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AN IMPROVED ALGORITHM FOR CALCULATION OF THE NATURAL GAS COMPRESSIBILITY FACTOR VIA THE HALL YARBOROUGH EQUATION OF STATE

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- Shanks Transform

Abstract

A numerical computational method-Adomian Decomposition, is being used to find the compressibility factor of natural gases using The Hall Yarborough Equation of States. To provide faster convergence, Shanks transform is also being implemented. This method doesn't require any initial guess to approximate the final results unlike common methods such as the Newton Raphson method and thus is more advantageous and computationally efficient. The comparison of results and computation speeds have been provided for several cases. Comparisons have also been done against the compressibility factors obtained using the Standing and Katz compressibility factor chart (experimental) to determine the accuracy of above methods.

Introduction

Gas compressibility is quite an important parameter that is used in various calculations involving natural gases. To find this parameter, we can use the experimental methods. However, these methods are not efficient with regards to time and cost. Therefore, several empirical relations were developed to closely approximate the value of z-factor. These values are often very close to those observed in Standing-Katz chart of z-factor vs pseudo reduced pressure [7].
Some of these relations are as follows:

1. Papay Equation (1968)
2. Hankinson Thomsan Philips relationship (1969)
3. Hall-Yarborough Equation (1973)
4. Brill and Begg's correlation (1974)
5. Dranchuk Purvis Robinson Correlation (1974)

In this work, we will be using the Hall-Yarborough equation to find the z-factor for various cases. We will then be using several numerical methods (Newton-Raphson, Adomian Decomposition and Shanks Transformation) to solve the non-linear equation(12) that we encounter in the Hall-Yarborough method. We will show how the Newton-Raphson method depends on initial guess if we fix the number of iterative steps. We will also show that the Adomian Decomposition method (ADM) and Shanks Transformation on ADM are computationally efficient methods.

Problem-Formulation

ADM Method

The Adomian Decomposition Method (ADM) was developed by an American mathematician George Adomian. This method provides an accurate and computationally efficient solution for a large variety of problems, starting from system of linear and non-linear equations to non-linear integral and differential equations. It has a wide range of applications in many different fields. So here we have presented a brief review of this method[9].
Let us take a general differential equation:

$$Lu + Nu + Ru = g \tag{1}$$

Here L is a linear operator, N is a nonlinear operator and R is the remaining part. Let us denote the inverse operator of L as L^{-1}. Now, if we multiply this L^{-1} on both sides of equation(1) then we will get:

$$L^{-1}Lu + L^{-1}Nu + L^{-1}Ru = L^{-1}g \tag{2}$$

Let us take L to be an n-th order derivative operator. So, L^{-1} will become nth order integration operator Since Integration is inverse of differentiation. So, it can be concluded that $L^{-1}Lu = u + a$, where a is a constant which is present due to integration. By ADM, the solution of this equation would be of the form: $u = \sum_{n=0}^{\infty} u_n$. Since the solution is divided into many, possibly infinite parts therefore this is called a decomposition method. Taking u_0 as $L^{-1} - ga$, we get:

$$u = u_0 - L^{-1}Nu - L^{-1}Ru \tag{3}$$

Now by ADM, Nu decomposes to an infinite series of polynomials, known as Adomian Polynomials.(represented by A_n)

$$Nu = \sum_{n=0}^{\infty} A_n \tag{4}$$

$$A_n(u_0, u_1, ..., u_n) = \frac{1}{n!}\left[\frac{d^n}{d\lambda^n} N\left(\sum_{i=0}^{\infty} \lambda^i u_i\right)\right]_{\lambda=0} \tag{5}$$

The method through which we have calculated these Adomian polynomials is listed in [5]. So now, a recurring relation is set to calculate the solution terms:

$$u_{i+1} = -L^{-1}A_i - L^{-1}Ru_i \quad ; \quad i \geq 0 \tag{6}$$

We have used the Hall-Yarborough equation for finding Z-factor for various cases which contains these parameters:(t_r is reduced temperature, which is obtained as $\frac{1}{T_{pr}}$. T_{pr} is pseudo reduced temperature.)

