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Web-Based Application for Calculation of Physical Properties of Hydrocarbon Fluids Using Compositional Approach

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Abstract. The objective of this study is to develop a web-based application that can be used to generate phase diagram and calculate the physical properties of hydrocarbon fluids using a compositional approach. This study applies a combined calculation of critical temperature and pressure, bubble point pressure, dew point pressure, and dew point temperature to generate phase diagram. Calculation of critical temperature is carried out using the Chueh and Prausnitz equations, while the calculation of bubble point pressure, dew point pressure, and dew point temperature is carried out using the Newton-Rapshon method. Calculation of the physical properties of hydrocarbon fluids using a compositional approach includes parameters apparent molecular weight, compressibility factor, density, specific gravity, and viscosity for gas and liquid phases. The calculation of the compressibility factor uses the Equation of State (EOS). There are 2 choices of EOS correlation, namely Peng-Robinson and Soave-Reidlich-Kwong. Flash calculation using Newton-Rapshon method. Based on the results of the flash calculation, the physical properties of the hydrocarbon fluids for each of the above phases are calculated. The calculation of the viscosity of the gas phase uses the Lee-Gonzales-Eakin correlation, while the calculation of the viscosity of the liquid phase uses the Lohrenz-Bray-Clark correlation. The both model of generates phase diagram and calculation of the physical properties of the hydrocarbon fluids is then implemented into a web-based application using the Dash Plotly framework. Dash plotly includes 3 components, namely the main programming language using Python3, a framework for building interfaces using ReactJS, and a framework for the backend using Flask. Testing results by using a set of hydrocarbon fluid data show the model can be used to predict volumetric properties and associated phase diagram as well as physical properties such as compressibility factor, density, specific gravity, and viscosity of gas and liquid phase of the fluid. Comparison with desktop version software results show that the model gives good results.

Keyword(s): compositional approach; hydrocarbon fluids; phase diagram; physical properties; web-based application

1 Introduction

Understanding behavior of fluid properties (oil, gas, water, and their mixtures) in various conditions plays a crucial role in the oil and gas production. In case fluid composition data not available, estimation of physical properties of fluid in various pressure and temperature conditions is carried out using empirical correlation. However, if fluid composition data is available, estimation of physical fluid properties using compositional approach will usually provide more accurate and realistic results. The physical properties of a petroleum fluid vary significantly as a function of temperature and pressure. These changes in temperature and pressure will often lead to a change in the state of the mixture from a single-phase state to a two-phase state where the two phases will each have a different composition in comparison to the original petroleum fluid. Therefore, the properties of the new phases will change with the change in composition, temperature, and pressure. A major step in modelling the physical properties of reservoir fluids is to calculate volumetric properties and associated phase equilibria as well as other important physical properties such as density, viscosity, compressibility, and heat capacity. In this study, we develop a PVT analysis model using compositional approach to estimate physical properties of a petroleum fluid based on several Equation of State correlations. In addition, the developed model can also be used to generate phase diagram.

2 Methodology

2.1 Gas–Liquid Phase Equilibrium

The two fluid phases, gas and liquid, are in equilibrium in the region bounded by the bubble point curve and the dew point curve on a multicomponent mixture phase diagram. The amount and composition of the two phases varies at various points within this phase envelope boundary. If n_L is the number of moles of liquid phase and n_V is the number of moles of gas phase, then the number of moles of hydrocarbon mixture, n is

$$n = n_{\mathrm{L}} + n_{\mathrm{V}} \tag{1}$$

The material balance in the i -th component produces:

$$z_{\mathrm{i}} n = x_{\mathrm{i}} n_{\mathrm{L}} + y_{\mathrm{i}} n_{\mathrm{V}} \tag{2}$$

