# SP-Wax: Solid-liquid equilibrium thermodynamic modeling software for paraffinic systems

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# Abstract

The open-source software (SP-Wax) for the solid-liquid equilibrium (SLE) calculation of paraffin is presented. Paraffin modeling is important to many industries and engineering applications. SP-Wax provides reliable predictions for phase behavior of paraffinic solutions, which is crucial for petroleum industry. The Coutinho et al. thermodynamic model was primarily used and coded in SP-Wax. The developed simulation was validated by experimental data of binary and multicomponent systems. Solid-phase compositions were successfully estimated, and aging process of wax deposition problem was analyzed. Within the software, core calculations were coded in C++ and OpenMP parallel programming technique was incorporated to improve the performance. A C# Windows Forms user interface was created to ensure the reusability of the software for both technical and non-technical users.

# Motivation and Significance

The continuous increase of energy demand and depletion of existing conventional oil reserves have driven the exploitation of petroleum resources in harsh and deep-water environments. Such locations require long subsea pipelines for the transportation of hydrocarbons. The cold subsea environment (about 5 °C) poses several flow assurance concerns including hydrate formation and paraffin (or wax) deposition. In such conditions, wax starts depositing on the inner wall of the pipe and periodic remedial treatments are needed to maintain continuous hydrocarbon flow. Therefore, a complete understanding of this phenomenon is imperative to plan any remedial action in the most optimal and cost-effective way possible. In one instance, financial loss of $100 million was reported due to a severe paraffin deposition problem [1]. Wax deposition problems are usually treated by mechanical (“pigging”) and chemical methods. In the first method, a mechanical device (“pig”) is placed inside the pipe and is used to scrape any deposit from the wall [2]. The chemical approach is performed by adding chemicals to crude oil including solvents, paraffin inhibitors and dispersants. [3]. It is important to note that both methods are expensive. Aside from the operation costs, deferment of production can be very costly [4].

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Pigging frequency and selection of chemicals are determined by three factors including deposit thickness, solid wax fraction [5] and carbon number distribution (CND) of the deposit [6,7]. Current paraffin deposition models estimate the deposit’s thickness and solid wax fraction based on heat and mass transfer calculations [6–9]. The mass transfer calculation section requires a reliable thermodynamic model to accurately predict the deposit’s composition. SP-Wax provides an open-source thermodynamics package which can be used in the modeling of paraffin deposition and other related fields.

# Software Description

In this section, theoretical framework of the SP-Wax software is presented. SP-Wax is based on the thermodynamic model of Coutinho et al. [10–17] and other literature [18–31]. Coutinho thermodynamic model describes the non-ideality of liquid and solid phases fairly accurately. In SP-Wax, governing equations [29] are solved for non-ideal paraffinic solutions and different SLE characteristics are reported. The following governing equation relates each carbon number component’s equilibrium constant () to its thermophysical properties using activity coefficients ().

|  |  |
| --- | --- |
| *C:\Users\epanacha\Desktop\Arya\Untitled.png* | (1) |
|  | (2) |

where R is universal gas constant and T is the mixture temperature.

The mole fraction of precipitated phase in n-alkane system () is determined from Eq. (3*3*) based on input n-alkane mole fraction data () and equilibrium constant values [23].

|  |  |
| --- | --- |
|  | (3) |

Finally, the liquid and solid phase compositions () are calculated from

|  |  |  |
| --- | --- | --- |
|  |  | (4) |
|  |  | (5) |

Researchers have used different models to express the non-ideality of liquid phase in thermodynamic modeling of paraffin. In SP-Wax, the Entropic-free-volume model (E-FV2/3) was used to express the activity coefficient of liquid phase as [17]:

|  |  |
| --- | --- |
|  | (6) |

where and are combinatorial contribution and composition fraction parameters, respectively.

Coutinho et al. [17] showed that E-FV2/3 model is an accurate approach to quantify the non-ideality of liquid phase. From E-FV2/3 model, is calculated as:

|  |  |
| --- | --- |
|  | (7) |

where, and are molar and Van der Waals volumes, respectively.

For carbon numbers larger than six and smaller than twenty-one (), molar volume () is calculated by DIPPR correlations [20]. For the rest of carbon number components ( or ), is predicted by the GCVOL group contribution method [22]. In addition, Van der Waals volumes ) for different carbon number components are calculated from Bondi et al. [21].

The solid-phase activity coefficient of each carbon number component () is needed for the equilibrium constant () calculation in Eq. (1). UNIQUAC and Wilson models were proposed by Coutinho et al. [10,12] to express . Results from both models were compared against several experimental data sets and it was shown that predictions from both models are very similar [10]. However, the Wilson model only considers one solid phase and requires simpler numerical scheme. Therefore, Wilson model [12] was used in SP-Wax to express the activity coefficients of solid-phase. The Wilson model is as follows:

|  |  |
| --- | --- |
|  | (8) |

where is the major interaction term and is calculated based on the minor binary interaction energy parameter between two similar () and two different () carbon number components

|  |  |
| --- | --- |
|  | (9) |
|  | (10) |
|  | (11) |

where and are correction factor and heat of sublimation respectively. is calculated as:

|  |  |
| --- | --- |
|  | (12) |

where enthalpy of fusion and solid-phase transition () are calculated using Coutinho’s proposed correlations [15]. For enthalpy of vaporization (), Extension of Pitzer CSP model [28] was used. For more details, please refer to the developer’s manual.

In Eq. (9), or is the interaction energy parameter which is used to quantify the interaction energy between a pair of short and long n-alkane molecules. Generally, it is assumed that the interaction energy between a long and a short n-alkane () is the same as the interaction between two short n-alkanes ()or [14]. However, if molecules are too different in size, then they can bend over further and cause more interactions, which invalidates the assumption of . Therefore, a correction factor *(*) has been introduced to account for such abnormalities. Although plays an important role in correct prediction of solid-phase composition and precipitation curve, it has not been evaluated thoroughly. has been modeled differently in the literature [10,14,25,27]. All proposed models either contain adjustment parameters or additional empirical correlations to evaluate . We analyzed all models and found that Coutinho et al. [10] type model is the best candidate to use in SP-Wax. In their paper [10], several multicomponent paraffinic systems were successfully analyzed using the proposed correction factor (. In SP-Wax, an adjustable coefficient was used instead of a constant value of which was used by Coutinho et al. [10]. This worked well for all analyzed multicomponent systems in this paper.

|  |  |
| --- | --- |
|  | (13) |
|  | (14) |

In Eq. (14), the parameter “” is needed to be adjusted to tune the precipitation curve prediction to experimental precipitation data. Among three of our analyzed oil samples (Rittirong [32], Panacharoensawad [33], Zheng et al.[7]), was chosen as the optimum value which resulted in the best match between software’s prediction and experimental data. In all three oil cases, wax content was less than 15% in the oil sample. For the other multicomponent system (Fleming et al. [25]), the solution only contained n-alkanes and a smaller correction factor was needed (). Based on the four analyzed oil samples, we provided a general suggestion for the value of “” when experimental precipitation data are not available.

|  |  |
| --- | --- |
|  | (15) |
|  | (16) |
|  | (17) |

where is the weight fraction of n-alkanes in the total system which should be provided as an input.

The above equations were solved iteratively in SP-Wax to predict the phase equilibria of paraffin. In addition to experimental precipitation data, composition data of waxy deposits in pipe was analyzed by SP-Wax. This was done by assuming that the composition can be approximated from the deposit’s temperature at a certain instance. The purpose of this analysis is not to replace the compositional wax deposition model from Zheng et al.[7]. This additional analysis is to show that SP-Wax can estimate the deposit composition (especially at early time), even though only the deposit temperature at a certain instance is available. Moreover, this wax deposit analysis proves that solid-phase composition prediction from our developed software is reliable. SP-Wax approximation matches reasonably well with the experimental data of Rittirong [32] and Panacharoensawad’s [33] single-phase wax deposition cases (See the Illustrative Example section). Partially, it is due to the fact that the deposit temperature values were obtained from Rittirong [32] and Panacharoensawad’s [33] calculations that have already been accounted for the deposit thickness and the solid fraction of the deposit. Nevertheless, their heat transfer calculations are not sensitive to the deposit’s composition and SP-Wax can be used to predict the CND.

## 2.1 Software architecture

In SP-Wax, C++ was used for the development of the thermodynamic model with OpenMP parallel computation technique. C# GUI was used to create a front-end which takes inputs, allows save and load operations, and shows the results. C# creates text files for the C++ calculation and displays the results. SP-Wax calculates the solid and liquid phase compositions by solving the SLE governing equation (Eq. (1)). The pre-calculated equilibrium constants () are used to solve for the precipitated solid mole fraction) and the compositions of both phases( and ). The pre-calculated equilibrium constants are used as estimates of to ensure the numerical stability of the software. Then, the activity coefficients (), are calculated from Eq. (6) and Eq. (8) and are used to calculate the new values of . The iteration of calculation ends when the summation of all differences between the last two iterations is smaller than a certain tolerance. The full details of the calculation steps are given in the developer’s manual of the software. Figure 1 shows a summary of SP-Wax thermodynamic software for the precipitation curve prediction.