$$A = 0.06125 t_r e^{-1.2(1-t_r)^2} \tag{7}$$

$$B = t_r(14.76 - 9.76t_r + 4.58t_r^2) \tag{8}$$

$$C = t_r(90.7 - 242.2t_r + 42.4t_r^2) \tag{9}$$

$$D = 2.18 + 2.82t_r \tag{10}$$

From these, the gas compressibility factor is calculated as:

$$Z = \frac{AP_{pr}}{Y} \tag{11}$$

Here Y is the reduced density. Y is calculated from the following equation:

$$f(Y) : \frac{Y+Y^2+Y^3-Y^4}{(1-Y)^3} - AP_{pr} - BY^2 + CY^D = 0 \tag{12}$$

In order to apply ADM to equation(12), we must first bring it to its canonical equivalent form:

$$\begin{aligned} Y &= -\tfrac{B}{3AP_{pr}+1}Y^5 + \tfrac{3B+1}{3AP_{pr}+1}Y^4 \\ &-\tfrac{AP_{pr}+3B+1}{3AP_{pr}+1}Y^3 + \tfrac{3AP_{pr}+B-1}{3AP_{pr}+1}Y^2 \\ &+\tfrac{C}{3AP_{pr}+1}Y^{D+3} - \tfrac{3C}{3AP_{pr}+1}Y^{D+2} \\ &+\tfrac{3C}{3AP_{pr}+1}Y^{D+1} - \tfrac{C}{3AP_{pr}+1}Y^D \\ &+\tfrac{AP_{pr}}{3AP_{pr}+1} \end{aligned} \tag{13}$$

From ADM now we can tell that the solution of this highly nonlinear equation will be computed as $Y = \sum_{i=0}^{\infty} Y_i$. Since summation upto infinite terms is not practically possible therefore, we will try to find an approximate solution to this equation $\tilde{Y}(n) = \sum_{i=0}^{n} Y_i$. Different components of the solution are calculated as:

$$\begin{aligned} Y_0 &= \tfrac{AP_{pr}}{3AP_{pr}+1}, \\ Y_{i+1} &= -\tfrac{B}{3AP_{pr}+1}\Theta_{(i,1)} + \tfrac{3B+1}{3AP_{pr}+1}\Theta_{(i,2)} \\ &-\tfrac{AP_{pr}+3B+1}{3AP_{pr}+1}\Theta_{(i,3)} + \tfrac{3AP_{pr}+B-1}{3AP_{pr}+1}\Theta_{(i,4)} \\ &+\tfrac{C}{3AP_{pr}+1}\Theta_{(i,5)} - \tfrac{3C}{3AP_{pr}+1}\Theta_{(i,6)} \\ &+\tfrac{3C}{3AP_{pr}+1}\Theta_{(i,7)} - \tfrac{C}{3AP_{pr}+1}\Theta_{(i,8)} \end{aligned} \tag{14}$$

Here $\Theta_{(i,1)}$ is used to denote the ith order Adomian polynomial. We have considered the general nonlinear term to be Y^x and used the general form of Adomian Polynomials for this nonlinear function[5].

Shanks Transformation

Shanks transformation was first derived by R.Schmidt in 1941, but it was Daniel Shanks who rediscovered this transformation. Thus, this transformation is named after Daniel Shanks. This transformation is a nonlinear transformation which increases the rate of convergence of any series. Let there be a sequence of number $\{U_n\}$. Then, Shanks transformation $Sh\{Un\}$ of a sequence $\{Un\}$ is defined as:

$$Sh(U_n) = \frac{U_{n+1}U_{n-1} - U_n^2}{U_{n+1} - 2U_n + U_{n-1}} \tag{15}$$

We can increase the rate of convergence by applying this Shanks transform more than once to a particular sequence. For example, $Sh^2(U_n) = Sh(Sh(U_n))$,$Sh^3(U_n) = Sh(Sh(Sh(U_n)))$ etc. If we combine both ADM and Shanks then we can achieve convergence really fast. For doing this, we can consider the $U_n = \tilde{Y}(n) = \sum_{i=0}^{n} Y_i$.