The calculation of the phase equilibrium is usually carried out on the basis of one mole of the hydrocarbon mixture, that is, n = 1, so equation (1) can be written as

$$n_{\mathrm{L}} + n_{\mathrm{V}} = 1 \tag{3}$$

so that for a given composition of the fluid,

$$x_{\mathrm{i}} n_{\mathrm{L}} + y_{\mathrm{i}} n_{\mathrm{V}} = z_{\mathrm{i}} \tag{4}$$

or

$$x_{\mathrm{i}} n_{\mathrm{L}} + (x_{\mathrm{i}} K_{\mathrm{i}}) n_{\mathrm{V}} = z_{\mathrm{i}} \tag{5}$$

where K_i is the equilibrium ratio of a given component, i.e. the ratio of the mole fraction of the component in the gas phase, y_i, to the mole fraction of the component in the liquid phase x_i.

$$K_i = \frac{y_i}{x_i} \tag{6}$$

2.2 *Flash Calculations*

Flash calculations are required to know the amount of hydrocarbon liquid and gas coexisting in the pipeline at a given pressure and temperature. Furthermore, these calculations are also performed to determine the composition of the existing hydrocarbon phases that are needed to determine:

- moles of the gas phase (n_V),
- moles of the liquid phase (n_L),
- composition of the liquid phase (x_i),
- composition of the gas phase (y_i).

The objectives function of flash calculation is to meet

$$f(n_V) = \sum_i \frac{z_i(K_i - 1)}{n_V(K_i - 1) + 1} = 0 \tag{7}$$

In this study, we use modified Newton-Rapshon iteration technique to solve equation (7).

2.3 *Equation of State*

An Equation of State (EOS) is an analytical expression relating the pressure P, to the temperature T, and the volume V. There are numerous empirical cubic equations of state. This study uses Peng-Robinson (PR) and Soave-Reidlich-Kwong (SRK) equations of state to calculate the equilibrium ratio K_i, compressibility factor, Z_i and the fugacity coefficient, Φ_i. The equations of state for PR and SRK are expressed in terms of the compressibility factor variables, respectively, which can be written as follows:

$$Z^3 + (B-1)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \tag{8}$$

and

$$Z^3 + Z^2 + (A - B - B^2)Z - AB = 0 \tag{9}$$

where,

$$A = \frac{(a\alpha)_m\, p}{(RT)^2} \tag{10}$$

and

$$B = \frac{b_m\, p}{RT} \tag{11}$$

with,

$$(a\alpha)_m = \sum_i \sum_j [x_i x_j (a_i a_j \alpha_i \alpha_j)^{0.5} (k_{ij} - 1)] \tag{12}$$

and

$$b_m = \sum_i [x_i b_i] \tag{13}$$

The parameter k_{ij} is an empirically determined correction factor, commonly called a binary interaction coefficient, which describes the interactions that occur between the i -th component and the j -th component in a hydrocarbon mixture.

2.4 PVT Calculation

The following model is used to calculate the physical properties of fluids using a compositional approach.

2.4.1 Apparent Molecular Weight

Gas-phase

$$MW_g = \sum_i y_i \, MW_i \tag{14}$$

Liquid-phase

$$MW_o = \sum_i x_i \, MW_i \tag{15}$$

2.4.2 Compressibility factor (Z-factor)

According to the equation of state selected for each phase using the correlation described in the previous section.

2.4.3 Density

Gas-phase

$$\rho_g = \frac{pMW_g}{Z_g RT} \tag{16}$$

Liquid-phase

$$\rho_o = \frac{pMW_o}{Z_o RT} \tag{17}$$

2.4.4 Specific Gravity

Gas-phase

$$\gamma_g = \frac{MW_g}{29} \tag{18}$$

Liquid-phase

$$\gamma_o = \frac{\rho_o}{62.4} \tag{19}$$

2.4.5 Viscosity

Gas viscosity is calculated using the Lee-Gonzales-Eakin correlation as follows,

$$\mu_g = 10^{-4} \, K \, EXP \left[X \left(\frac{\rho_g}{62.4} \right)^Y \right] \tag{20}$$