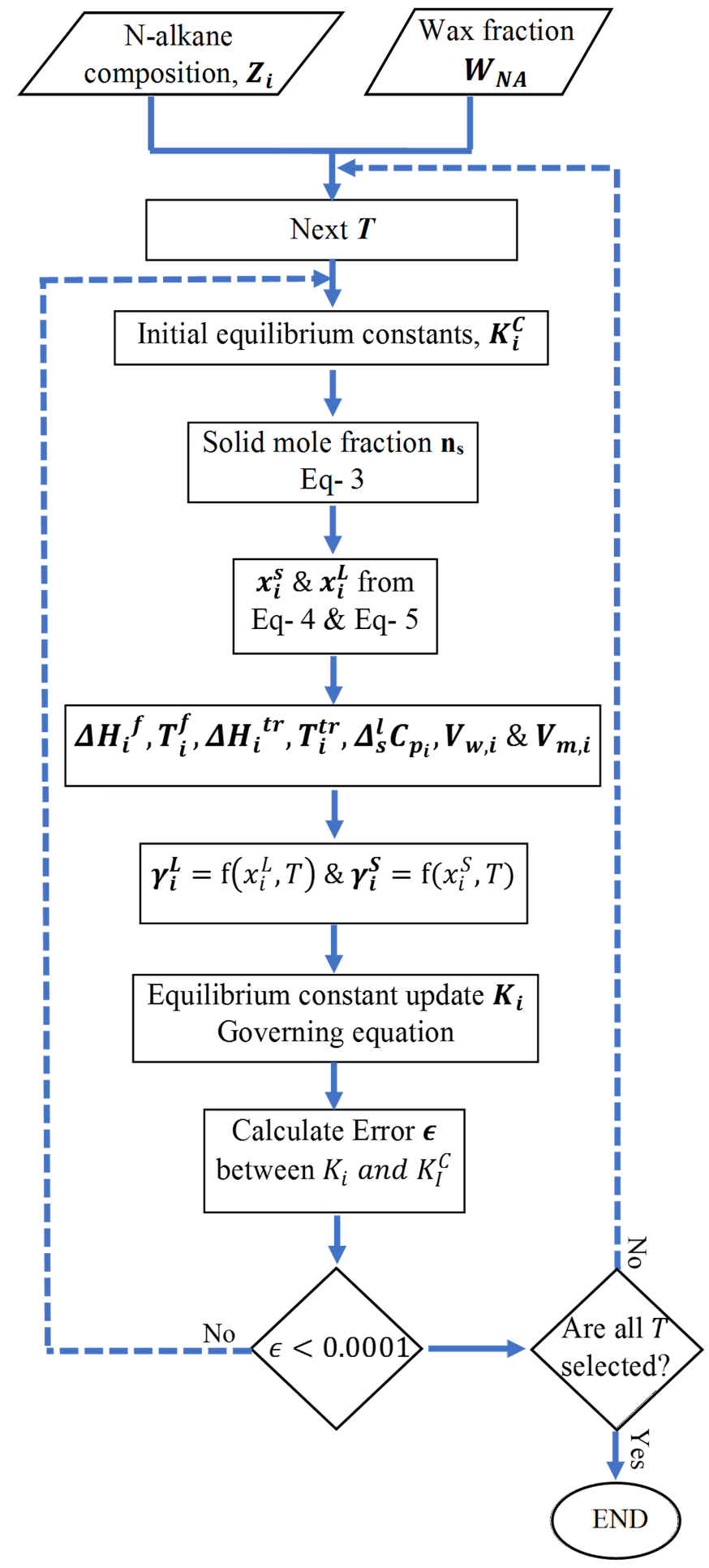


Figure 1: Flowchart of SP-Wax for precipitation curve prediction

## 2.2 Software functionalities

SP-Wax functionality is categorized into two binary and multicomponent systems. In binary systems, solid solubilities are calculated based on provided solute mole fractions in the solution (SPWaxBinary.cpp). For comparison purposes, experimental data can be inserted and plotted versus the software’s prediction. In multicomponent systems, there are three major program options including 1) Precipitation curve and WAT, 2) One temperature SLE calculations and, 3) Critical Carbon Number (CCN) estimation (see Figure 2). The first option allows users to predict the precipitation curve and WAT based on the provided input data (SPWaxPrecipitation.cpp). SP-Wax calculates the weight fractions of the precipitated wax in the total fluid at certain temperatures and plots them. The generated curve is called a precipitation curve and is used extensively in wax deposition simulations [1,32–35]. SP-Wax allows users to plot experimental solid fraction points versus the predicted precipitation curve for adjustment of correction factor coefficient in the thermodynamic model (Eq. (13)). Moreover, the solid-phase composition can be plotted at any temperature within the given range using a track-bar.

The second simulation option for a multicomponent system is to calculate and report various SLE properties of the system at one desired temperature (SPWaxOneTemperatureCase.cpp). The user can choose the desired output parameter from a combo-box and plot it. In SLE modeling, equilibrium constant values can vary from to for different carbon number components. Therefore, a convergence problem could be encountered near WAT. Choosing the right initial values for is enough to avoid any convergence problem. In SP-Wax, sets of initial values are calculated and reported by SPWaxKInitialization.cpp which are used by other C++ source files including SPWaxOneTemperatureCase.cpp and SPWaxPrecipitation.cpp. By this method, we eliminated the convergence problem near WAT.

The third multicomponent simulation option enables the user to calculate and plot the relative concentration gradients of all carbon numbers. In this graph, the smallest carbon number with positive relative concentration gradient is the Critical Carbon Number and it is reported by SP-Wax. Please refer to the developer’s manual for more information about required inputs and program options. The Figure 2 the shows SP-Wax software interface for multicomponent systems.