Newton Raphson Method

We have studied Newton Raphson method in class. For applying this method for solving equation(12), We consider equation(12) as f(Y) and

Table 1: Characteristics of the natural gases used in Examples 1, 2, and 3

Example 1	Example 2	Example 3
Temperature = 337.872 K	Temperature = 355.372 K	Temperature = 310.928 K
Pressure = 13.7895 MPa	Pressure = 34.4737 MPa	Pressure = 6.8947 MPa
Gas specific Gravity = 0.7	Gas specific Gravity = 0.65	Pseudo-Critical Temperature = 237.2 K
$y_{N_2} = 0.05$	$y_{N_2} = 0.1$	Pseudo-Critical Pressure = 4.4815 MPa
$y_{CO_2} = 0.05$	$y_{CO_2} = 0.08$	
$y_{H_2S} = 0.02$	$y_{H_2S} = 0.02$	

find out f'(Y).

$$f'(Y) = \frac{Y^4-4Y^3+4Y^2+4Y+1}{(Y-1)^4} - 2BY + DCY^{D-1} \tag{16}$$

Then we use this iterative algorithm to further solve for the value of Y as:

$$Y_{i+1} = Y_i - \frac{f(Y)}{f'(Y)} \tag{17}$$

For finding the pseudo critical pressure(P_{pc}) and pseudo critical temperature(T_{pc}) (When specific gravity and mole fraction of gases are given) we use these formulas[The gas under consideration is assumed to be a mixture of H_2S, CO_2, N_2 and rest of the gases combined]. These formulas would give the temperature in Rankine and pressure in psia.

$$P_{pc} = 678 - 50(\gamma_g - 0.5) - 206.7y_{N_2} + 440y_{CO_2} + 606.7y_{H_2S} \tag{18}$$

$$T_{pc} = 326 + 315.7(\gamma_g - 0.5) - 240y_{N_2} - 83.3y_{CO_2} + 133.3y_{H_2S} \tag{19}$$

Here, γ_g denotes the specific gravity of gas and y_i denotes the mole fraction of gas i.

Numerical Analysis

We will first consider 3 examples mentioned in Table[1]. We will be using Newton-Raphson, ADM and ADM-Shanks transformation to evaluate the value of Y and eventually the Z - factor of gases.

Example 1

We use ADM for approximating Z. Using Table 1 and equations (18) and (19) we can calculate the pseudo critical temperature and pseudo critical pressure. For this example, $P_{pc} = 4.76979$ MPa and $T_{pc} = 208.689$ K . Now, the reduced temperature can be calculated as $t_r = T_{pc}/\mathrm{T} = 0.617658$ and pseudo reduced pressure as $p_{pr} = p/P_{pc} = 2.89101$. On putting these values in equations (7),(8),(9) and (10), we get the values of A,B,C and D :
A = 0.0317445
B = 6.4724
C = -26.3870
D = 3.9218
Now we can use these parameters obtained to get the values of $Y_0, Y_1, Y_2...Y_{10}$ from equation(14). Their final computed values are:

$Y_0 = 0.07196140$	$Y_6 = 0.000960638$
$Y_1 = 0.01831020$	$Y_7 = 0.000614761$
$Y_2 = 0.00823824$	$Y_8 = 0.000399974$
$Y_3 = 0.00438462$	$Y_9 = 0.000263533$
$Y_4 = 0.00253244$	$Y_{10} = 0.00017536$
$Y_5 = 0.00153512$	

We can calculate the approximate value of $Y = \tilde{Y}(10) = \sum_{i=0}^{10} Y_i = 0.109376$. Now, value of the compressibility factor Z can easily be calculated from equation(11) as $Z = 0.839066$.

We now apply Shanks transform along with ADM to increase the rate of convergence. For applying Shanks Transform, we now define a new sequence of numbers $U_n = \tilde{Y}(n) = \sum_{i=0}^{n} Y_i$. On applying Shanks transform twice on the first five values of Y_i as shown in Table 2, we obtain the approximated value of $Y = 0.109511$. Thus, from equation(11) $Z = 0.838034$.