Liquid viscosity is calculated using the Lohrenz-Bray-Clark correlation as follows,

$$\mu_{ob} = \mu_{oL} + (\xi_m)^{-1}([a_0 + a_1\rho_r + a_2\rho_r^2 + a_3\rho_r^3 + a_4\rho_r^4]^4 - 0.0001) \quad (21)$$

2.5 *Phase Diagram*

Phase diagram generation is carried out in the following stages:

1. Calculation of critical temperature using the following equation:

$$T_{cm} = \sum_j (\Theta_j T_{cj}) + \sum_i \sum_j (\Theta_{ij}\tau_{ij}) \quad (22)$$

2. Calculation of critical pressure using the following equation:

$$f(p_d) = \sum_{i=1}^{n} \left[\frac{f_i^V}{\Phi_i^L}\right] - p_d = 0 \quad @T_{cm} \quad (23)$$

3. Calculation of bubble point pressure using the following equation:

$$f(p_b) = \sum_{i=1}^{n} \left[\frac{f_i^L}{\Phi_i^V}\right] - p_b = 0 \quad (24)$$

4. Calculation of dew point pressure using the following equation:

$$f(p_d) = \sum_{i=1}^{n} \left[\frac{f_i^V}{\Phi_i^L}\right] - p_d = 0 \quad (25)$$

5. Calculation of dew point temperature using the following equation:

$$f(T_d) = \sum_{i=1}^{n} \left[\frac{f_i^V(T_d)}{\Phi_i^L(T_d)}\right] - T_d = 0 \quad (26)$$

2.6 *Web-Based Application Development*

The both model of generate phase diagram and calculation of the physical properties of the hydrocarbon fluid are implemented into a web-based application using the Dash Plotly framework. Dash Plotly is a framework that allows developer making beautiful analytics web application with just using pure Python. Dash Plotly will cover both backend and front end, so deep knowledge about web development technology like HTML, CSS and Javascript are not mandatory anymore. Dash Plotly also offer clean user interface, great community support and its open source. Python is cross-platform software that may run on many platforms, so does Dash Plotly. Dash plotly includes 3 components, namely the main programming language using Python3, a framework for building interfaces using ReactJS, and a framework for the backend using Flask. Figure 1 and figure 2 shows respectively the front page of the web-based application to generate phase diagram (called PE Generator) and to calculate the properties of hydrocarbon fluid (called Compo Solver).

