the simpler one-parameter model will also be optimal. Thus, a characteristic viscosity scaling parameter, η_c , of 0.031799 mPa·s with an AAPD of 1.8% and a bias of 0.05% was found when compared to the reproduction of the data used in the regression. When compared to the primary data at temperatures greater than 200 K (i.e., excluding the MD simulations data, the data of Steele et al. and Monteil et al.) the one parameter model reproduce the primary data to within an AAPD of 3.8% and BIAS of –1.1%.

Overall, the one parameter model represents the saturation data reasonably well and the 1.013 bar gas viscosity very well. The results from the one parameter f-theory are compared to the experimental saturation data and the results from the reference viscosity equation in Figure 8. The deficiencies of the modeling approach at the low temperature region are expected as the one-parameter friction theory model was originally developed for fluids away from the triple point. Therefore, no attempt was made to force the one-parameter model to reproduce the data below 200 K, since the intrinsic mathematical structure of the model does provide for adequate performance at such low temperatures.

Figure 7 also shows the 1.013 bar gas viscosity determined from the DIPPR, AQUALibrium, SUPERTRAPP, and REF-

(43) Rowley, R. L.; Wilding, W. V.; Oscarson, J. L.; Yang, Y.; Zundel, N. A.; Daubert T. E.; Danner, R. P. *DIPPR Data Compilation of Pure Compound Properties*; Design Institute for Physical Properties, American Institute of Chemical Engineers: New York, NY, 2005.

(44) Huber, M. L. *NIST Thermophysical Properties of Hydrocarbon Mixtures Database. SUPERTRAPP 3.1, NIST Standard Reference Database 4*; National Institute of Standards and Technology: Gaithersburg, MD, 2003.

(45) Carroll, J. J. Gas Liquids Engineering Ltd., private communication, December, 2006.

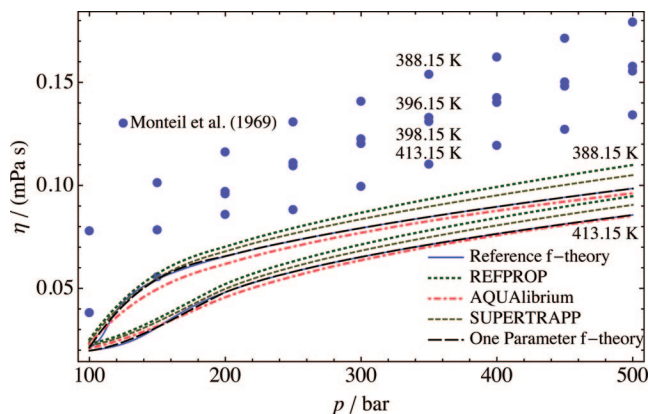


Figure 9. Comparison of the viscosity calculated with several relevant models (at the higher and lower temperatures of the data (388.15 and 413.15 K)) with the measurements of Monteil et al.⁹

PROP 7 models which are all quite similar in performance and compare well with that obtained from the viscosity reference equation for H₂S (generalized f-theory) and the one parameter f-theory.

The results from all the models vary significantly when the saturation liquid viscosity is considered. Figure 8 compares the experimental results with those obtained from the six viscosity modeling techniques. Results from molecular dynamics simulation¹⁴ are included in these plots and illustrate that the liquid viscosity data from Steele et al. are exceptionally high. AQUALibrium underestimates the liquid viscosity at all temperatures. DIPPR, SUPERTRAPP and REFPROP 7 tend to overestimate the viscosity at all temperatures, except at temperatures close to the triple point. The DIPPR correlation matches the higher temperature data better than these two models.

The f-theory reference equation reproduces the primary data of the liquid phase very well over essentially the full temperature range. The one parameter f-theory does a very good job of reproducing the temperature region above 200 K and it should not be considered applicable below this temperature. As previously discussed, the one parameter f-theory was developed at temperatures away from the triple point which results in its poor ability to capture the physics at temperatures near the triple point. In addition, it should be underlined that the Peng–Robinson EoS, which is the backbone of the one parameter f-theory model, performs poorly at capturing the physics of fluids near the triple point.

Despite, extending the model beyond its capabilities to the near triple point region, the one parameter model can reproduce the data to within 10% at a temperature of 200 K. No model, other than the viscosity reference equation captures the triple point region well (except for the DIPPR liquid viscosity correlation which is purely a data smoothing equation). Temperatures of this scale are rarely, if ever, experienced in the sour gas processing or acid gas injection industries and therefore the one-parameter f-theory model is fully applicable within the full range expected operating conditions.