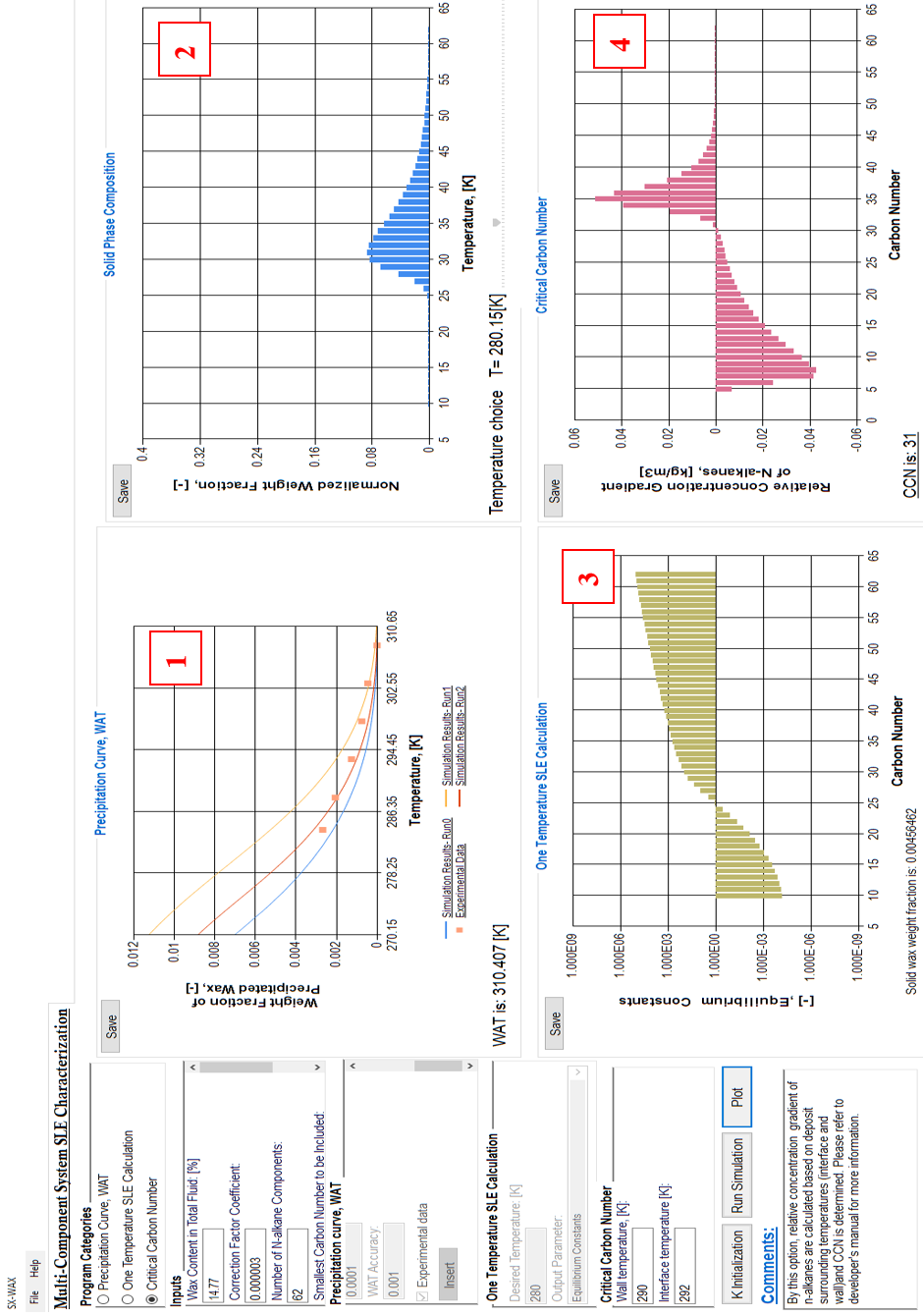


Figure 2: SP-Wax interface for multicomponent systems with various functionalities. The inputs are given through different textboxes on the left of the screen and the plots are created. In 2.1 the predicted and experimental precipitation curves can be plotted, in 2.2 the solid-phase composition can be plotted for the given temperature range using a trackbar, in 2.3 different SLE characteristics can be plotted (as desired) for the provided temperature point and, in 2.4 the relative concentration gradient is plotted for CCN determination

# 3.0 Illustrative Examples

SP-Wax software has been validated by binary and multicomponent data. The binary data of Provost et al. and Madsen [26,36] were used for validating the binary system prediction of SP-Wax. The data from these sources [26,36] are the syntactic binary system where n-C7 (n-heptane) was used as the solvent and the solute was either n-C23, n-C25, n-C28, n-C32, or n-C36. For multicomponent systems, experimental data of four different oil samples [7,25,32,33] were used for the validation process.

## 3.1 Binary System Validation

SP-Wax predictions have been validated by experimental data of five binary systems. The dissolved solute mole fractions at various WAT values from SP-Wax were compared to the literature data [26,36] and satisfactory agreement was obtained as shown in Figure 3. The dissolved solute mole fraction decreases as either the temperature decreases (or 1000/T increases) or the n-alkane chain length becomes longer, as expected.

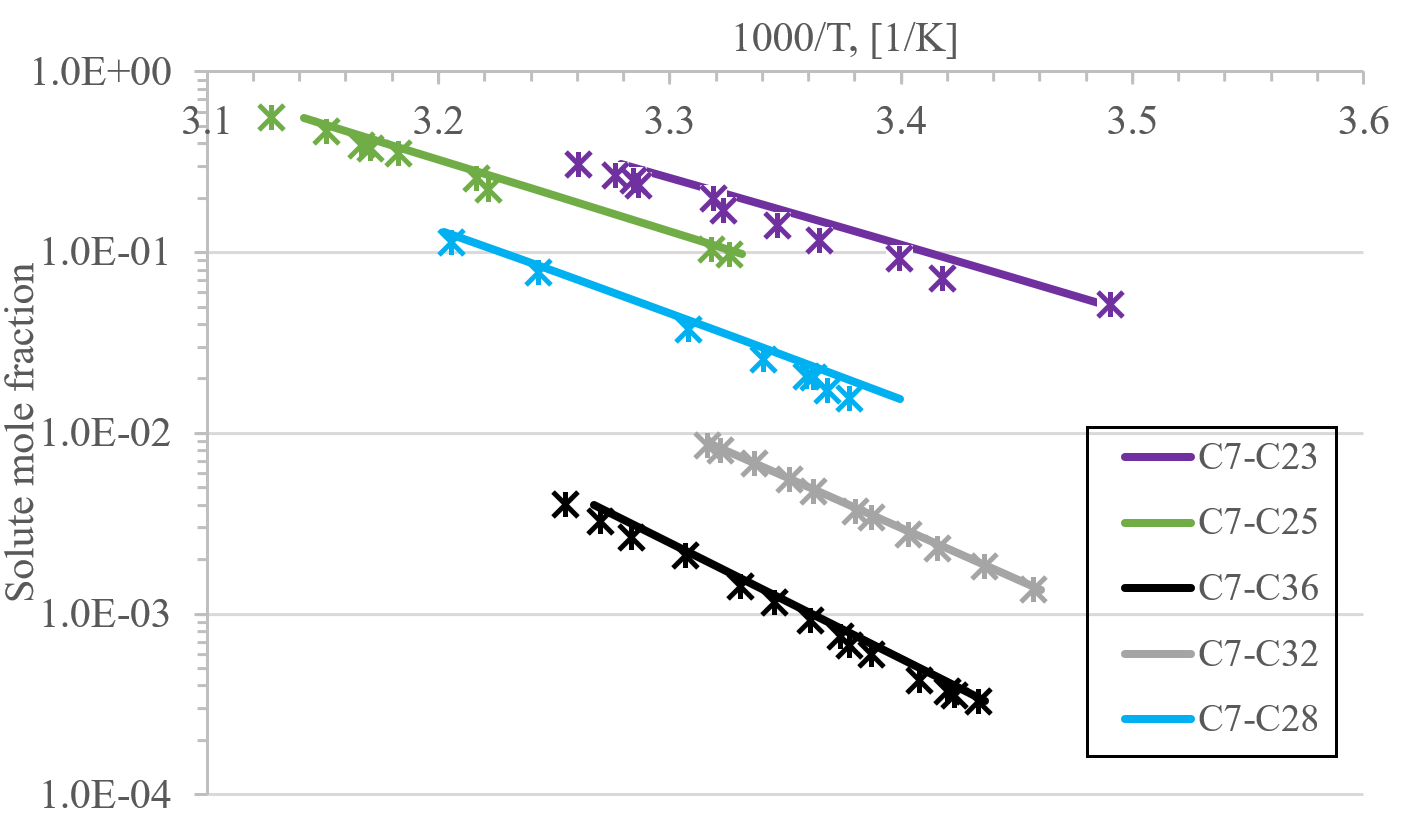


Figure 3: SP-Wax predictions and experimental data [26,36] ( symbol) of solid solubilities for five binary system at 1 bar

## 3.2 Multicomponent System Validation

One important aspect of a reliable thermodynamic model is its accuracy to predict the mass of precipitated paraffin in different temperatures (precipitation curve). Experimental precipitation data [7,25,32] were used to validate SP-Wax software. Fleming et al. [25] reported the experimental and predicted precipitation data points. Their prediction was based on Coutinho et al.’s model [16] using UNIQUAC approach for solid-phase non-ideality. For another case, Rittirong [32] reported experimental precipitation data along with simulation results from TUWAX and PVTsim thermodynamic software. Notably, SP-Wax is far more accurate than all other simulation results. Zheng et al.’s [7] precipitation data are from the direct centrifugal technique. The direct technique is subject to less uncertainty because it does not need to calculate the precipitated amount based on the estimated enthalpy of crystallization of wax [9]. Zheng et al.’s [7] input composition for n-alkanes were reported graphically from C15 to C36. In our study, we extrapolated the composition for the wider range of carbon numbers, however, the extrapolation is somewhat subjective, and it is not unique. SP-Wax predictions of precipitation curve are in very good agreement with all three experimental data sets. SP-Wax prediction is almost identical to Fleming et al.’s prediction. Both studies use Coutinho thermodynamic model. However, Fleming used UNIQUAC to express solid-phase’s activity coefficients and SP-Wax used the Wilson method. As per Coutinho’s comparison, both methods should result in similar predictions which is true in our analyzed case. This is another indication of the validity of our developed thermodynamic software.

For Fleming et al. [25], the precipitation curves with three different values of adjustment parameter were calculated and shown in Figure 4(a). In their case, only n-alkane components were present () and very small adjustment was needed. Among the three curves, the best fit resulted from with . For oil cases of Zheng et al. [7] and Rittirong [32], the optimum adjustment coefficient was chosen to be with of 0.95 and 0.96, respectively.