Now, we would apply Newton-Raphson method to calculate the value of Z. We use initial guess of Y to be 0.5 . Using equation(17) iteratively, we get the value of Y as 0.109744 . Now we put this value of Y and all other required parameters in equation(11) to obtain the value of Z as 0.83625

Table 2: Shanks+ADM in Example 1

n	$U_n = \tilde{Y}(n)$	$Sh(U_n)$	$Sh^2(U_n)$
0	0.0719614		
1	0.0902716	0.105248	
2	0.0985098	0.107883	0.109511
3	0.1028940	0.108889	
4	0.1054270		

Example 2

Example 2 is similar to example 1, the only difference between them being the numerical values. So we will proceed in a similar fashion.

For ADM, we get the values of initial parameters from Table 1. Using these parameters in equations(18) and (19) we obtain the values of $T_{pc} = 191.865K$ and $P_{pc} = 4.80678MPa$. Now, t_r and p_{pr} can be calculated as $t_r = T_{pc}/\mathrm{T} = 0.539899$ and $p_{pr} = p/P_{pc} = 7.17191$. Putting these values of t_r and p_{pr} in equations (7),(8),(9) and (10), we get the values of A,B,C and D as:
A = 0.0256504
B = 5.84474
C = -14.9575
D = 3.70252
Using A,B,C and D we get values of $Y_0, Y_1, ...Y_{10}$ as:
$Y_0 = 0.1185410$ $Y_6 = 0.00117341$
$Y_1 = 0.0335020$ $Y_7 = 0.000582361$
$Y_2 = 0.0154191$ $Y_8 = 0.000265313$
$Y_3 = 0.0079446$ $Y_9 = 0.000101570$
$Y_4 = 0.0042332$ $Y_{10} = 0.000022362$
$Y_5 = 0.0022548$
On adding $Y_0 + Y_1 + ... + Y_{10}$ we get final approximated value of $Y = 0.18404$. Using equation(11), we get $Z = 0.999579$.

Using Shanks Transform with ADM, we get the approximated value of $Y = 0.184614$. Using this in equation(11), we get $Z = 0.996473$. All the necessary calculations required for calculating Y is mentioned in table 3.

For Newton Raphson method, we take initial guess as 0.5 . This gives us the final value of $Y = 0.183929$. On putting this in equation(11) we get $Z = 1.00018$.

Table 3: Shanks+ADM in Example 2

n	$U_n = \tilde{Y}(n)$	$Sh(U_n)$	$Sh^2(U_n)$
0	0.118541		
1	0.152043	0.180610	
2	0.167462	0.183851	0.184614
3	0.175407	0.184468	
4	0.179640		

Example 3

Example 3 is a little different from Example 1 and 2. In this example, we have already been provided with the values of pseudo critical temperature T_{pc} and pressure P_{pc}. So this will reduce one step in our calculations for each of the three methods.

For ADM, since we already have the values of T_{pc} and p_{pc}, so now we can get the values of t_r and p_{pr} as $t_r = T_{pc}/\mathrm{T} = 0.762878$ and $p_{pr} = p/P_{pc} = 1.53846$. Putting these values of t_r and p_{pr} in equations (7),(8),(9) and (10), we get the values of A,B,C and D as:
A = 0.0436775
B = 7.61336
C = -52.9383
D = 4.33131

Using A,B,C and D we get values of $Y_0, Y_1, ...Y_{10}$ as:

$Y_0 = 0.05592280$ $Y_6 = 0.00104737$
$Y_1 = 0.01458750$ $Y_7 = 0.000724536$
$Y_2 = 0.00687953$ $Y_8 = 0.000511188$
$Y_3 = 0.00387912$ $Y_9 = 0.000366286$
$Y_4 = 0.00239029$ $Y_{10} = 0.000265755$
$Y_5 = 0.00155397$

On adding $Y_0 + Y_1 + ... + Y_{10}$ we get final approximated value of $Y = 0.0881284$. Using equation(11), we get $Z = 0.762481$.