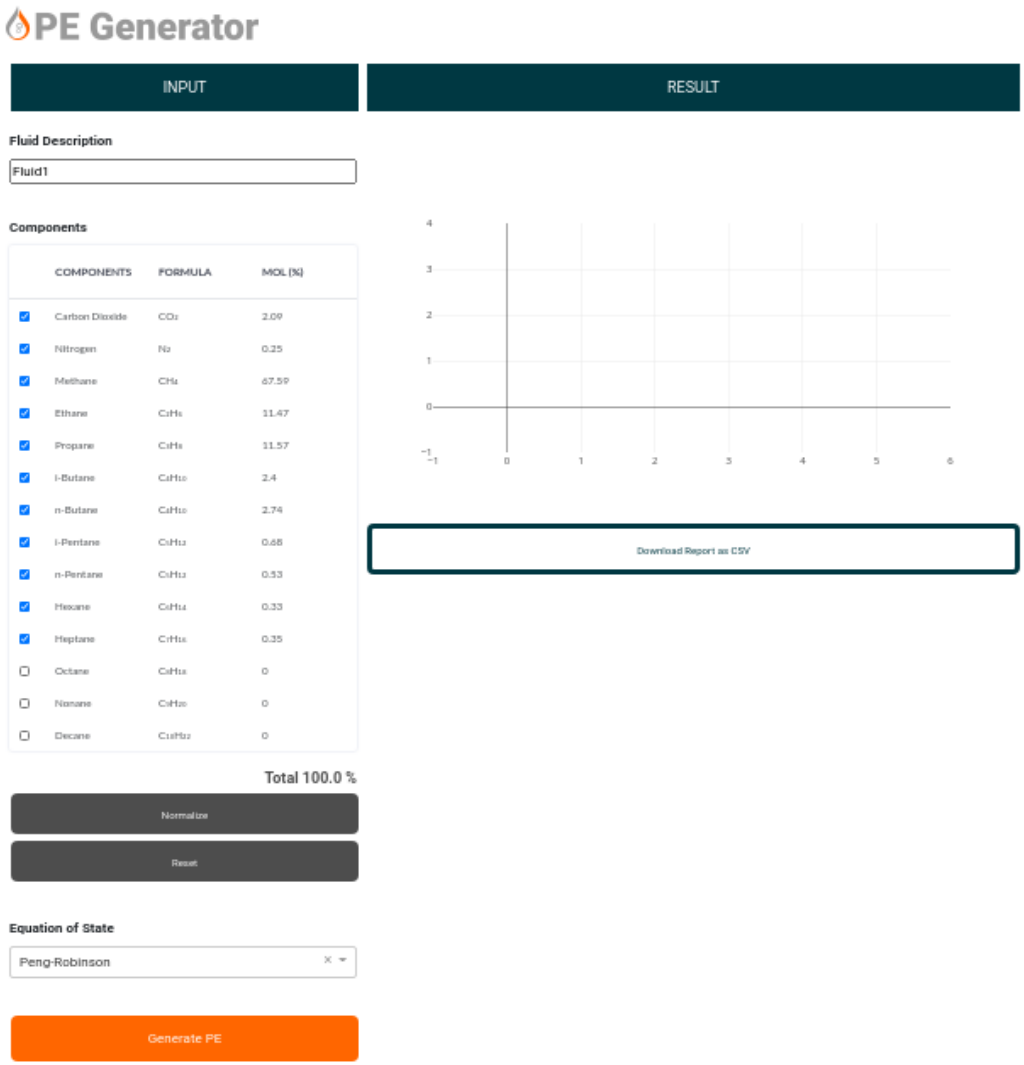

Figure 1. The front page of PE Generator

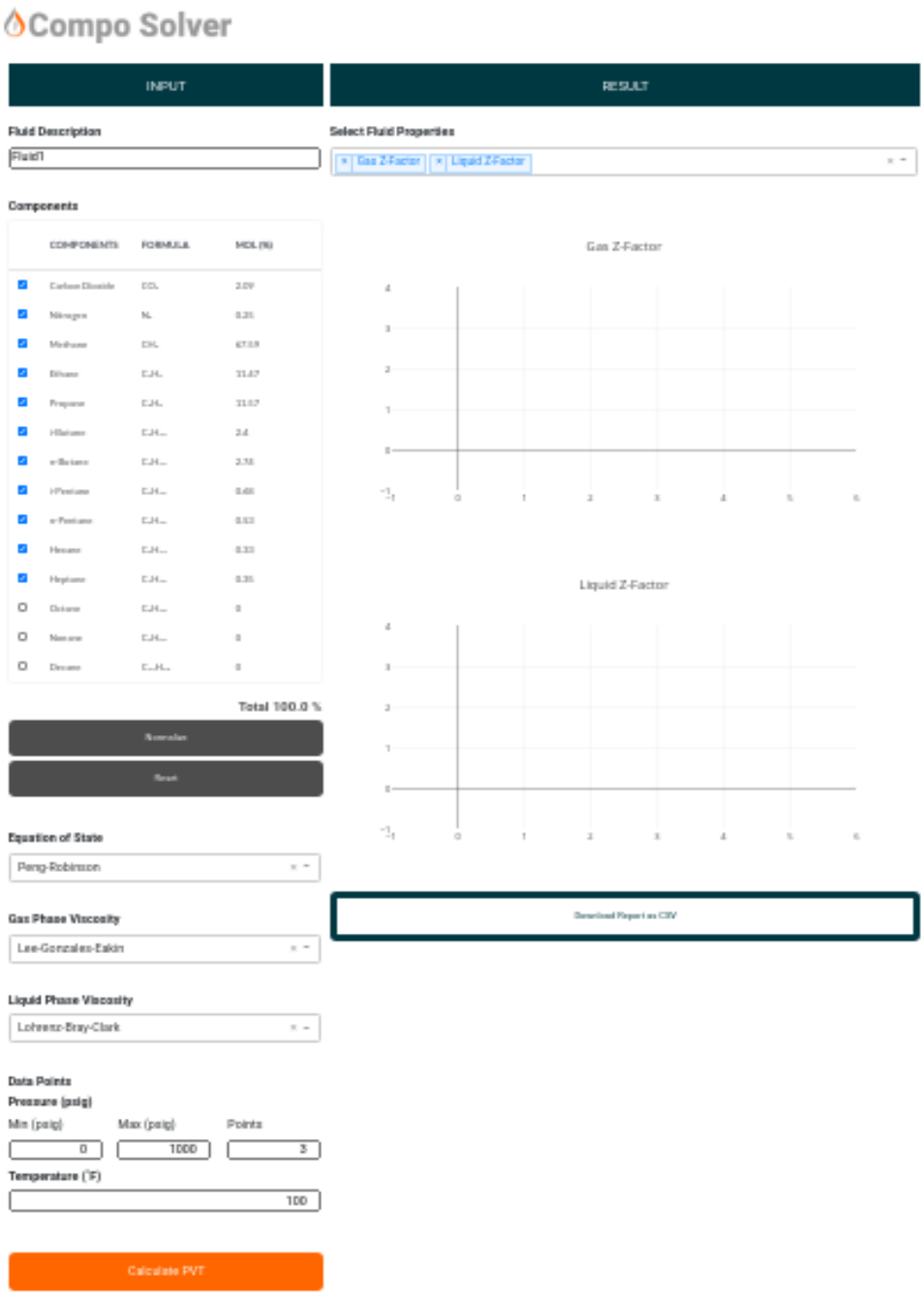

Figure 2. The front page of Compo Solver

3 Results and Discussion

3.1 Case Study

This section presents the simulation results to test the model developed in this study. The fluid composition data is given in table 1. The data is simulated using EOS correlation PR and SRK for both flash calculation and phase diagram simulation. Flash calculations are performed at multiple pressure points and single temperature point as given in table 2.

Table 1. Fluid composition data.

No	Component	Symbol	% Mole
1	Carbon dioxide	CO_2	2.09
2	Nitrogen	N_2	0.25
3	Methane	C_1	67.59
4	Ethane	C_2	11.47
5	Propane	C_3	11.57
6	iso-Butane	i-C_4	2.40
7	n-Butane	n-C_4	2.74
8	iso-Pentane	i-C_5	0.68
9	n-Pentane	n-C_5	0.53
10	Hexane	C_6	0.33
11	Heptane	C_7	0.35

Table 2. Pressure and temperature condition.

Temperature (°F)	Pressure (psig)
60	0
	500
	1000
100	0
	500
	1000

3.2 Results

3.2.1 Phase Diagram

The phase diagram results for each of the EOS correlation of PR and SRK are shown in figure 3 and figure 4 respectively.