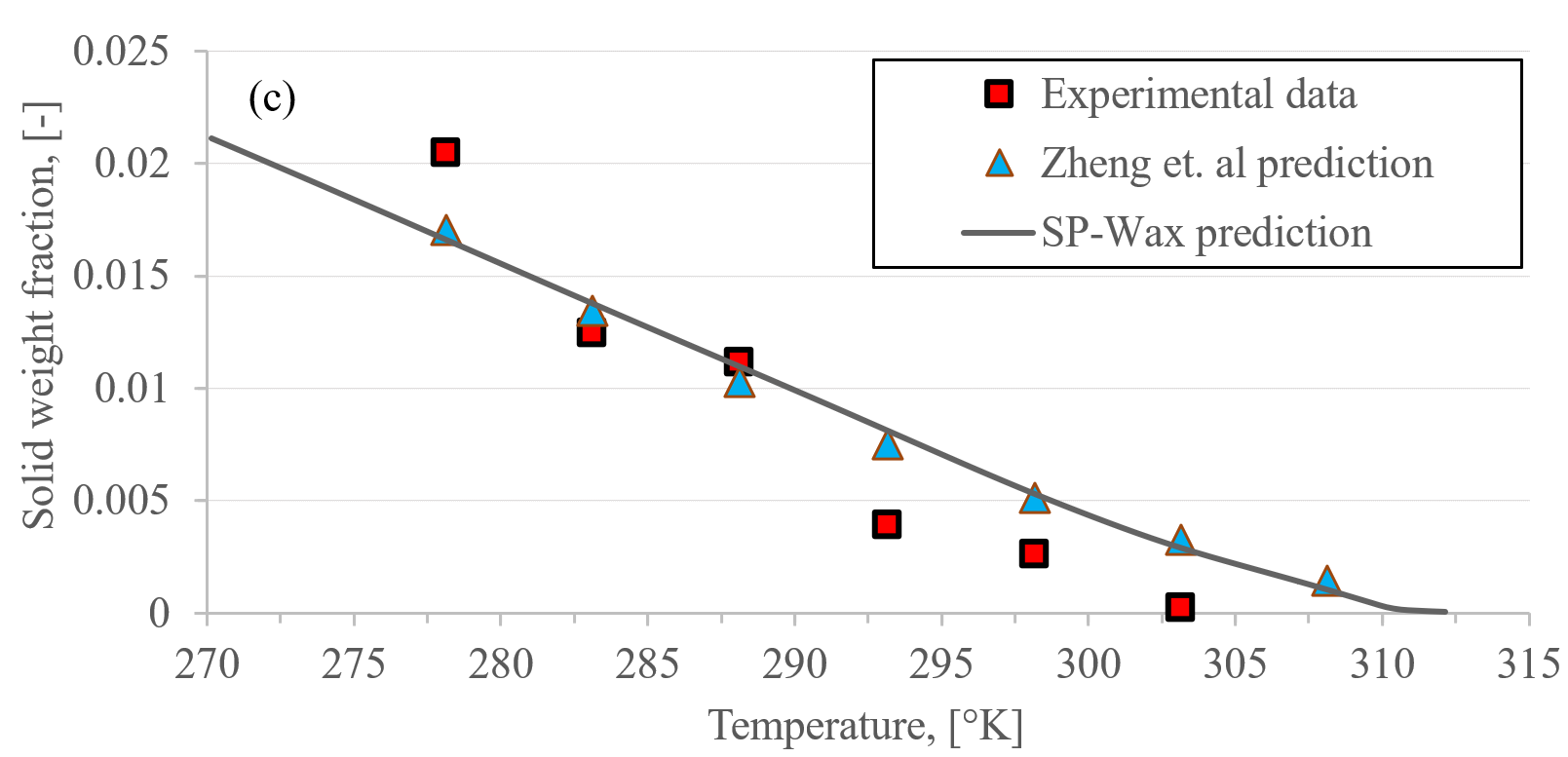
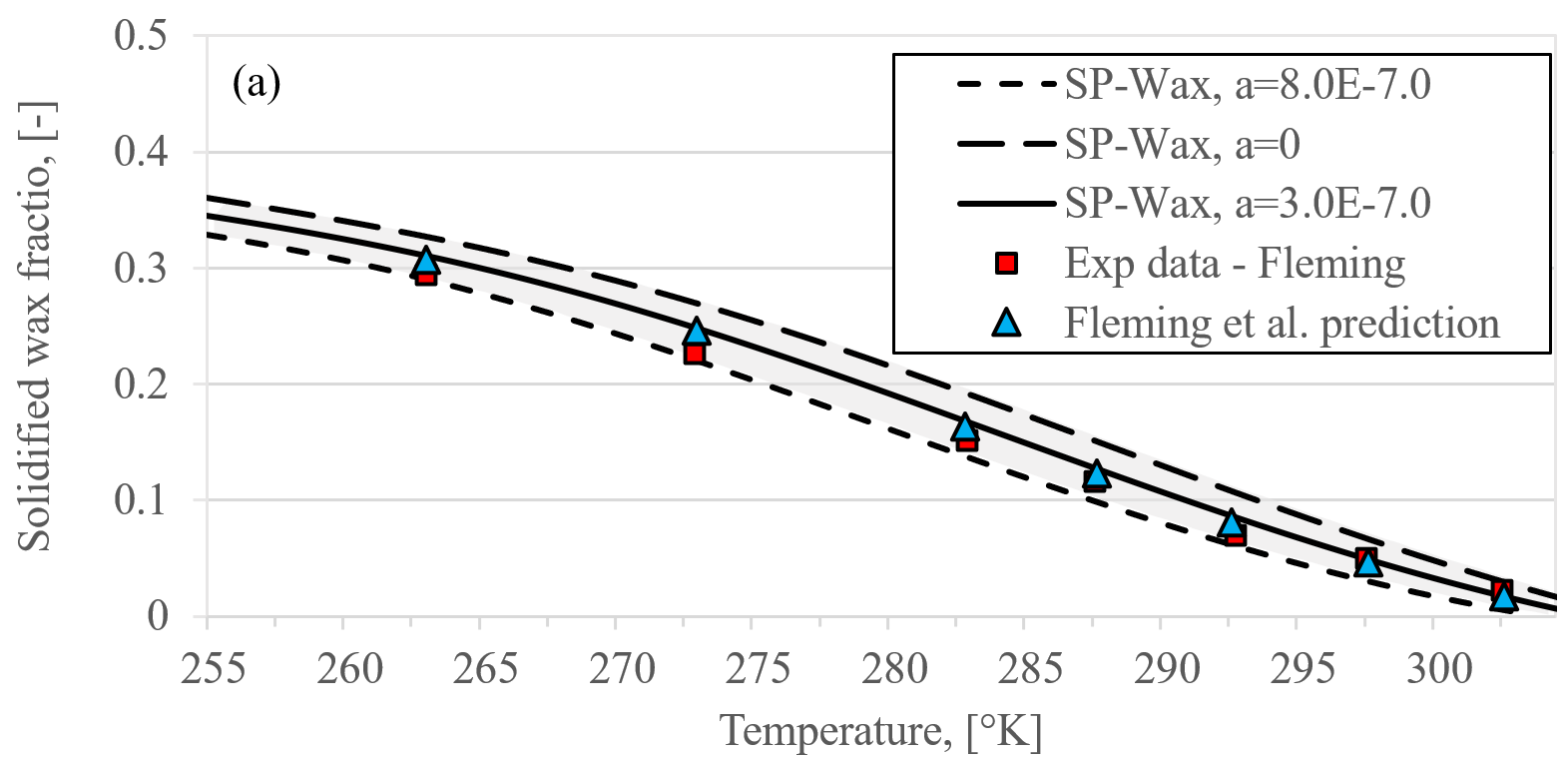
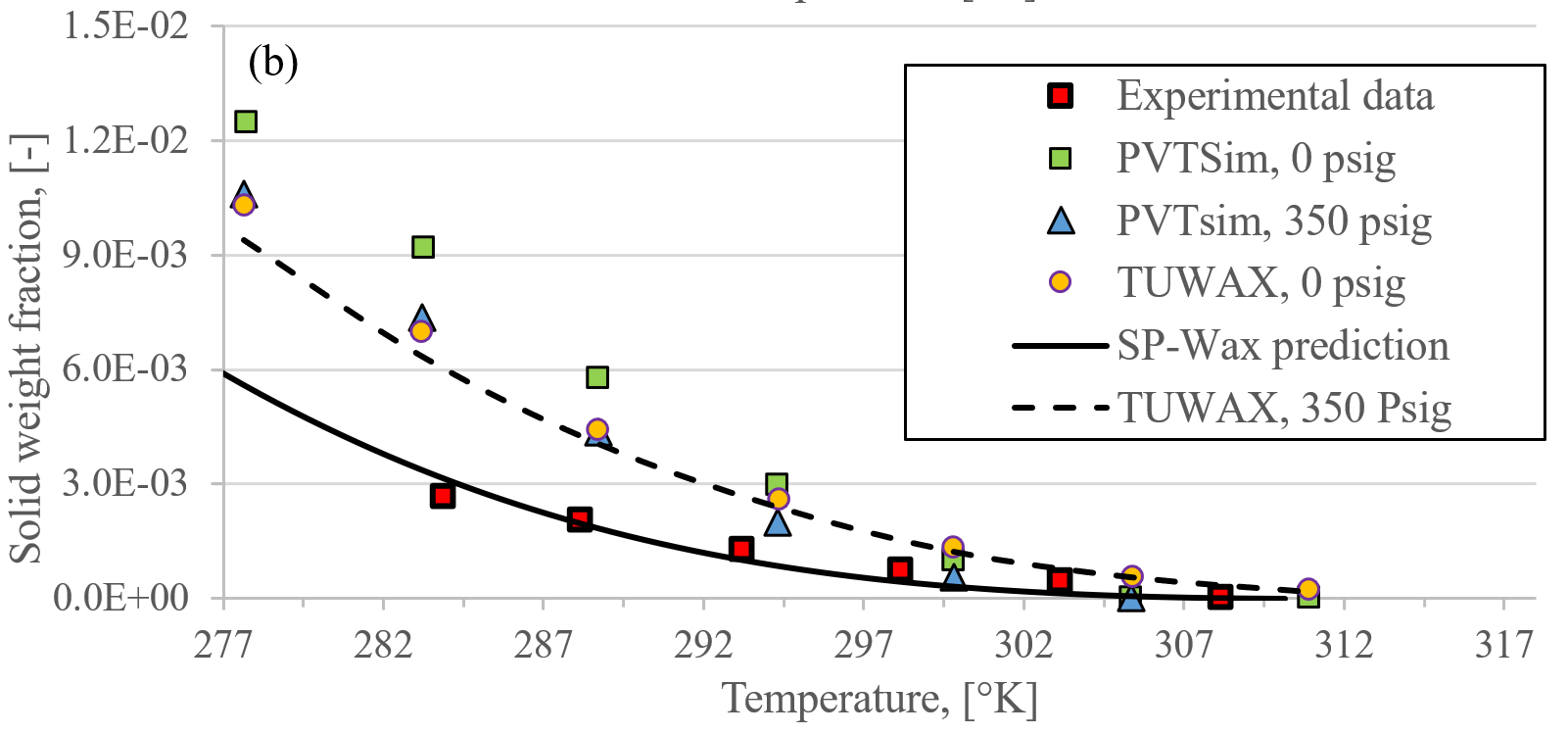