Using Shanks Transform with ADM, we get the approximated value of $Y = 0.0884508$. Using this in equation(11), we get $Z = 0.759702$. All the necessary calculations required for calculating Y is mentioned in table 4.

For Newton Raphson method, we have taken the initial guess as 0.5 . This gives us the final value of $Y = 0.088914$. On putting this in equation(11) we get $Z = 0.755744$.

Table 4: Shanks+ADM in Example 3

n	$U_n = \tilde{Y}(n)$	$Sh(U_n)$	$Sh^2(U_n)$
0	0.0559228		
1	0.0705103	0.083530	
2	0.0773899	0.0862842	0.0884508
3	0.0812690	0.0874968	
4	0.0836593		

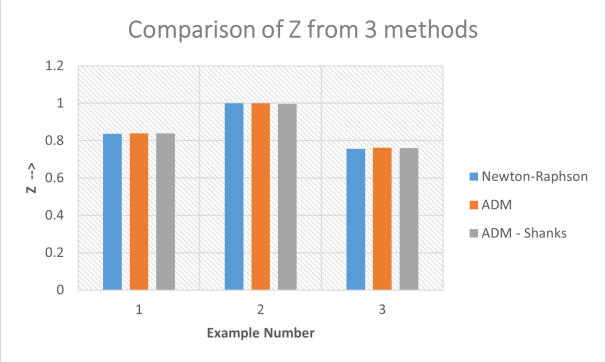
Apart from these 3 examples, we have also calculated Z for various t_{pr} and p_{pr} values using all the three methods: Newton-Raphson, ADM and ADM-Shanks. We have compared the Z obtained in each case from these three methods with the actual value of Z as obtained from Standing-Katz table[7]. We have also made a table of the absolute relative deviation of these values which is calculated as :$|Z_{experimental} Z_{theoretical}|/Z_{experimental}$

Results and Discussions

All the calculations were done in C++ language and the codes were developed using the discussed algorithms. Programs to measure the CPU time usage were also developed for all the three examples. These programs were finally compiled online using GDB C++ compiler. Calculations for Newton Raphson was done up to 10 iterations since we are going to compare CPU time usage and thus want to fix number of steps for any initial guess taken. The results obtained for input data set given in Table 1 are as follows (0.5 was used as initial guess used for N-R method in below output):

Table 5: Results

Method	Example 1	Example 2	Example 3
N-R	0.83625	1.00018	0.755744
ADM	0.839066	0.999579	0.762481
Shanks	0.838034	0.996473	0.759702



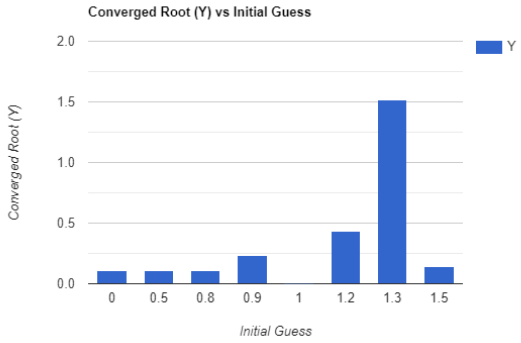
Graph 1

As visible in above data, results obtained from all the three algorithms are very close to each other. However, results from Newton-Raphson are highly dependent on initial guess if the number of iterations is fixed. The other two methods have no such shortcoming and so are at advantage from the very beginning. We have shown this dependency on initial guesses for Example 1 in Table[6]. If we try to find the converged value of Y using N-R Method using various initial guesses, the results obtained are as follows:

Table 6: Initial Guess vs Converged Root

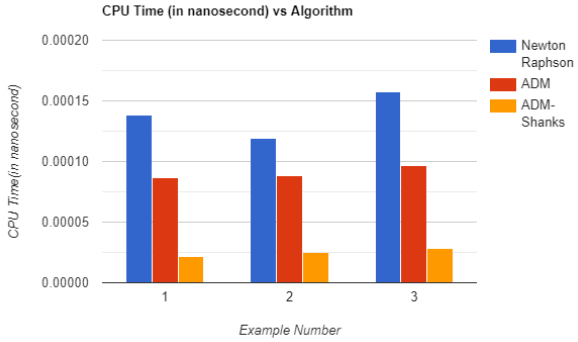
Initial Guess	Converged Root(Y)
0	0.109744
0.5	0.109744
0.8	0.109901
0.9	0.234796
1	Not Computable*
1.2	0.436773
1.3	1.51493
1.5	0.145156