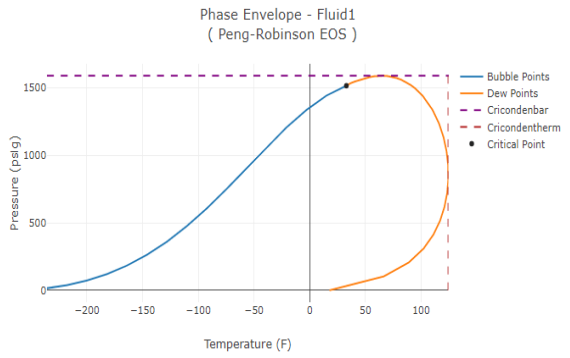

Figure 3. Phase diagram for EOS PR

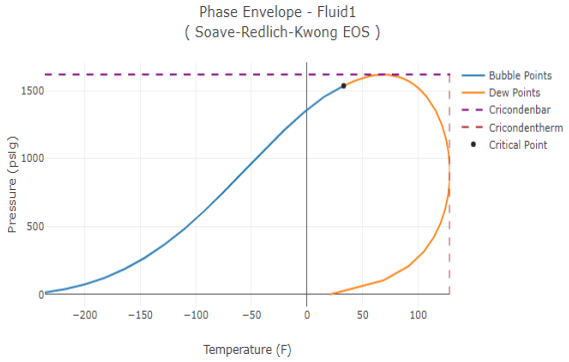

Figure 4. Phase diagram for EOS SRK

Figures 5 and figure 6 show a comparison of simulation results using the web application with the desktop version software for EOS correlation of PR and SRK respectively. It can be seen that the simulation results of the web version are the same as the results of the desktop version.

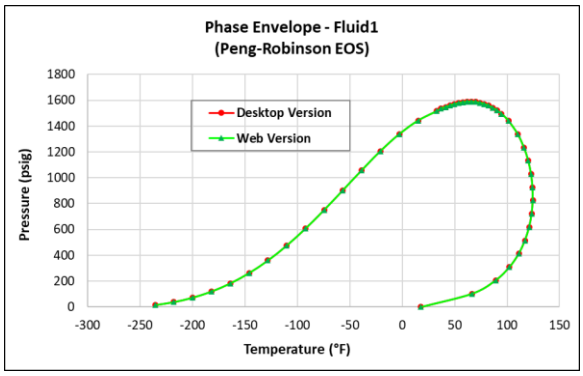

Figure 5. Phase diagram comparison (EOS PR)

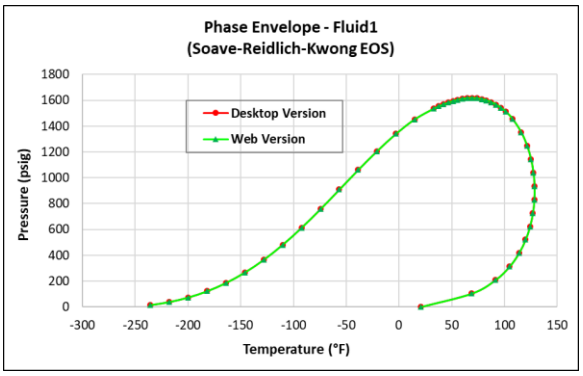

Figure 6. Phase diagram comparison (EOS SRK)

3.2.2 PVT Calculations

The results of PVT calculations using EOS correlation of PR are given in table 3. Table 4 shows the results of PVT calculations using the desktop version software for comparison. It can be seen that the results of the PVT calculation using the web version are the same as the results of the desktop version.

Table 3. PVT calculation results of web application for EOS correlation of PR.

Parameter	Results					
Temperature(F)	60	60	60	100	100	100
Pressure(psig)	0	500	1000	0	500	1000
nV(fraction)	1	0.9157	0.8174	1	0.9856	0.9504
nL(fraction)	0	0.0843	0.1826	0	0.0144	0.0496
MW_g(lbm/mole)	24.88	22.7906	22.071	24.88	24.426	23.961
MW_l(lbm/mole)	0	47.5866	37.4577	0	55.905	42.5077
Z_g(dim.)	0.9943	0.8289	0.6935	0.9955	0.846	0.7196
Z_l(dim.)	nan	0.1286	0.237	nan	0.1376	0.2462
rho_g(lb/ft3)	0.0659	2.5375	5.7906	0.0612	2.4742	5.6253
rho_l(lbm/ft3)	nan	34.1406	28.7546	nan	34.8085	29.1679
miu_g(cP)	0.0098	0.0111	0.0133	0.0106	0.0115	0.0136
miu_l(cP)	nan	0.1507	0.0912	nan	0.1524	0.089

Table 4. PVT calculation results of desktop version software for EOS correlation of PR.