Figure 4: SP-Wax precipitation curve validation against Fleming et al.(a) [25], Rittirong(b) [32], and Zheng et al.(c) [7].

In addition to the precipitation curve prediction that is used in the pseudo-single-wax-phase modeling approach [1,2,34,35], the solid phase composition information is also important for a compositional-based model [7] and for analyzing the CCN of wax deposit for both single-phase [2] and multiphase cases [37,38]. SP-Wax was validated through five sets of experimental CND data from Rittirong [32] and Panacharoensawad’s [33] single phase wax deposition test results. Figure 5 shows the SP-Wax predictions against experimental solid-phase CND data. SP-Wax predictions are in good agreement with experimental data for all cases. The slight overestimation is expected because, SP-Wax takes only the final-time temperature which is always higher than the average temperature over the time of the experiment.

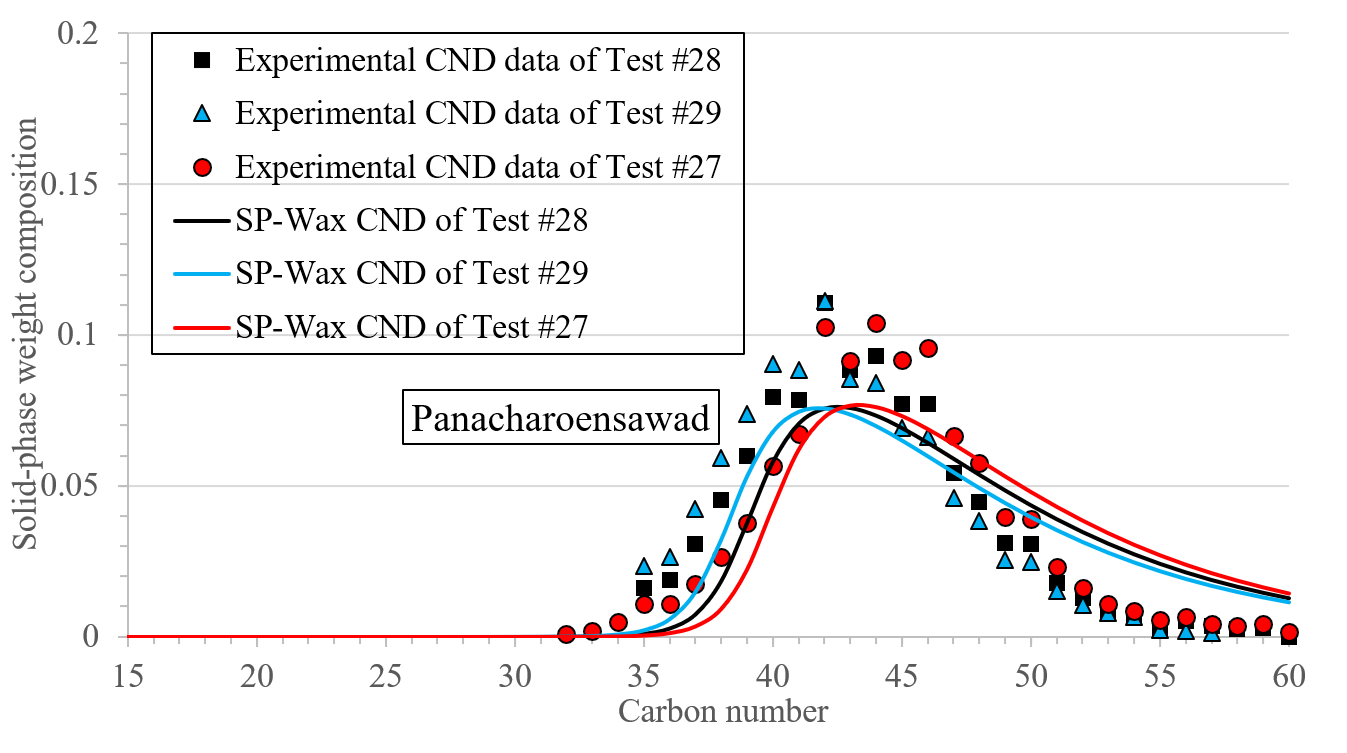
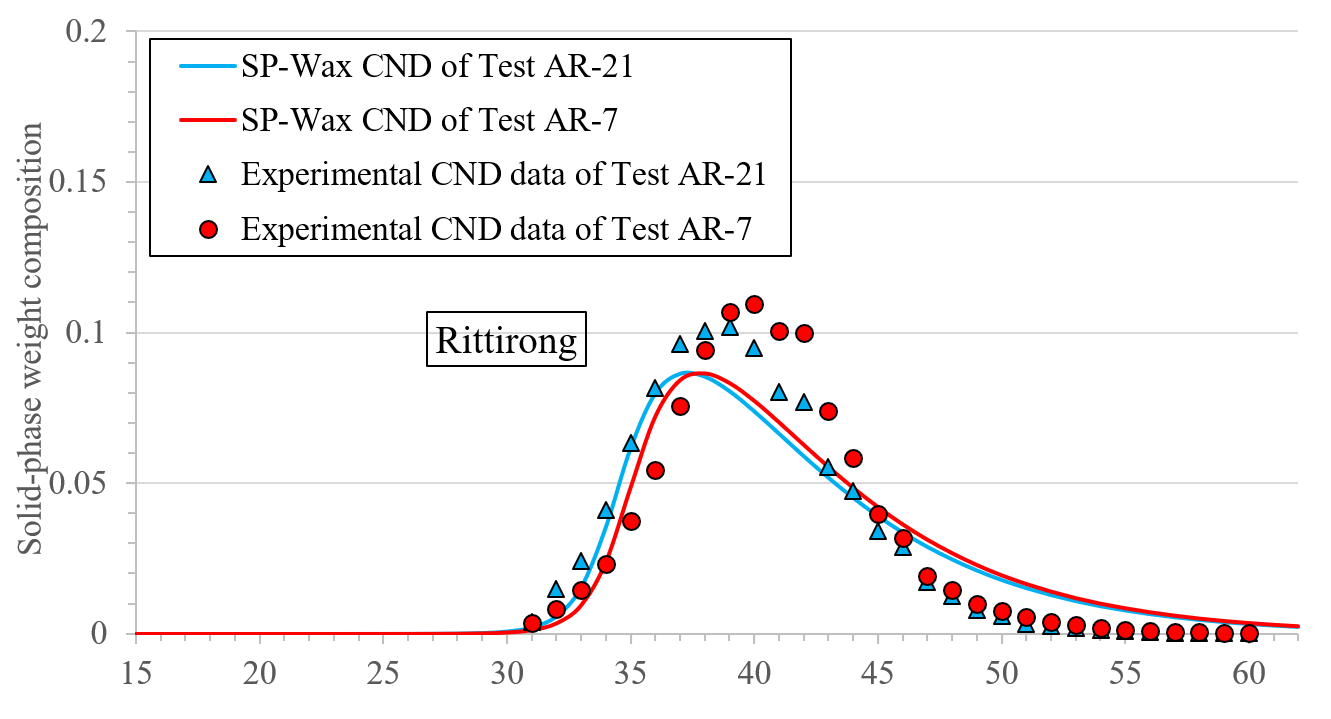