*Due to division by 0



Graph 2

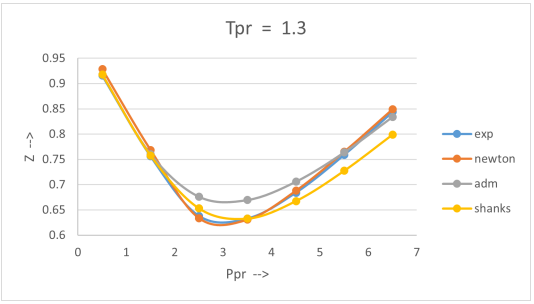
Clearly, using 0.5 as initial guess yielded quite accurate results. But if we would have taken any other initial guess such as 1.2 then the value of Z would have been deflected by a huge margin. Now, the main difference between these three algorithms lies in the computational efficiency. The CPU time usage would vary with every compilation, compiler, and device. However, their relative comparison is still observable. Plotting CPU Time usage vs algorithm on a random compilation generated following output (not bound to remain exactly same each time but close to this) :



Graph 3

Clearly ADM along with Shanks transformation took least time due to its faster convergence rate and half the number of decomposition component compared to ADM. Newton Raphson required maximum time among all. Hence ADM-Shanks is most efficient method in terms of computational speed.

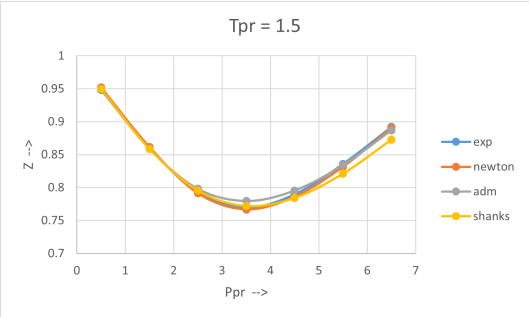
Other than these 3 case examples, we have also plotted values of Z factor vs pseudo reduced temperature for various experimental values obtained from Standing and Katz Z factor table[7] and compared the experimental data with the values obtained from our three algorithms. This would establish the validity of the estimates obtained by our algorithms. Initial guess used for N-R method is 0.8 . The Y-axis of graph represents value of Z and X-axis represents values of P_{pr}.



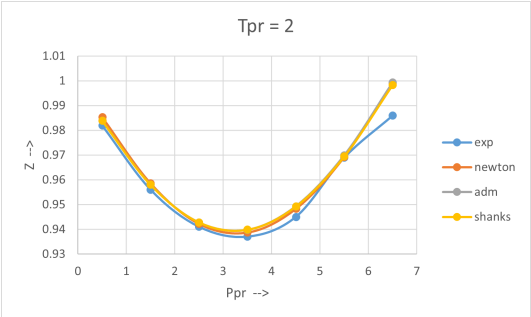
Graph 4

Table 7: Absolute Relative Deviation(in %)