As described earlier the supercritical data of Monteil et al.⁹ were rejected in the development of the reference equation. As can be seen in Figure 9, no model, not even the viscosity reference equation, can reproduce these data. For clarity sake, only the upper and lower isotherms from the models are presented in Figure 9. In contrast, it must also be underlined that, within reasonable ranges of uncertainty, all models

predictions are self-consistent for the supercritical region covered by Monteil et al.⁹

5. Sour Gas Viscosity Results

5.1. One Parameter f-theory: Unfortunately, there are also few H₂S mixture experimental viscosity data points relevant to the gas processing industry available in the open literature. In fact the amount of mixture data is significantly less than that for pure H₂S. A comprehensive literature review revealed only one experimental source of data.^{46,47} The databank used in these references contains a large number of data for reservoir fluids, however only eight viscosity data points of samples containing H₂S are available. The H₂S content of these fluids ranges from 0.02 to 70.03 mol %. The temperatures and pressures appear to be at reservoir conditions; however, no further information including experimental method or accuracy is given. The identification numbers of the fluids tested were Koc46, Koc59, 1111, 1881, 2076, 84, 439, and 926.

As previously mentioned, the original version of the Peng–Robinson EoS was used in combination with the one parameter f-theory. The critical temperatures, pressures and acentric factors of nitrogen, carbon dioxide hydrogen sulfide and the C₆– hydrocarbon components (methane - n-hexane) were taken from the compilation of Rowley et al. (DIPPR).⁴³ When a C₇₊ fraction was present in the mixture the critical temperature, critical pressure and acentric factor was determined with the supplied C₇₊ fraction molecular weight. The necessary equation of state parameters for the C₇₊ fraction was estimated using eqs 25–27, which are empirical correlations based the properties of normal alkanes.³¹

$$T_{c,i} = -423.587 + 210.152 \ln(MW_i) \quad (25)$$

$$P_{c,i} = f_c \exp(9.67283 - 4.05288 MW_i^{0.1}) \quad (26)$$

$$\omega_i = \exp\left(8.50471 - \frac{15.1665}{MW_i^{0.1}}\right) \quad (27)$$

In these three equations, MW is in g/mol in order to obtain T_c in K and P_c in bar. The parameter f_c in eq 26 represents a perturbation factor away from the f_c = 1 corresponding to n-alkanes. Typically, the perturbation parameter is iteratively modified (tuned) until the saturation pressure of the fluid of interest is matched³¹. Since, no saturation data was available, the f_c parameter could not be tuned and a f_c = 1 was used.

Since the C₇₊ composition was not significantly high, no attempts were made to split the C₇₊ fraction into smaller pseudocomponents.

The characteristic viscosity scaling parameter of the well-defined light compounds (i.e., methane, ethane, etc.) were taken from the tabulated values.²⁶ In the case of hydrogen sulfide, the characteristic viscosity scaling parameter, 0.031799 mPa·s determined in the previous section was used. When some of the lighter hydrocarbon compounds (up to C₆) were lumped together,^{28,31} the modified Ueyhara and Watson⁴⁸ correlation²⁸ was used

(46) Elsharkawy, A. M. Predicting the Properties of Sour Gases and Condensates: Equations of State and Empirical Correlations. Paper Presented at the SPE International Petroleum Conference and Exhibition held in Villahermosa, Mexico, February, 10–12, 2002; SPE 74369.

(47) Elsharkawy, A. M. Predicting Volumetric and Transport Properties of Sour Gases and Gas Condensates Using EOSs, Corresponding State Models, and Empirical Correlations. *Pet. Sci. Technol.* **2003**, *21*, 1759–1787.

(48) Ueyhara, O. A.; Watson, K. M. A Universal Viscosity Correlation. *Natl. Pet. News* **1944**, *36* (40), R-714–R-722.

$$\eta_c = 7.9483 \frac{\sqrt{MWP_c}^{2/3}}{T_c^{1/6}} \quad (28)$$

with the properties of the lumped groups. Without more than one viscosity data point to tune the critical scaling parameter, η_c , of the C₇₊ fraction to, the $\eta_{c,C7+}$ was assumed to be the value of that of the corresponding *n*-alkane determined with eq 28. Naturally the amount of C₇₊ fraction and the way it is characterized will affect the results, and the calculated viscosity could be significantly improved if the relaxed form of the Uyehara and Watson correlation²⁸ was used:

$$\eta_c = K_c \frac{\sqrt{MWP_c}^{2/3}}{T_c^{1/6}} \quad (29)$$

and the K_c parameter was adjusted until the available viscosity data was matched. Since there was only one data point available for each fluid the full viscosity characterization technique^{28,31} was not used. As such, the obtained results are predictions based on the pure fluid component properties and the C₇₊ fraction properties determined with the techniques described above (i.e., $f_c = 1$ and $K_c = 7.9483$).