Figure 5: Solid-phase CND of paraffin deposit. SP-Wax predictions versus CND experimental data of Ritirrong [32] and Panacharoensawad [33] at average deposit temperature at the end of each test

Lastly, the relative concentration gradient from SP-Wax (Figure 6) is used to estimate the CCN in five different tests. In our analysis, pre-calculated deposit’s temperatures, which were reported in the literature [32,33], were used to calculate the relative concentration gradient for CCN estimation. The relative concentration gradient is defined as the ratio of the dissolved mass of ith carbon number over the volume of all n-alkanes in liquid phase (in m3). In SP-Wax, CCN is estimated by determining the smallest carbon number with positive relative concentration gradient (Figure 6). We note that the CCN estimation typically requires significant overhead calculations as part of wax deposition modeling. However, this thermodynamic property (CCN) can be estimated as a function of deposit’s temperature. Since the deposit’s temperature can be determined using experimental measurements at the final time (the time at which the composition was determined by HTGC), CCN can be predicted by SP-Wax.

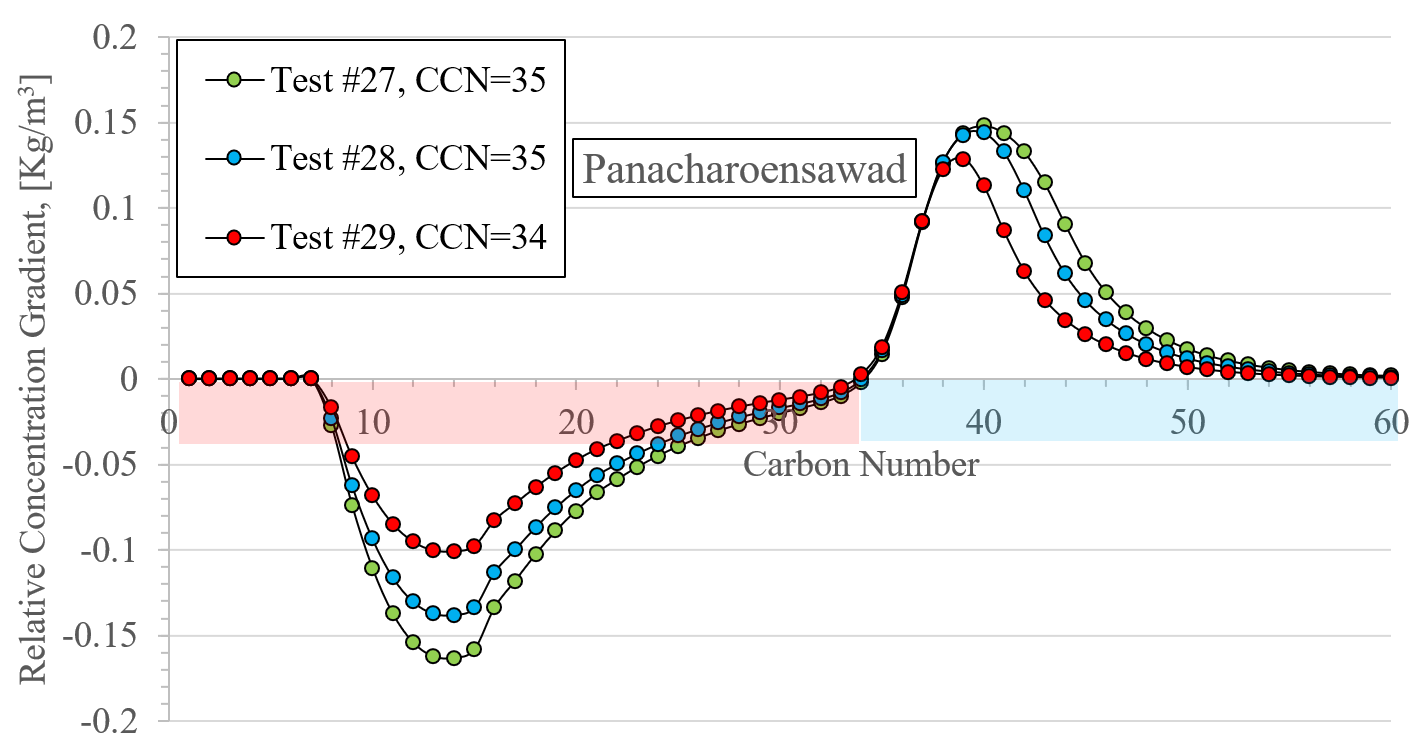
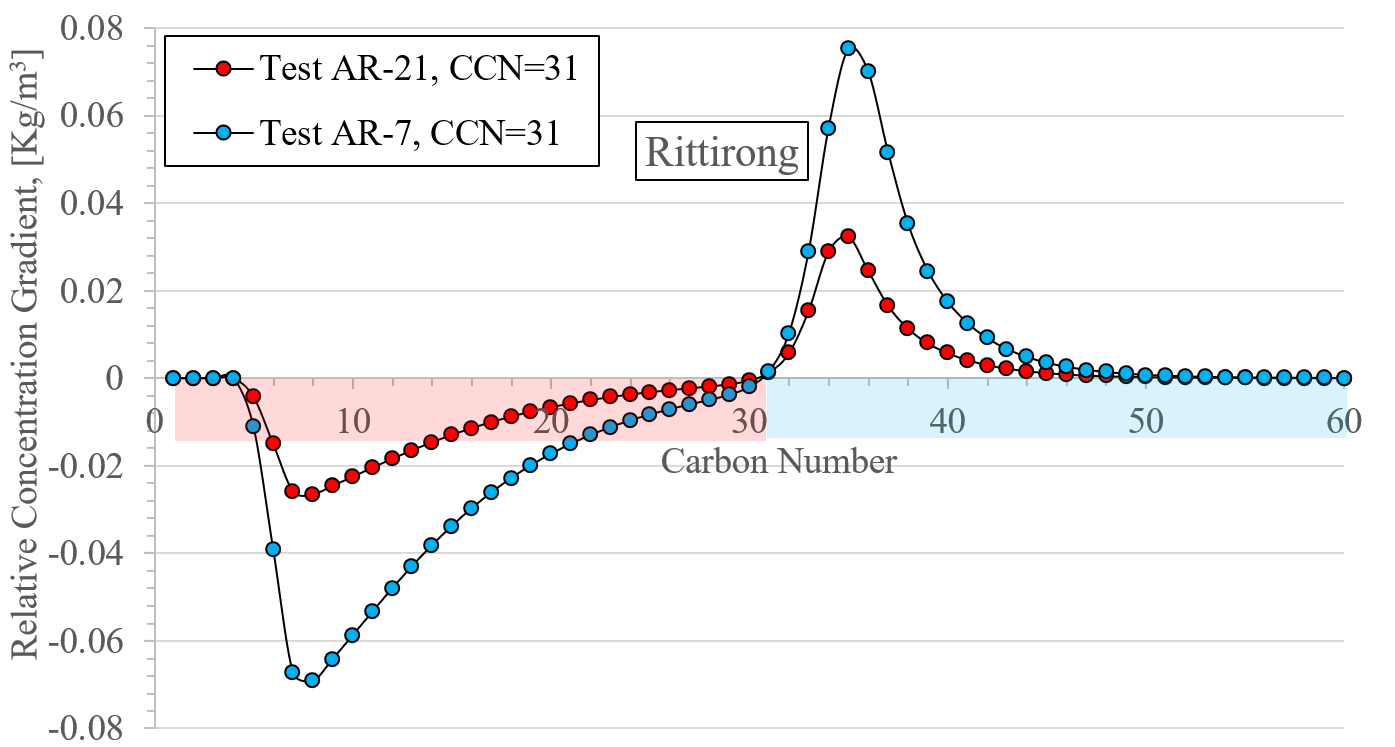


Figure 6: SP-Wax relative concentration gradient predictions for five tests of Ritirrong [32] and Panacharoensawad [33]. Associated CCN values are annotated in the graph for each test. Blue and red highlighted sections are referred to carbon number components that diffuse in and out of the deposit, respectively.

The numerical values of solid-phase Average Carbon Number (ACN), mode and CCN predictions with test temperature values used in SP-Wax simulation are shown in Table 1. In addition to the comparison in the above graphical form, the numerical value shown below confirm the match of SP-Wax to the literature data.