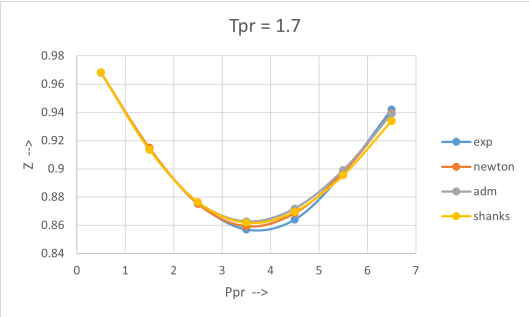
p_{pr}	0.5	1.5	2.5	3.5	4.5	5.5	6.5
$t_{pr} = 1.3$							
N-R	1.378	1.666	0.672	0.352	0.573	0.810	0.637
ADM	0.178	0.569	5.976	5.783	3.182	0.641	1.183
Shanks	0.181	0.193	2.351	0.031	2.429	4.156	5.316
$t_{pr} = 1.5$							
N-R	0.414	0.278	0.337	0.404	0.499	0.541	0.158
ADM	0.177	0.038	0.514	1.256	0.705	0.219	0.568
Shanks	0.178	0.024	0.197	0.258	0.708	1.761	2.167
$t_{pr} = 1.7$							
N-R	0.029	0.091	0.084	0.270	0.528	0.052	0.268
ADM	0.026	0.051	0.045	0.662	0.902	0.218	0.328
Shanks	0.026	0.040	0.048	0.557	0.646	0.177	0.866
$t_{pr} = 2.0$							
N-R	0.339	0.268	0.129	0.181	0.346	0.024	1.330
ADM	0.185	0.209	0.183	0.295	0.454	0.093	1.355
Shanks	0.185	0.211	0.192	0.304	0.447	0.048	1.250



Graph 5



Graph 7



Graph 6

On observing, we can see that taking 0.8 as initial guess for Newton-Raphson has led to significant deviations from actual experimental data. If we would have taken 0.5 as initial guess then results would have been much better for Newton-Raphson method.

Newton Raphson method is completely dependent on the initial guess. There isn't any exact way to find which guess would yield better results. Thus, it all narrows down to hit and trials. Graph[2] clearly illustrate this drawback. This could become very problematic. However, there isn't any such requirement in ADM and ADM Shanks method. ADM and ADM Shanks algorithm yielded results which were quite within the acceptable relative deviation range

establishing the validity of our estimates. Computationally, ADM and ADM Shanks are much more efficient than Newton Raphson. This is well summarised and illustrated in Graph[3].

Conclusion

Adomian decomposition method proposed to find Z factor using Hall Yarborough Method. The method is simple to understand like any other numerical method. To provide ever faster convergence, Shanks transformation was proposed. The results obtained were compared with the conventional Newton Raphson method and the experimental data, which is due to Standing and Katz table[7]. Both the methods were found to be advantageous over Newton Raphson due to non-requirement of initial guesses for approximation. CPU times were also compared for all methods and ADM methods were found to be much better. Estimates from all methods were found to be very close to the experimental data, however Newton Raphson showed large deviations for inappropriate initial guess. Thus, proposed algorithms could be used for precise calculations of real-world problems.

Self Assessment

Level 1

We have given our sincere effort to replicate the original papers. We were successful in replicating most of the results and hence approximate the z-factor using discussed algorithms. We have used C++ language to develop our codes and all the codes are in working condition. This report has been prepared using TeX studio(LaTeX) There are few things in original paper that needs to be pointed out.

The data set for case example 1 and 2 have some printing error. In example 1, temperature and mole fraction of hydrogen sulphide were wrongly printed. In example 2, Mole fraction of hydrogen was wrong. We have confirmed this error from the actual reference [8] from where these data sets were obtained. We noticed this error when we found that our codes were giving correct results for any data set but not for Example 1 and 2. After making necessary changes in the input, we were able to yield correct results.

The number of iterations to be fixed in Newton-Raphson was also not given which was used to make table[6]. Thus, we had to check results for various iterations to find it out.

Since the initial guess for Newton Raphson was not given for table[7] in the original paper, we chose 0.8 as our guess to replicate the deviations in Newton Raphson method for table[8]. The conclusion still remained the same, i.e. results from Newton Raphson can vary from guess to guess if the number of iterations are fixed and initial guess is not correctly chosen.

Also, the original paper provided us with a MATLAB code to find Adomian polynomials for a given non-linearity in the appendix. However, we decided to calculate those polynomials manually using the general formula given in [5]. The obtained polynomials were so large that we decided not to present those polynomials in this paper and instead have provided with the reference from which those polynomials were obtained.

Finally, from selecting the journal, to finally able to replicate the results, it has been a great learning experience for us. We have devoted a very good amount of time in this paper in order to generate quality results.

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