In this work, a variety of H₂S binary interaction parameters for the Peng–Robinson EoS were considered. H₂S binary interaction parameters were obtained from Carroll and Mather⁴⁹ or Stamataki and Magoules;⁵⁰ all other binary interaction parameters were taken from either Nagy and Shirkovskiy⁵¹ or Knapp and Doring.^{52,53} The combination of the binary interaction parameters from Knapp and Doring^{52,53} and Stamataki and Magoules⁵⁰ gave the best results in the viscosity and in the Z-factor^{46,47} (albeit slightly). Overall, the one parameter f-theory predicted the viscosity of these eight fluids to within 13.1%. The detailed results are presented in Table 5.

The predictions from the one parameter model are better than the models tested by Elsharkawy.⁴⁶ Some of the models tested by Elsharkawy included viscosity models only applicable to the gas phase. One significant advantage of the f-theory is that it can be used to model the viscosity of fluids ranging from dilute gases to dense heavy oils. This one equation applicable to the vapor and liquid phases, similar to an equation of state, ensures that there is no discontinuity in the T - η - P space. Based on the pure and sour gas mixture results, the inclusion of H₂S extends the one parameter f-theory model to sour systems.

The results are quite satisfactory despite the limited number of data points and the unascertained quality of the data. The viscosity of the high H₂S fluid was quite good, suggesting that this approach may be extended to acid gas injection schemes. Although more testing of the model is warranted when more data relevant to these schemes becomes available.

(49) Carroll, J. J.; Mather, A. E. A Generalized Correlation for the Peng–Robinson Interaction Coefficients for Paraffin–Hydrogen Sulfide Binary Systems. *Fluid Phase Equilib.* **1995**, *105*, 221–228.

(50) Stamataki, S.; Magoules, K. Prediction of Phase Equilibria and Volumetric Behavior of Fluids with High Concentration of Hydrogen Sulfide. *Oil Gas Sci. Technol.* **2000**, *55*, 511–522.

(51) Nagy, Z.; Shirkovskiy, A. Mathematical Simulation of Natural Gas Condensation Processes Using the Peng–Robinson Equation of State. Paper Presented at the 57th Annual Fall Technical Conference and Exhibition of the Society of Petroleum Engineers of AIME held in New Orleans, LA, on September 26–29, 1982; SPE 10982, 1982.

(52) Knapp, H.; Doring, R. Vapor–Liquid Equilibria for Mixtures of Low Boiling Substances. *DECHEMA Chemistry Data Series Part I - Binary Systems*; Berhens, D., Eckeman, R., Eds.; DECHEMA: Frankfurt am Main, Germany, 1986.

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Table 5. Comparison of the Predicted Viscosity of the Tested Sour Gas Mixtures

gas ID no. ⁴⁶	H ₂ S mol %	<i>T</i> (K)	<i>P</i> (bar)	η (mPa·s) ^{exp}	η (mPa·s) ^{calc}	AAPD %
Koc46	0.57	348.7	144.8	1.72×10^{-2}	1.72×10^{-2}	0.0
Koc59	0.02	388.7	179.2	1.91×10^{-2}	2.01×10^{-2}	5.2
1111	22.60	352.6	344.8	3.00×10^{-2}	3.00×10^{-2}	0.1
1881	49.37	322.0	172.4	3.00×10^{-2}	3.30×10^{-2}	10.0
2076	70.03	352.6	94.0	2.20×10^{-2}	2.04×10^{-2}	7.3
84	7.10	419.8	321.9	4.20×10^{-2}	3.71×10^{-2}	11.7
439	28.16	394.3	288.9	1.00×10^{-1}	6.04×10^{-2}	39.6
926	0.34	377.0	332.7	9.00×10^{-2}	6.24×10^{-2}	30.7

Table 6. Comparison of the Predicted Viscosity of the Tested Binary and Ternary Mixtures

gas ID no. ⁵⁴	H ₂ S mol %	<i>T</i> (K)	<i>P</i> (bar) ^a	η (mPa·s) ^{exp}	η (mPa·s) ^{calc}	AAPD % ^b
B1	40	350	1008	7.79×10^{-2}	7.83×10^{-2}	0.6
B2	60	350	441	6.21×10^{-2}	6.24×10^{-2}	0.5
T1	27	290	201	9.27×10^{-2}	9.42×10^{-2}	1.6
T1	27	290	744	1.482×10^{-1}	1.507×10^{-1}	1.7
T1	27	320	408	9.36×10^{-2}	9.44×10^{-2}	0.9
T1	27	320	1069	1.492×10^{-1}	1.483×10^{-1}	0.6
T1	27	350	601	9.34×10^{-2}	9.32×10^{-2}	0.2
T1	27	335	1247	1.481×10^{-1}	1.487×10^{-1}	0.4