Table 1: Temperatures data at the end of experiments for five tests plus experimental data [32,33] and predictions of Average Carbon Number (ACN), Mode, and Critical Carbon Number (CCN). South Pelto and Garden Banks are the names of oil samples that have been used by Panacharoensawad [33] and Ritirrong [32], respectively.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Oil Type** | **South Pelto** | **South Pelto** | **South Pelto** | **Garden Banks** | **Garden Banks** | **Mean Absolute Relative percentage error %\*** |
| **Test #** | 27 | 28 | 29 | AR-21 | AR-7 |  |
| **Tb [C]** | 40.6 | 40.5 | 40.3 | 25.1 | 26.0 |
| **Tw [C]** | 29.5 | 29.3 | 29.5 | 16.8 | 16.5 |
| **Ti [C]** | 37.5 | 36.0 | 34.0 | 18.0 | 19.7 |
| **ACN (Exp)** | 44.8 | 43.6 | 42.8 | 40.5 | 39.6 |
| **ACN (Pred)** | 47.3 | 46.6 | 45.9 | 41.9 | 41.4 | 5.49 |
| **Mode (Exp)** | 44 | 42 | 42 | 40 | 39 |  |
| **Mode (Pred)** | 43 | 43 | 42 | 38 | 37 | 2.96 |
| **CCN (Exp)** | 35 | 35 | 35 | 30 | 30 |  |
| **CCN (Pred)** | 35 | 35 | 34 | 31 | 31 | 1.90 |
| **Correction Factor Coefficient** | 3.0E-06 | | | | |  |

\* Mean relative percentage error % is defined as .

Table 2 contains the relative error of the model for solid solubilities of binary systems and precipitation curves of multicomponent systems. The calculations and the numerical values can be found in (<https://bit.ly/2zQYt7r>). The relative error formula which is used in Table 2 is as follows:

|  |  |
| --- | --- |
|  | (19) |

where, NN, and are the total number of cases, simulated and experimental sample parameters, respectively

Table 2 shows that the model has the average estimated relative error of about 22% and 3.7% for the case of multicomponent precipitation curve and the binary system WAT, respectively. SP-Wax requires accurate input n-alkane compositions. In multicomponent systems, the accumulative error of input compositions is higher than in binary systems, simply because more components are present. In some multicomponent cases, such as in Zheng et al. [7], the n-alkane input composition data are incomplete and the extrapolation of the n-alkane composition is needed. This contributes to the model prediction’s uncertainty.

Table 2: Estimated relative error of the SP-Wax prediction for precipitation curves (Figure 4) of multicomponent systems.

|  |  |  |
| --- | --- | --- |
| Case | System | Estimated Relative error [%] |
| Rittirong | Multicomponent | 20.0 |
| Zheng et al. | Multicomponent | 28.7 |
| Fleming et al. | Multicomponent | 17.1 |

Furthermore, the average absolute errors of WAT prediction for the binary systems are calculated and shown in Table 3. The results show that SP-Wax can successfully predict the solid solubility of binary systems.

Table 3: Temperature differences between predicted and experimental WAT parameter of five binary systems.

|  |  |
| --- | --- |
| System | Average temperature difference [°C] |
| C7-C23 | 1.83 |
| C7-C25 | 1.10 |
| C7-36 | 0.74 |
| C7-C32 | 0.22 |
| C7-C28 | 1.28 |

# Impact and Conclusions

The currently available thermodynamics software in the literature is either not open-source [39], or is open-source and does not have the SLE calculation for n-alkanes [40]. SP-Wax is the first open-source thermodynamic software for modeling various SLE characteristics of paraffin in binary and multicomponent systems. Furthermore, for the first time, a simplified CCN estimation method is proposed via the use of thermodynamic modeling without the need to fully solve the whole wax deposition equations.

SP-Wax will directly benefit various researchers and industries that need the SLE calculation of paraffinic solutions, including petroleum and chemical industries. Specifically, paraffin deposition research will significantly benefit from the software and the provided source code, because it enables the composition prediction of wax deposit.

SLE thermodynamic model from Coutinho and co-workers [10–17] and other literature [18–31] were coded in C++ with a user-friendly C# interface. SP-Wax is, equipped with OpenMP parallel programming technique to maximize the performance. SP-Wax comes with complete user and the developer manuals. The user manual provides step-by-step instructions and enough information to reproduce case-runs shown in this article. For developer’s manual, theoretical framework and technical parts are explained. SP-Wax predictions were validated by forty-nine solid-solubility data points from five different binary systems. Furthermore, various aspects of SP-Wax were verified through multicomponent data of four different oil compositions.

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# Declaration of Interest

The authors declare no potential conflict of interest with any entities that could inappropriately influence or be perceived to influence their work.

# Nomenclature

## Variables

Correction factor coefficient

Molecular diffusivity of wax in oil,

Enthalpy,

Equilibrium constant, [-]

Equilibrium constant from previous iteration, [-]

Molecular weight,

N Number of carbon number components

NN Total number of cases used to calculate the mean absolute relative error.

Solid mole fraction in n-alkane system (or [mole of solidified n-alkanes] / [total moles of all n-alkanes]), [-]

Universal gas constant,

Temperature,

Volume,

Weight fraction of n-alkane system in total liquid sample (paraffin and non-paraffins), [-]

Weight fraction of all n-alkanes in the system, [-]

Mole composition, [-]

Sample parameter in relative error equation

Input mole composition of n-alkanes (), [-]

Difference between specific heat capacity of component in liquid and in solid phase

## Greek letters

Correction factor, [-]

Activity coefficient, [-]

Relative error, [-]

Major binary interaction energy parameter in Wilson equation, [-]

Minor binary interaction energy parameter,

Volume fraction for n-alkanes in total fluid, [-]

Composition fraction, [-]

Combinatorial contribution in liquid phase non-ideality

## Subscripts

Bulk

Experimental

carbon number

cases used in the mean absolute relative error calculation.

Interface

carbon number

carbon number

Long

Molar

Short

Simulation

Van der Waals

## Superscripts

Fusion

Liquid

Solid

Sublimation

Solid-phase transition

Vaporization

# References

[1] P. Singh, R. Venkatesan, H.S. Fogler, and N. Nagarajar, Formation and aging of incipient thin film wax-oil gels. American Institute of Chemical Engineers. 2000, 46 (5): 1059–1074 http://goo.gl/ugZndp.

[2] A. Singh, E. Panacharoensawad, and C. Sarica, A Mini Pilot-Scale Flow Loop Experimental Study of Turbulent Flow Wax Deposition by Using a Natural Gas Condensate. Energy & Fuels. 2017, 31 (3): 2457–2478 http://goo.gl/8m5gzR.

[3] D. Jennings and K. Weispfennig, Effect of shear on the performance of paraffin inhibitors: coldfinger investigation with Gulf of Mexico crude oils. Energy & fuels. 2006, 20 (6): 2457–2464 https://goo.gl/7bBNtA.

[4] Y. Lu, Z. Huang, R. Hoffmann, L. Amundsen, and H.S. Fogler, Counterintuitive effects of the oil flow rate on wax deposition. Energy & Fuels. 2012, 26 (7): 4091–4097 http://goo.gl/Qcz2Ss.

[5] C. Labes-Carrier, H. Rønningsen, and J. Kolnes, Wax deposition in North Sea gas condensate and oil systems: Comparison between operational experience and model prediction. SPE Annual Technical Conference and Exhibition. 2002, http://goo.gl/auaRNz.

[6] Z. Huang, H.S. Lee, M. Senra, and H. Scott Fogler, A fundamental model of wax deposition in subsea oil pipelines. AIChE Journal. 2011, 57 (11): 2955–2964 http://doi.wiley.com/10.1002/aic.12517.

[7] S. Zheng, F. Zhang, Z. Huang, and H.S. Fogler, Effects of operating conditions on wax deposition carbon number distribution: Theory and experiment. Energy and Fuels. 2013, 27 (12): 7379–7388 http://goo.gl/or2hdz.

[8] E. Panacharoensawad, A. Rittirong, and C. Sarica, A Self-Sufficient Wax Deposition Model for Horizontal Gas-Oil Slug Flow. American Institute of Chemical Engineers (AIChE) Spring Meeting and Global Congress on Process Safety. 2015, http://goo.gl/kbCitV.

[9] C. Sarica and E. Panacharoensawad, Review of paraffin deposition research under multiphase flow conditions. Energy & Fuels. 2012, 26 (7): 3968–3978 http://goo.gl/xfeb2K.

[10] J.A.P. Coutinho, B. Edmonds, T. Moorwood, R. Szczepanski, and X. Zhang, Reliable Wax Predictions for Flow Assurance. Energy & Fuels. 2006, 20 (3): 1081–1088 http://goo.gl/5U7WMB.

[11] J. Coutinho, C. Gonçalves, I.M. Marrucho, J. Pauly, and J.L. Daridon, Paraffin crystallization in synthetic mixtures: Predictive local composition models revisited. Fluid Phase Equilibria. 2005, 233 (1): 28–33 http://goo.gl/2LyMQc.