Parameter	Results					
Temperature(F)	60	60	60	100	100	100
Pressure(psig)	0	500	1000	0	500	1000
nV(fraction)	1	0.9157	0.8174	1	0.9856	0.9504
nL(fraction)	0	0.0843	0.1826	0	0.0144	0.0496
MW_g(lbm/mole)	24.88	22.7906	22.0710	24.88	24.426	23.9610
MW_l(lbm/mole)	0	47.5866	37.4577	0	55.905	42.5077
Z_g(dim.)	0.9943	0.8289	0.6935	0.9955	0.846	0.7196
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rho_l(lbm/ft3)	nan	34.1406	28.7546	nan	34.8085	29.1679
miu_g(cP)	0.0098	0.0111	0.0133	0.0106	0.0115	0.0136
miu_l(cP)	nan	0.1507	0.0912	nan	0.1524	0.089

The results of PVT calculations using EOS correlation of SRK are given in table 5. Table 6 shows the results of PVT calculations using the desktop version of the software for comparison. It can be seen that the results of the PVT calculation using the web application are the same as the results of the desktop version of the software.

Table 5. PVT calculation results of web application for EOS correlation of SRK.

Parameter	Results					
Temperature(F)	60	60	60	100	100	100
Pressure(psig)	0	500	1000	0	500	1000
nV(fraction)	1	0.9132	0.8092	1	0.9836	0.9417
nL(fraction)	0	0.0868	0.1908	0	0.0164	0.0583
MW_g(lbm/mole)	24.88	22.7205	21.9195	24.88	24.3632	23.7999
MW_l(lbm/mole)	0	47.6132	37.4365	0	55.8135	42.3301
Z_g(dim.)	0.9951	0.8506	0.7309	0.9961	0.8668	0.7559
Z_l(dim.)	nan	0.1453	0.2659	nan	0.1552	0.276
rho_g(lb/ft3)	0.0659	2.465	5.4566	0.0611	2.4085	5.3192
rho_l(lbm/ft3)	nan	30.2453	25.612	nan	30.8108	25.9075
miu_g(cP)	0.0098	0.011	0.0131	0.0106	0.0115	0.0134
miu_l(cP)	nan	0.0921	0.0673	nan	0.0926	0.0657

Table 6. PVT calculation results of desktop version software for EOS correlation of SRK.

Parameter	Results					
Temperature(F)	60	60	60	100	100	100
Pressure(psig)	0	500	1000	0	500	1000
nV(fraction)	1	0.9132	0.8092	1	0.9836	0.9417
nL(fraction)	0	0.0868	0.1908	0	0.0164	0.0583
MW_g(lbm/mole)	24.88	22.7205	21.9195	24.88	24.3632	23.7999
MW_l(lbm/mole)	0	47.6132	37.4365	0	55.8135	42.3301
Z_g(dim.)	0.9951	0.8506	0.7309	0.9961	0.8668	0.7559
Z_l(dim.)	nan	0.1453	0.2659	nan	0.1552	0.276
rho_g(lb/ft3)	0.0659	2.465	5.4566	0.0611	2.4085	5.3192
rho_l(lbm/ft3)	nan	30.2453	25.612	nan	30.8108	25.9075
miu_g(cP)	0.0098	0.011	0.0131	0.0106	0.0115	0.0134
miu_l(cP)	nan	0.0921	0.0673	nan	0.0926	0.0657

4 Conclusion

A web-based application has been successfully developed for calculating the properties of hydrocarbon fluids and generating phase diagrams using a compositional approach. The testing results show that the web-based application can be used to generate phase diagram and calculate the physical properties of the hydrocarbons fluid at various pressure and temperature conditions. The results of generating phase diagram and calculating the properties of hydrocarbon fluids using this web-based application show the same results as the results of the desktop version software.

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