^a Average pressure.⁵⁴ ^b Compared to the average viscosity.⁵⁴

Recently, molecular dynamics simulations for the viscosity of binary and ternary mixtures of H₂S with CH₄ and CO₂ have been performed.⁵⁴ The mixtures consisted of: B1 (40 mol % H₂S + 60 mol% CH₄), B2 (60 mol % H₂S + 40 mol% CH₄), and T1 (27 mol % H₂S + 63 mol% CO₂ + 10 mol% CH₄). These three mixtures are dense phase fluids (liquid like) at the conditions of the MD simulations. The results from the one parameter f-theory model are compared to the results of the numerical experiments in Table 6. As can be seen, the one parameter model predicted the viscosity of these mixtures to within an AAPD of 0.8%. Although these viscosity values are the results from molecular dynamics simulations, the results do supplement the sour gas viscosity database and appear to be consistent to those obtained from the one parameter model f-theory.

The molecular dynamics simulations viscosity results for pure H₂S and its mixtures definitely supplement the experimental results and agree well with those obtained from the f-theory and the trends of the experimental data set. However, more experimental data with supplemental MD simulations of these systems is necessary. The data, experimental and simulations should be compared at the same conditions and, initially, be compared to the database collected here. This will expand the data set for H₂S and its mixtures and to verify the existing experimental data which have been suggested to be inconsistent with the data set as a whole.

6. Conclusions and Recommendations

The optimal design of an acid gas injection scheme requires various physical properties. The viscosity is important in order to establish the optimum pipeline diameter for the transport of the acid gas from the compressor to the injection well and for

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the estimation of the pressure loss due to fluid friction in the well bore. This is especially true for the larger injection schemes. In addition, the viscosity is an important parameter for performing reservoir simulations.

As such, an exhaustive literature survey to obtain all the pure hydrogen sulfide viscosity data available was performed. All the published data was reviewed and the f-theory was successfully applied to obtain a H₂S reference viscosity model. Although, based on limited data, this model has a strong background and with the critical evaluation of the data and sound physical reasoning this model appears to deliver superior modeling results over the T - η - P surface for H₂S. This work was first presented at the 86th Annual Convention of the Gas Processors Association, March 11–14, San Antonio, Texas, U.S.A. (2007).⁵⁵ The model presented at the conference and in this work are the same and this model is now incorporated in REFPROP 8.⁵⁶

Results from the reference equation were then used to derive the scaling parameters used in the one-parameter f-theory models which have been shown to model the viscosity of a wide variety of reservoir fluids under broad conditions. When tested against the available sour gas experimental data, the predictions from the one-parameter model were quite satisfactory when compared to previous modeling investigations. When compared to the numerical experiments results of binary and ternary systems, the one parameter f-theory performed exceedingly well.

The literature review and the development of the H₂S reference viscosity model identified significant regions where additional data are needed to fill voids, resolve discrepancies of existing data sets and to extend regions where the viscosity may be insufficiently modeled with the current techniques. New experimental measurements or molecular dynamics simulations,

based on the findings are required to expand the data set, not only for pure H₂S but for mixtures necessary found in the sour gas treating and acid gas injection industries.

Increasing the available data for viscosity of hydrogen sulfide is only the starting point. The acid gas found in injection schemes is a mixture of H₂S, CO₂, light hydrocarbons, and water. It is the mixture properties that are important in the design of an optimum acid gas injection scheme. It should also be pointed out that the conditions (temperature and pressure) of the experiments should be at the relevant operating conditions found in industry.^{57–59} Pressures in acid gas injection schemes range from near atmospheric at the overhead of the solvent regenerator to up to 500 bar in the reservoir. Temperatures are rarely below 273 K and are a maximum of about 423 K. The composition of these acid gas systems can range from nearly pure H₂S to nearly pure CO₂. There is always a small amount of hydrocarbon present, but this is typically less than 5 mol%. Also the mixture always contains some water: the overhead of the solvent regenerator column is saturated with water. Experimental data of these mixtures are nonexistent in the literature and along with pure H₂S are needed at the conditions described above.

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