[12] J. Coutinho and E.H. Stenby, Predictive Local Composition Models for Solid/Liquid Equilibrium in n-Alkane Systems: Wilson Equation for Multicomponent Systems. Industrial & Engineering Chemistry Research. 1996, 35 (3): 918–925 http://goo.gl/JhQg13.

[13] J. Coutinho, S. Andersen, and E. Stenby, Solid-liquid Equilibrium of N-alkanes Using the Chain Delta Lattice Parameter Model. Fluid Phase Equilibria. 1996, 117 (1–2): 138–145 http://goo.gl/YPPFXU.

[14] J. Coutinho, K. Knudsen, and S. Andersen, A local composition model for paraffinic solid solutions. Chemical Engineering Science. 1996, 51 (12): 3273–3282 http://goo.gl/EqMoE7.

[15] J. Coutinho and J. Daridon, Low-Pressure Modeling of Wax Formation in Crude Oils. Energy & Fuels. 2001, 15 (6): 1454–1460 http://goo.gl/WAoxJU.

[16] J.A.P. Coutinho, Predictive UNIQUAC: A New Model for the Description of Multiphase Solid−Liquid Equilibria in Complex Hydrocarbon Mixtures. Industrial & Engineering Chemistry Research. 1998, 37 (12): 4870–4875 http://goo.gl/C6gE3z.

[17] J. Coutinho, S. Andersen, and E. Stenby, Evaluation of Activity Coefficient Models in Prediction of Alkane Solid-liquid Equilibria. Fluid Phase Equilibria. 1995, 103 (1): 23–39 http://goo.gl/CNGpy1.

[18] R. Hutchings, Molar volumes in the homologous series of normal alkanes at two temperatures. Fluid Phase Equilibria. 1985, 21 (1–2): 165–170 http://goo.gl/k5Kjiw.

[19] H.S. Elbro, A. Fredenslund, and P. Rasmussen, A new simple equation for the prediction of solvent activities in polymer solutions. Macromolecules. 1990, 23 (21): 4707–4714 http://goo.gl/2d73mn.

[20] T. Daubert and R. Danner, Physical and thermodynamic properties of pure compounds: data compilation. Hemisphere Publishing Corporation. 1989, https://goo.gl/TsUcib.

[21] A. Bondi, Physical Properties of Molecular Crystals Liquids, and Glasses. 1968, http://goo.gl/18sWfW.

[22] H.S. Elbro, A. Fredenslund, and P. Rasmussen, Group Contribution Method for The Prediction of Liquid Densities as a Function of Temperature for Solvents, Oligomers, and Polymers. Industrial & Engineering Chemistry Research. 1991, 30 (12): 2576–2582 http://goo.gl/gaKEaE.

[23] K. Pedersen, P. Christensen, and J. Shaikh, Phase behavior of petroleum reservoir fluids. CRC press. 2006, https://goo.gl/1zB53q.

[24] P.J. Flory, Fifteenth spiers memorial lecture. Thermodynamics of polymer solutions. Discussions of the Faraday Society. 1970, 49 7–29 http://goo.gl/o7k689.

[25] F. Fleming, J. Daridon, L. Azevedo, J.P.-F.P. Equilibria, and U. 2017, Direct Adjustment of Wax Thermodynamic Model Parameter to Micro Differential Scanning Calorimetry Thermograms. Fluid Phase Equilibria. 2017, 436 20–29 http://goo.gl/HciXwW.

[26] H. Madsen, R.B.-J. of the C. Society, U. Faraday, and U. 1979, Solubility of Octacosane and Hexatriacontane in Different N-alkane Solvents. Journal of the Chemical Society, Faraday Transactions. 1979, 75 1254–1258 http://goo.gl/tgEQ9J.

[27] J. Yang, W. Wang, B. Shi, Q. Ma, P. Song, and J. Gong, Prediction of wax precipitation with new modified regular solution model. Fluid Phase Equilibria. 2016, 423 128–37 http://goo.gl/9KXfYS.

[28] D.L. Morgan and R. Kobayashi, Extension of Pitzer CSP Models for Vapor Pressures and Heats of Vaporization to Long-chain Hydrocarbons. Fluid Phase Equilibria. 1994, 94 51–87 http://goo.gl/JErqCJ.

[29] J.M. Prausnitz, R.N. Lichtenthaler, and E.G. de Azevedo, Molecular thermodynamics of fluid-phase equilibria. Pearson Education. 1998, http://goo.gl/57gDdU.

[30] J.J. Marano and G.D. Holder, General Equation for Correlating the Thermophysical Properties of n-Paraffins, n-Olefins, and Other Homologous Series. 2. Asymptotic Behavior Correlations for PVT Properties. Industrial & Engineering Chemistry Research. 1997, 36 (5): 1895–1907 http://goo.gl/tCgEwX.

[31] M.G. Broadhurst, An Analysis of The Solid Phase Behavior of The Normal Paraffins. Journal of Research of The National Bureau of Standards. 1962, 241–249 http://goo.gl/axg2mB.

[32] A. Rittirong, Paraffin Deposition Under Two-Phase Gas-oil Slug Flow in Horizontal Pipes. Ph.D. Dissertation, University of Tulsa. 2014, http://goo.gl/ja7G1F.

[33] E. Panacharoensawad, Wax deposition under two-phase oil-water flowing conditions. Ph.D. Dissertation, University of Tulsa. 2012, http://goo.gl/JzL1nw.

[34] H.S. Lee, Computational and Rheological Study of Wax Deposition and Gelation in Subsea Pipelines. Ph.D. Dissertation, University of Michigan. 2008, http://goo.gl/X2onHc.

[35] R. Venkatesan, The deposition and rheology of organic gels. Ph.D. Dissertation, University of Michigan. 2004, https://goo.gl/V33PPw.

[36] E. Provost, V. Chevallier, M. Bouroukba, D. Petitjean, and M. Dirand, Solubility of Some n -Alkanes (C 23 , C 25 , C 26 , C 28 ) in Heptane, Methylcyclohexane, and Toluene. Journal of Chemical & Engineering Data. 1998, 43 (5): 745–749 http:goo.gl/ks7BaZ.

[37] A. Rittirong, E. Panacharoensawad, and C. Sarica, An Experimental Study of Paraffin Deposition under Two-Phase Gas-Oil Slug Flow in Horizontal Pipes. Offshore Technology Conference. 2015, http://goo.gl/b7XPZH.

[38] E. Panacharoensawad and C. Sarica, Experimental Study of Single-Phase and Two-Phase Water-in-Crude-Oil Dispersed Flow Wax Deposition in a Mini Pilot-Scale Flow Loop. Energy & Fuels. 2013, 27 (9): 5036–5053 http://goo.gl/9tyLgS.

[39] R.. Davies, A.. Dinsdale, J.. Gisby, J.A.. Robinson, and A.. Martin, MTDATA-thermodynamic and phase equilibrium software from the national physical laboratory. Calphad. 2002, 26 (2): 229–271 http://goo.gl/gSRvji.

[40] B. Sundman, U.. Kattner, C. Sigli, M. Stratmann, R. Le Tellier, M. Palumbo, and S.. Fries, The OpenCalphad thermodynamic software interface. Computational Materials Science. 2016, 125 188–196 http://goo.gl/Qx83En.

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| **Nr** | **Code metadata description** | ***Please fill in this column*** |
| C1 | Current Code version | *1.0* |
| C2 | Permanent link to code / repository used of this code version | *https://github.com/epmmko/sp-wax/* |
| C3 | Legal Code License | *The Unlicense (unlicensed.org)* |
| C4 | Code Versioning system used | *None* |
| C5 | Software Code Language used | *C++, C#, OpenMP* |
| C6 | Compilation requirements, Operating environments & dependencies | *C++11, Windows* |
| C7 | If available Link to developer documentation / manual | *https://github.com/epmmko/sp-wax/Manuals* |
| C8 | Support email for questions | [*ekarit.panacharoensawad@ttu.edu*](mailto:ekarit.panacharoensawad@ttu.edu)  *arya.shahdi@ttu.edu* |

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| **Nr** | **(executable) Software metadata description** | ***Please fill in this column*** |
| S1 | Current software version | *1.0* |
| S2 | Permanent link to executables of this version | *example : https://github.com/combogenomics/DuctApe/releases/tag/DuctApe-0.16.4* |
| S3 | Legal Software License | *The Unlicense (unlicensed.org)* |
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| S5 | Installation requirements & dependencies | *Microsoft Windows operating system* |
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| S6 | Support email for questions | [*ekarit.panacharoensawad@ttu.edu*](mailto:ekarit.panacharoensawad@ttu.edu)  *arya.shahdi@ttu.edu* |